We thank both reviewers for their insights, which we will use to improve the manuscript. In the following, we give the point-by-point responses to both reviews. Please also note the short comment placed earlier, which addressed some general issues in a more compact fashion.

Response to Gerrit de Rooij

Dear Gerrit de Rooij, thank you for you comments on our manuscript and additional literature provided, and pointing out some errors. In the following we give a point-by-point response to all comments and also describe the changes we will do in the revision of the manuscript.

We have slightly changed the order of the comments, since the last two paragraphs of the review are a summary, and we respond to them first as a general response:

[GdR 01] Overall, I think the paper presents a fresh way of looking at root water uptake that merits attention. On analyzing the paper I found several assumptions that I find unconvincing, but that do not appear to be crucial to the model. Most of these assumptions were implicit. I would recommend a more rigorous mathematical derivation of the model equations based on fewer assumptions and simplifications. I think this is feasible. Those assumptions that remain should be stated explicitly, and their validity tested if possible.

We will certainly aim at improving the mathematical description, and point out the specific places below.

[GdR 02] More fundamentally, I believe the way the authors used and interpreted Figure 2 is incorrect. I do not think one can use a representation of the average features of a non-linear system to derive the behavior of the system when that behavior is the sum of local processes driven by the local values of the averaged quantities

We fully agree on the fact that water fluxes are driven locally.

We believe that there is a misunderstanding with the overall procedure applied in this paper, and we will improve the narrative in the revision to prevent this misunderstanding.

From the comments, it seems that Gerrit de Rooij assumed that the actual model calculations are performed with a thermodynamical model, with fluxes driven based on average soil states. This is not the case. We will add a description along the following lines in the revision:

The predictive flux model was driven based on distributed (local) water potentials (very similar to complex three dimensional root water uptake models, although simplified and reduced to four compartments), of which the equations are given in section 2.

The model is distributed, and uptake is based on solving the equations given in Section 2. When omitting water fluxes between compartments, which we have done here for

simplicity, the xylem water potential (root collar potential, ψ_x) can be calculated as follows:

$$\psi_x = \frac{-J_{wu} + \sum_{i=1}^{n} (\psi_{M,i} * K_{r,i})}{\sum_{i=1}^{n} K_{r,i}}$$
(D1)

where $J_{\rm wu}$ is the total plant transpiration, $\psi_{\rm M,i}$ the matric potential of compartment i, $K_{\rm r,i}$ the root conductivity in compartment i.

Root water uptake in each compartment ($J_{wu,i}$) can then be calculated based on Eq. 4, and water content is updated accordingly in each compartment. Thus, the model dynamically adapts the location of uptake based on the local water potential and root distribution in a typical, although simplified, resistance framework.

The model is a toy model, and we will change the heading of section 2 to reflect this. "A conceptual model" as a heading seems to suggest a great deal of generality, which is not at all implied. Instead, we wish to demonstrate the power of diagnosing model output of root water uptake models using thermodynamics.

The thermodynamical evaluation of the fluxes was applied *a posteriori* to the results of the flow model, with the purpose to demonstrate the calculation of energy fluxes and change of energy content from water fluxes and soil water states. The averaging was done **after** those distributed fluxes were calculated.

The advantage of calculating the energy fluxes lies in the possibility to express the distributed processes in a compact way and different processes (soil drying vs. water flow) in the same units by evaluating their dissipation. We therefore propose it as a diagnostic tool for studying efficiency of root water uptake. The purpose of the paper is to illustrate this based on a simple example. Surely, much more will be learnt when applying it to more realistic 3-dimensional models, but at this point we want to emphasize and illustrate the general approach. At this point a complex 3-dimensional model would distract from this general illustration and the insights that can be gained.

[GdR 03] Abstract: The root water is most efficient if water is extracted uniformly from the soil. In what way does this have implications for forests (with significant lateral redistribution of water through stem flow), or any other systems with non-uniform distributions of water? Whatever the distribution of water in a soil is, this is a given for the root system. The root network does not drive infiltration patterns, so in what way does its desire for a uniform water content have implications?

In fact, perhaps one can reason the other way around: co-evolution of species in natural ecosystems in all likelihood has led to an optimal root network in terms of energy-efficiency of root water uptake, effectiveness of capturing water in times of water stress, and energy-efficiency of root development to populate the entire root zone with roots. Despite heterogeneity of soil properties as well as spatial distribution of infiltration this led to root systems that take up water most efficiently in terms of energy use when the initial water distribution in the soil is uniform.

Yes, we also believe that root systems may have evolved to capture heterogeneous soil water.

In our example, we want to first state that heterogeneous water distribution per se requires greater effort, or greater dissipative losses, to taking up water. This is an impediment to water uptake that has not been considered so far, to our knowledge. In order to show we impose heterogeneity of soil water such that the same initial volume of water is felt by the same root length, just the distribution differs.

And yes, if heterogeneity of soil water potential is somewhat stable in time (as is the case for vertical soil water potential profiles, and may also be to some extent the case in forests), root systems can and should adjust. However, with unpredictable heterogeneity (as may also be the case for forests), heterogeneity imposes an additional constraint to root water uptake, and it could be a future avenue of research to understand the relation between heterogeneous water input from canopies and related patterns of root water uptake.

[GdR 04] In the last few lines, are you really claiming to predict in which direction evolution will go? That seems a bit bold. Also, plants have been evolving in heterogeneous soils (and probably co-evolving as they influenced the trajectory of the soil genesis) for the past few hundred million years. They seem to have done quite well so far, yet your phrasing seems to suggest this challenge is a relatively recent evolutionary driver.

No, we are not claiming to predict the direction of evolution, this was apparently not well formulates. Rather, we are using a diagnostic tool to learn about how efficiency is achieved in already existing (heterogeneous) environments. This should help gather process understanding to improve prediction.

We will reformulate this.

Old: "Our diagnostic in the energy domain should be useful in future model applications for quantifying how plants can evolve towards greater efficiency in their structure and function, particularly in heterogenous soil environments."

New: "Our diagnostic in the energy domain should be useful in future model applications targeted at evaluating strategies of efficient root water uptake, particularly in heterogeneous soil environments"

[GdR 05] p. 133856, l. 25 The soil water retention curve may not have a resistance analog, but the matric potential is a direct analogue to the electrical potential. The potential difference between the atmosphere and the soil provides the driving force for transpiration, and thus for root water uptake. Gradient-driven water flow and soil drying both have an effect on the soil water potential that can be readily compared, I would say. One obvious difficulty is the non-linear relationship between the water loss and the drop in water potential. I doubt if this poses a fundamental objection against comparing the effect of different processes leading to water loss at the same location in the soil.

Yes, the influence of water loss and flow on soil water potential can be evaluated.

However, the statement refers to a different point, which is the question posed at the beginning of the paragraph (we need to make this connection clearer): Which of the processes (soil drying or flow over a resistance) impedes the total plant root water uptake how much? To evaluate this, we need to compare them with the same units,

which is possible in the energy domain, and more complicated when working with potentials.

We will formulate this more precisely in the revision:

Old: "Both processes (gradient-driven water flow and soil drying) may each impede the water flow to the atmosphere, but comparing their mutual contribution in form of resistances is not suitable, amongst others, since the soil" water retention relation has no resistance analogue."

New: "Both processes (flow over a resistance network and increasing soil water retention) impede transpiration, but comparing their mutual contribution in form of resistances is not suitable, since the change of soil water retention per water removed has no proper resistance analogue."

[GdR 06] p. 13387, Equation (1) I believe the second flux needs to be summed over all j not equal to i. Also, I do not understand the limitation to fluxes between neighboring reservoirs in a conceptual model. It implies that the outer two reservoirs have only one neighbor and the inner two have two neighbors. But their arrangement is arbitrary. Why not permit fluxes between all reservoirs, in which cases my suggestion to sum over all j unequal to i applies. According to your text and figure you need to consider one value of j for the two outer compartments, and two values of j for the inner compartments, which is inconsistent.

Yes, we will include the sum in the revised version of the manuscript.

[GdR 06] p. 13391, Equation (5) I disagree with the integration over the entire soil volume that is implied here. This integration should only take place over the waterfilled portion of the soil volume, and thus the volume of integration will change with the water content. The integral here is similar to that of Zehe et al. (2006), which I compared with other averaging methods in de Rooij (2011). I do not like having to put my own paper forward here, but it covered the various methods of averaging potentials presented in the literature in some detail, and therefore has direct relevance to this paper.

Equation (3) only sums the energy (not the potential) over the model compartments, thus spatially integrating (not averaging) the local energy contents (binding energy and gravitational energy).

The binding energy is obtained based on Equation (7). By definition, it applies to the water phase, because it corresponds to the latent heat of immersion. Thus, the spatial summation (not an average) of the binding energy in equation (5) only relates to the water filled pore space. The same is true for the gravitational energy, which values are also calculated for the water phase only in equation (6), separately for each compartment.

Since both types of energy contents already account for the fact that the soil is unsaturated, there is no need to account for this anymore in Equation (3).

Thus, we do not see a similarity of Equation (3) to Zehe et al. (2006), or the intrinsic phase average.

We will clarify this in the manuscript. We will reformulate Equation (5) to make it a sum over the modeled soil compartments, and include comments at several occasions to avoid confusion with established averaging techniques.

[GdR 07] Equation (5) and (6) in combination are wrong if the water content is not only a function of z but also of x and y (the horizontal coordinates). By including the volumetric water content, but only permitting it to vary with z, you implicitly establish the requirement of a horizontally uniform water content. But in reality, you in fact require the average water content at elevation z multiplied by the area at elevation z. The latter permits you to use soil volumes of arbitrary shape.

Yes, we will change the notation, including a dependency on the x and y positions as well.

[GdR 08] These complications can be avoided by integration over the water-filled pore space, as suggested in the previous comment. Doing so amounts to multiplying the intrinsic average of the binding energy (or any other property of the soil water) by the water volume, and thereby links the paper more clearly to the considerable body of literature that studies scale transitions like the one you are interested in here. See for instance the series of papers by Quintard and Whitaker that appeared in Transport in Porous media in the 1980s and 1990s. The reference below (Quintard and Whitaker, 1988) elaborates on upscaling through volume averaging most extensively, I trust you can trace the rest if you start your search there.

The work of Quintard, Whittaker and colleagues has dealt with flux equations, where spatial averages of flow velocity are related to spatial averages of potentials.

Here, we sum however not in the potential, but in the energy domain. Also, we do not use the total energy to drive the flow model (see response to [GdR 02] above for more detail). The application of Equation (3) is diagnostic on the already calculated fluxes, and only shows how heterogeneous soil drying affects internal energy.

[GdR 09] p. 13392, l. 14-17. Please rephrase. I believe 'replace' means 'to be transferred to the soil'. Can energy be negative?

We will change the formulation as proposed.

Yes, energy can be negative, because its absolute value is arbitrarily defined to a reference level. For the binding energy of soil water, this reference level is free, unbound water. Hence, bound water has a negative binding energy with respect to free water, indicating that it requires energy to unbind the water from the matrix. Likewise, the gravitational energy is arbitrarily defined by a reference level as well. This can be the surface of the soil, or the groundwater level. As flow processes act on differences and not the absolute value, the reference level plays no role for the physics of the system.

[GdR 09] l. 18-22. I believe this applies to non-uniform wetting of a uniform soil. A heterogeneous soil should be heterogeneously wetted to minimize the binding energy. The distribution of the water will clearly conform to the soil heterogeneity,

and as such is a deterministic function of the configuration of the heterogeneous pore architecture, but it will definitely be non-uniform.

Yes, our wording applies to homogenous soil physical soil properties. It is also true that in a heterogeneous soil the minimum binding energy state would be found for heterogeneous soil water contents (i.e. because the equilibrium state is with non-uniform soil water contents).

But any soil with heterogeneous potentials, suitable to drive flow, will be characterized by higher binding energy. We will reformulate as follows:

Old: "When soil water is distributed heterogeneously, the binding energy increases (is less negative)."

New: If the soil water potential is distributed heterogeneously, the binding energy increases (is less negative).

[GdR 10] l. 26-28. I can imagine a scenario where the opposite applies, and which makes more sense from the plant's point of view. The curves in Fig. 2b are themselves based on volume averaging: they represent the relationship between the average water content and the binding energy integrated over the volume of water in the soil volume for which the average water content was calculated. Around these graphs are clouds of dots of local water contents with their local binding energies. The root hairs of a plant experience these local values, not the average. The population of root hairs of a single plant will therefore experience at any time a range of bounding and gravitational energies among its root hairs. I argue that plants either take up the water only from those spots where the least amount of energy needs to be spent to get it, or (more general) that the local magnitude of water uptake is a function of the local energy status of the water that is such that the water uptake decreases if the local potential energy of the water is lower.

The first hypothesis implies that the root hairs that are in wet spots take up the water there until the energy of the remaining water equals that of root hairs in drier spots. Initially, a soil with a markedly heterogeneous water distribution will have a considerable amount of water that is more easily taken up by root hairs than one would expect based on the average curve. An uneven water distribution will therefore result in less energy expended for water uptake than in case of an even distribution of water, contrary to your statement. This is the case because the water uptake will take place preferentially from those spots where the sum of the gravitational and binding potential is highest. As root water uptake progresses, the water remaining in the initially wet spots will reach energy levels comparable to drier spots, and the root hairs tapping those locations then also start taking up water. This process continues to ever drier soil spots with root hairs in them until the water demand of the plant is met, water stress stops the water uptake altogether (wilting), or rainfall/irrigation resets the water status in the soil profile and the root hairs adjust their uptake accordingly.

[The following paragraph was replaced, according to the correction in hessd-12-C6350-2016]

Thus, root water uptake itself is a major factor in making the soil water distribution more uniform, while simultaneously reducing the overall water content. Since the root water uptake preferentially targets water with higher potential energy, the red

arrow in Fig. 2b is the conglomerate of many local water extractions that, on average, start at a point above the lines in Figure 2. Only in the case of a perfectly uniform soil will the red arrow appear as indicated, but this is a case that is purely hypothetical and can only be realistically produced in the laboratory when the soil is saturated (which presents its own problems for root water uptake). For the other lines, the red arrow will start somewhere above the line, and as the soil dries out and the roots homogenize the water distribution by extracting mainly from the wettest spots, the arrow will come closer towards the line as it moves to the left.

We actually only included the red arrow in Figure 2b, to help orientation. We did not imply the exact trajectory of root water uptake here (it is given in Fig. 4b however, for the different scenarios, calculated based on a distributed model, where the water uptake is driven by local potentials). Figure 2b only gives the relation between the total hydraulic energy and average water content for different levels of heterogeneity. It is meant to illustrate that besides the stored volume of water, also its distribution affects the total hydraulic energy. It also illustrates the physical meaning of this, which is the availability of additional energy to drive flow.

We will change the caption of Figure 2 as follows

Old: "The red arrow along the solid curve indicates (homogenous) root water uptake."

New: "For orientation, the red arrow indicates the general direction of (homogenous) soil drying."

[GdR 11] In short: when discussing root water uptake I think it is crucial to not only look at average soil water properties, but also to account for the distribution of the local variations around these average water contents and binding energies since these drive the root water uptake strategy of a root system with a large population of root hairs that each can only experience one of many local values.

Yes, we agree, the water uptake is driven by local variations in root water uptake, and this heterogeneity is also represented in our model, although quite crudely. They are calculated using the root water uptake model described in Section 2. Local uptake is calculated with Equation 4. See also our response to comment [GdR 02] above.

Again, please note that Fig 2b illustrates only that heterogeneous soil water potentials increase total hydraulic energy compared to homogenous situations. In the results section of the paper, it turns out that this increase of hydraulic energy constitutes an additional impediment to root water uptake, and uptake is more efficient (occurs at lower xylem potentials, lasts longer), when soil water potentials are homogenous and uptake is homogenous.

[GdR 12] p. 13393-13394, Eqs. (8) – (12) The energies of the water in the compartments is kept constant in these equations. This implies that steady state conditions are assumed. But for both root water uptake and large scale applications, both key to the paper, such a limitation would be too strict to yield anything of relevance. You apply your model to transient conditions, which leads me to believe that you also derived the equations for transient conditions. If believe these involve expressions that indicate how water contents and energies are updated between time steps. This basically amounts to presenting discretized

versions of the conservation laws of energy and mass. (I expect that the use of the intrinsic average as suggested above will prove beneficial in formulating these equations.) Please present the full set of equations for transient conditions to give us a complete overview of the model.

Yes, we applied them to transient conditions. The calculation of energy for a given distribution of soil water is independent of time. The transient conditions come in through the soil water balance equation. In the revised manuscript, we will clarify this aspect in the set of equations.

[GdR 13] Eqs. (13) – (14). This are energy balances. For clarity and completeness, it would perhaps be good to include the heat term to show explicitly what the dissipated binding and gravitational energy is converted to, and to add the corresponding mass balance equations. The latter would be useful to address my next comment.

As these are not balance equations of all forms of energy in the soil, but only for binding and gravitational energy, it would be physically inconsistent to add a heat term to these balances. Unfortunately we can therefore not do this. In the revision, we will clarify this aspect and explain that the heating term can be seen in the dissipation, which is shown in Fig 4c.

We are not sure what is meant with "adding the corresponding mass balance equations", as the water balance equations are provided in form of the flux model in Section 2. Maybe this is a misunderstanding?

[GdR 14] One thing that makes Eqs. (8) to (15) a bit hard to interpret is the fact that they combine two contributions to the change in gravitational and binding energy: a change in the gravitational and/or matric potential (integrated over the water content in the soil volume of interest), and the change of the volumetric water content (integrated over the soil volume of interest). I believe more can be learned about energy dissipation if these terms are separated out in the equations.

We agree that this makes it a bit hard to interpret, yet it is a general issue in thermodynamics where the entropy of a system can change due to internal processes or by entropy exchange at the system boundary. The changes in energy associated with soil water are no different, as shown by eqn. (13) and its discussion in the manuscript. We will try to make this difficulty in interpretation clearer in the revised manuscript.

We do not think the contribution of gravitational and binding energy can be separated out easily, simply because it is really the spatial distribution (including heterogeneity) that causes much of the overall change in total hydraulic energy. In Equations 8-12 we only calculate the local values.

However, there is a way to learn about gravitational contribution *a posteriori*, by calculating the minimum increase in gravitational energy needed for a specific amount of soil drying. This should be demonstrated in a model application where the z dimension is resolved.

[GdR 15]. 13395, l. 10-14. I agree with the first part of the statement (the collar xylem potential would need to be lower when water is taken up from a drier soil),

but disagree with the second (... and also when soil water potentials are more heterogeneously distributed). Similar to my argument above, I believe plants take up water preferentially from areas where it is energetically advantageous to get (Adiku et al, 2000). Your statement is based on an interpretation of Fig. 2, and thereby implicitly assumes that plant roots obtain water indiscriminately from the entire root zone irrespective of the local energy status of the extracted water.

We did some work some time ago with measuring root water uptake in a root zone (from the local water depletion) while at the same time measuring the matric potential (van der Ploeg et al, 2008). The gravitational potential was known of course at each measurement location. We saw root water uptake start in the top of the profile (where irrigation caused relatively wet conditions initially). Under water-stressed conditions, we saw evidence of root water uptake activity moving deeper into the profile. Clearly, the root water uptake had a 'strategic' element in it, although we suspect it was not strictly energy-related, but also seemed to be largest in locations where the slope of the retention curve was small, i.e., a small drop in xylem potential energy could yield a sizeable amount of water delivered to the roots. This is the only piece of direct experimental evidence that I am aware of, but there is a lot of literature on this topic.

This comment addresses one of the major points of the paper. We would like to respond in separate steps:

- (1) As mentioned in the response to comment [GdR 02] above, we present the results of a distributed model, where fluxes are driven by local soil states and not, as suggested above, by average states. This is really important for the following.
- (2) We agree that presented with heterogeneous soil water distribution, roots would take up water, where it is most efficient to get it. Here we raise an additional point however. We say that from the perspective of the plant, it would increase the efficiency (further), if the soil water potential and uptake distribution were homogenous. Those two considerations are not at all mutually exclusive.
- (3) We understand your intuition that touching moist spots with the root system may render water uptake efficient. We thought similarly, when we set out on this project. But the results prove to the opposite. The evolution of the xylem potential of the purely hydrological and distributed (!) water flow model shows that water limitation occurs earlier (in wetter average soil condition) in soils with initially heterogeneous soil water potentials (Figure 3a). And the thermodynamical diagnostics show that the cause lies in both a greater dissipation during uptake and a greater change of internal energy per time.

Thus, we believe that the thermodynamic diagnostics presented here help gaining process understanding particularly in situations where heterogeneity occurs, such as root water uptake.

We will add a paragraph to the discussion to explicitly address this.

[GdR 15] p. 13395, l. 21-23. Ignoring soil water redistribution is a rather dangerous assumption in the case of root water uptake. Roots only take up water during daytime, and the re- distribution of water around the roots during night time is crucial for next day's uptake. Indeed, evidence is beginning to mount that roots excrete substances that facilitate water flow towards them, perhaps to increase the hydraulic conductivity in their immediate surroundings, where the radially

converging flows create need high gradients to get the water through to the root hair. Furthermore, roots acting as passive but conductive conduits for water at night allow water within the root zone to be redistributed more uniformly in the root zone during the night (although there still is some debate about this process).

The day-night rhythm in root water uptake also makes the constant-flux boundary condition debatable, doesn't it? Do you really need this assumption? It seems to me that it compromises the validity of your study considerably. That being said, for a proof of principle, this should not be major problem. But for any quantification of energy dissipation of root water uptake in ore natural systems, it will be.

Yes, it will be important to include more realistic conditions in order to make quantitative predictions on the overall energy dissipation. In fact, we hope that the thermodynamic diagnostics may support the assessment of the importance of those different processes (mucilage, aquaporin regulation, stomatal regulation, hydraulic redistribution, root system architecture and morphology), with regard to efficiency of root water uptake and improve our process understanding on strategies to optimize water relations in plants.

This paper does not attempt to do this. We think that because thermodynamics is not routinely used in soil hydrology it is critical to first use simple examples to demonstrate its use and have straightforward interpretations that are not obscured by model complexity stemming from the many processes and the highly variable forcing of the real world.

Result section

[GdR 16] Unfortunately, since I believe that the basic assumption about the nature of root water uptake being independent of the local soil water energy status is invalid, I do not consider the model runs and their outcome valid. I think this assumption needs to be replaced (or compared) to one that takes into account energy-sensitive root water uptake strategy before the model can yield meaningful results.

We believe that this remark is based on the assumption that the model is run on average soil states, which is not the case. We have responded to this in [GdR 02]. We will make sure to re-formulate the Methods section to avoid this misunderstanding with the readers.

[GdR 17] Also, both the model in its current state and the example problem that is examined are very simple. I believe the authors can be a bit more ambitious in their model development. The underlying equations are not wildly complicated. There is no need for a proof of principle on a problem that is too simple to have any relevance for realistic systems to be published separately before the model can be applied to more realistic scenarios. At this time, this second stage is entirely missing, and that clearly weakens the paper.

Yes, the model is simple, and with it we do not claim to make a general contribution to the dynamics of root water uptake. Instead, we wish to show the relevance of using a thermodynamic approach to assessing root water uptake. We demonstrate it deliberately on a simple model, because this has helped us (and we hope will help others), to capture the dynamics of this new approach, even if it may yield counterintuitive results. One of them being that heterogeneous soil water potentials inhibit

water flow. In a next step, this approach can be applied to more complex root water uptake models for improving process understanding.

On important reason, why we have not included soil water re-distribution is because the thermodynamic formulation is very sensitive to numerical errors. Hence, we would not be able to close the energy balance with the simple four compartment model due to numerical inconsistencies. It would require a proper discretization and much more complex representation of soil hydrology, which would defeat the purpose of the paper.

We believe that the simple model serves the intended purpose. We will motivate the purpose better in the revision.

[GdR 18] When a more comprehensive modeling exercise has been performed the advantages of this approach should be much clearer. I would welcome a paragraph explaining what the main contribution of this approach is. I expect it will be in bringing soil hydrology and thermodynamics closer together. The relevance for more application-oriented research may be less clear. If this is indeed the case, than what is missing is a connection with other works striving to do the same: the work of Gray, Hassanizadeh, and Miller on the pore scale and larger scales (with most paper appearing in the 1990s but still ongoing I believe in Advances in Water Resources), but also some very useful work by Groenevelt and Bolt in the 1960s already.

We will describe our contribution more clearly in the revised version of this paper.

The main contribution of the paper lies providing a tool that allows assessing where the impediments to root water uptake lie along the flow path between soil and atmosphere. Their relative contribution can be quantified. We show this using thermodynamic representation of each of the processes, which we derive.

We also show as a proof of concept that the energy balance is closed using the simple distributed uptake model. This is, in fact, not trivial, because a less careful numerical implementation may not achieve this balance. This insight may provide a useful diagnostic on how to implement soil water flows numerically in a physically consistent way.

We may also point out that the references by Grey, Miller etc. deal with quite a different issue in the thermodynamics of soils as these go into depth on how the statistical scaling should be done. We do not suggest new formulations, but simply combine what is already commonly being used, except that these are not evaluated in terms of energy. As we show, this evaluation of energy clearly reveals effects of heterogeneity that cannot be found simply by looking at water fluxes or matric potentials.

[GdR 19] I would also like to see simulations of continuous root water uptake vs. day-night cycles with redistribution at night to see how that affects the energy needed.

We have followed this suggestion and looked at day-night cycles. A model application in transient conditions, and with passive hydraulic redistribution during the night is shown in Figs S01 and S02 below. The effects of heterogeneity are enhanced with this variable forcing, but qualitatively yield the same insights. What is, however, difficult to interpret in these simulations is that water-stressed conditions set in much earlier in the heterogeneous setups. This makes it difficult to compare to the homogeneous case and

goes back to the point that the total hydraulic energy changes because of dissipiation but also because of how much water is removed.

We therefore think that the idealized setup chosen in the manuscript is more instructive as the cases are easier to be compared. We will include the additional simulations as an Appendix in the revised manuscript.

[GdR 20] On a different note: does the plant actively expend energy when taking up water? It does not need to actively lower its water potential, but instead can rely on the generally very low water potential in the atmosphere. Through its capillaries and its tissues that potential is passed on to the roots. All it needs to do is to regulate its stomatal resistance and possibly other resistances that plant physiologists know better than I do to moderate that potential to the degree best suited for its purpose and then let the resulting potential drop draw the water in. There is a biological advantage of minimizing the energy dissipation when the plant is water-stressed because the plant that can generate the lowest water potential in its root hairs can get more water in than less efficient plants with roots nearby. Under non-stressed conditions, is there an advantage to minimizing energy dissipation that I am overlooking?

Yes, the plant does not actively expend energy, it really only connects water potentials in the air and in the soil, and along this gradient water flows. The advantage in minimizing dissipation lies in delaying the time until water stress is reached.

The formost goal of this research however on learning where along the flow path the impediment to root water uptake lies. However, similar considerations can be applied to maximizing efficiency of water uptake, given certain constraints. Generally, it can also be applied in water limiting conditions (as shown above)

Detailed Comments (comments in the attached supplement)

[GdR 21] P 13384, L 15 I am not quite sure. If you really mean 'exported', from where does the energy come and where does it go?

"Export" is a typical term in describing systems, but we will clarify this meaning in the revision. It refers to the export of water (and binding energy) from the soil as roots take up soil water.

[GdR 22] P 13387, L 9: Please explain 'collar xylem potential'.

We will omit the reference to the xylem potential at this position, because it is better explained later in the text. We will change as follows:

Old: "Soil water is extracted by root water uptake with a collar xylem potential ψx from all reservoirs."

New: "Soil water is extracted from the soil reservoirs by root water uptake."

[GdR 23] P 13388, Eq (3): n = 4

Will be changed.

[GdR 24] P 13388, L 8-10: The conductivities represent the soil between the roots, and definitely not the root system itself. They do take into acount the geometry of the flow tubes towards the roots as affected by the root network density.

We believe this relates to the description of $K_{r,i}$ in Table 1, which should be improved. We will change this:

Old: "Effective conductivity of the root system in compartment i"

New: "Effective radial conductivity of the active roots in compartment i"

[GdR 25] Figure 1: This entire caption is rather confusing, please rewrite. The final sentence seems to imply that the initial water content in the two densely rooted reservoirs is equal, but different from the water content in both reservors with few roots. This contradicts the earlier sentence stating that each rooting density had one initially moist and one intially dry reservoir.

We will reformulate the caption.

Old: Schematic of the numerical split root experiment. The soil volume of each reservoir is explored by roots of a given root length thus changing the effective root conductivity. Reservoirs are paired with two reservoirs of high and low rooting density, and high and low initial water content each, while the evolution of average soil water content is the same in all simulations. Also, at the beginning of all simulations the average soil water content is the same in both reservoirs with high and low rooting density respectively.

New: Schematic of the numerical split root experiment. One plant has access to four soil compartments, two densely rooted (left) and two sparely rooted (right). Color shading of the containers indicates high (dark color) and low (bright color) initial soil water content. The *average* initial soil water content is the same in all simulations. In the same way, the *average* water content over the two left (densely rooted) and two right (sparsely rooted) containers is the same in all simulations.

[GdR 26] Figure 2: Spelling error

Will be corrected, thank you!

Response to Uwe Ehret

Dear Uwe Ehret, thank you very much for your feedback on the manuscript. We have divided the review in several sections in order to provide a point-by-point response. We start with the heading "Evaluation".

4. Evaluation

[UE 01] The study is conducted and written in a clear and precise way, all assumptions are clearly stated, the text is well-written and the figures are illustrative. The energy-centered approach to formulate and diagnose dynamics across connected subsystems is interesting and innovative.

Thanks.

However, in the way the study is presented now, the simplifying assumptions are so strong that the study lacks transferability of its insights to real-world soil-plant systems. Although the authors claim that this is not their intention, and they rather seek a proof-of-concept of the energy-based diagnosis system only, the study stays clearly below its potential. Also, without showing that the chosen model parameters are at least in a realistic range and realistic with respect to their relative values, it is not clear whether the overall findings of the paper are transferable to real-world systems.

We do not think that our assumptions are that strong, and in fact the formulations are comparatively easy to transfer, as, e.g., shown in the study by Bechmann et al. (2015). Yet, complex models and complex forcings can easily hide the basic mechanisms that are at work, as shown by the simulations that include a diurnal cycle (see below for details). There, the interpretation is much less straightforward, because the total hydraulic energy changes because of dissipation, but there is also a difference due to the earlier onset of water limitation in the heterogeneous simulations. This obscures a clear interpretation. We therefore think that the idealized setup is more instructive to illustrate the use of thermodynamics to look at root water uptake.

The parameters are within reasonable ranges of observations, as described in greater detail below.

In the revision, we will describe these points more clearly and specifically address the transferability of the insights to more complex settings.

More specific:

[UE 02] Are the absolute and relative values of total root water uptake, root system size (and with it the Kr,i conductivities) and soil hydraulic properties realistic? Compare to observations.

Although it is explicitly not the goal of this study to model real world systems, we have chosen the parameters to match nature. The model is representative of a plant having access to a soil volume of 0.5 m^2 , consisting of a soil monolith of 0.5 m depth and a surface area of 1 m^2 . Each of the compartments is same size (0.125 m^2) . The transpiration rate is indicative of a hot summer day, with 6 mm d^{-1} . With the indicated radial conductivities, we assumed them be around of $3 \text{ 10}^{-6} \text{ m s}^{-1} \text{ MPa}^{-1}$, which is on the upper end of the values summarized in Draye et al. 2010. and the total root length in the compartments thus varying between 1 cm cm^{-3} (most densely rooted), 0.5 cm cm^{-3} (average) and 0.1 cm cm^{-3} (least densely rooted). This is within the range of observed root length densities (Kuchenbuch et al., 2009).

[UE 02] Give proof that the negative feedback of soil water availability on the total transpiration rate is not a major constraint and can thus be neglected in the study without compromising the results.

Soil water does limit transpiration in our model as soon as the xylem potential drops below a critical value. This is a formulation commonly assumed in distributed models of root water uptake (i.e. Javaux et al. 2008, Schneider et al. 2010), and is meant to represent the regulation of transpiration expected of isohydric plants.

[UE 03] Why is the process of soil water movement and the associated dissipation in-between the boxes described in the manuscript, but not used in the experiments? It would seem to me that the relative magnitudes of soil water fluxes and root water uptake are a major control on the effectiveness (and strategies) of root water uptake and hence should not be omitted.

We described soil water flow because we wanted to show how dissipation due to soil water flow enters the total energy export in Eq. 15.

The reason why we did not include soil water flow in the simulations is because a model of unsaturated flow requires appropriate discretization to avoid numerical errors that can result in artificially high water flow rates. Those numerical errors strongly affect whether or not the energy balance can be closed. This is because, the dissipation is calculated based on the gradients in one time step, but the change in binding energy based on two consecutive time steps.

Remember that the total hydraulic energy is elevated in soils with heterogenous soil water potentials compared to homogenous ones, with the extra energy available to drive flow to equilibrate potentials. This extra energy will dissipate in the equilibrating flow process. If the water flux calculation is faulty due to numerical errors, for example assuming an overestimation of water flow between two compartments, then the change in internal energy does not match the dissipation due to the flow. This is a very sensitive issue.

Ideally, unsaturated flow and related dissipation is best accounted for in a sophisticated numerical scheme for flow and root water uptake like RSWMS or OGS. Such an application would however sacrifice the intuitive character of the paper and take away the focus from the thermodynamics. This is why we did not include the representation of unsaturated flow, but we hope Eq. 15 will be applied to sophisticated model results in the future.

In the revision, we will extend this discussion on how important it is to adequately represent the numerics in solving the water balance.

[UE 05] In this context, the diurnal cycle of transpiration can also play a role (there is time for soil water recharge during the night, where no transpiration occurs). At least show that soil water heterogeneity can indeed persist long enough that it plays a role for root water uptake.

As the first reviewer (Gerrit de Rooij) also mentioned this aspect, we respond equivalently to the first point:

We have followed this suggestion and looked at day-night cycles. A model application in transient conditions, and with passive hydraulic redistribution during the night is shown in Figs S01 and S02 below. The effects of heterogeneity are enhanced with this variable forcing, but qualitatively yield the same insights. What is, however, difficult to interpret in these simulations is that water-stressed conditions set in much earlier in the heterogeneous setups. This makes it difficult to compare to the homogeneous case and

goes back to the point that the total hydraulic energy changes because of dissipiation but also because of how much water is removed.

We therefore think that the idealized setup chosen in the manuscript is more instructive as the cases are easier to be compared. We will include the additional simulations as an Appendix in the revised manuscript.

Regarding the persistence of heterogeneity: In this model setup, we also allow for hydraulic redistribution in the night, which occurs passively. In the model this takes place when the xylem potential calculated with Eq. D1 (response to GdR 02 above) falls between the actual soil water potentials. However, this redistribution is slow.

Heterogeneity of soil water potentials is omnipresent, and may have many causes. For example, root water uptake itself is a major causing disequilibrium in soil water potentials. Thus, we believe soil water potential heterogeneity plays an important role in many real life situations and therefore also for closing the energy balance, thus meriting a treatment in this paper.

In this paper, we do not insist on the exact magnitudes of the represented processes, but we wish to show how they can be represented in models and that heterogeneity has a general effect on the thermodynamics of the system.

Some minor points

[UE 06] 13385/24-25: Why can the soil water relation not be formulated in a resistance analogue (e.g. piece-wise linear)? Please clarify.

What we mean is that unlike in the Darcy Equation, the water retention function cannot be described as a resistance in an electrical circuit as it relates to storage changes. Thus, we cannot calculate the respective contribution of different resistors within the network. We will reformulate this.

Old: "Both processes (gradient-driven water flow and soil drying) may each impede the water flow to the atmosphere, but comparing their mutual contribution in form of resistances is not suitable, amongst others, since the soil" water retention relation has no resistance analogue."

New: "Both processes (flow over a resistance network and increasing soil water retention) impede transpiration, but comparing their mutual contribution in form of resistances is not suitable, since the change of soil water retention per water removed has no proper resistance analogue."

[UE 07] 13391/6: Jm-3 (the 'J' is missing)

Yes. Thank you!

[UE 08] 13392/20: I suggest 'this additional free energy'

Yes, we will change this.

[UE 09] 13396/9: I suggest 'optimal (from the plant's point of view)'. Also give a link to the later section where you discuss (and resolve) the apparent disagreement of maximum and minimum dissipation states.

Ok. We will change as follows:

Old: The scenario called "optimal" is one where both initial soil water content and root distribution are homogenous. It can be seen as the optimal 10 scenario as it minimizes dissipation.

New: The scenario called "optimal" is one where both initial soil water content and root distribution are homogenous. It can be seen as the optimal scenario (from a plants point of view) as it minimizes dissipation.

Ok, we will refer to the discussion section.

References

Javaux, M., Schroder, T., Vanderborght, J. and Vereecken, H.: Use of a three-dimensional detailed modeling approach for predicting root water uptake, Vadose Zo. J., 7(3), 1079–1088, 2008.

Draye, X., Kim, Y., Lobet, G. and Javaux, M.: Model-assisted integration of physiological and environmental constraints affecting the dynamic and spatial patterns of root water uptake from soils, J. Exp. Bot., 61(8), 2145–2155, doi:10.1093/jxb/erq077, 2010.

Kuchenbuch, R. O., Gerke, H. H. and Buczko, U.: Spatial distribution of maize roots by complete 3D soil monolith sampling, Plant Soil, 315, 297–314, doi:10.1007/s11104-008-9752-8, 2009.

Schneider, C. L., Attinger, S., Delfs, J.-O. and Hildebrandt, A.: Implementing small scale processes at the soil-plant interface – the role of root architectures for calculating root water uptake profiles, Hydrol. Earth Syst. Sci., 14(2), 279–289, doi:10.5194/hess-14-279-2010, 2010.

Figures

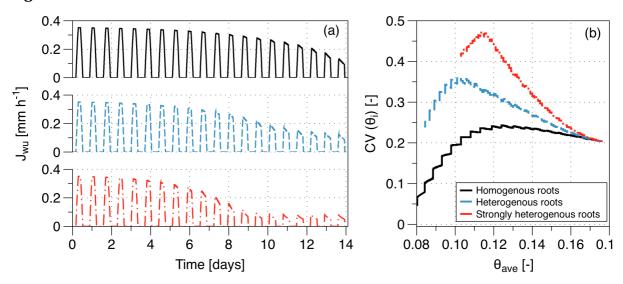


Fig. S01: Evolution of a distributed, transient root water uptake model. Total potential daily transpiration is 3 mm d⁻¹. Root water uptake follows potential transpiration, unless root collar potential drops below the permanent wilting point (-150 m). **(a)** Evolution of the calculated root water uptake, **(b)** Coefficient of variation of water content in the three compartments.

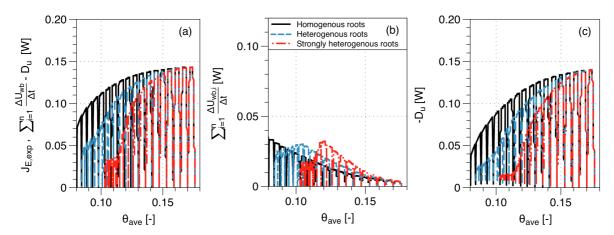


Fig S02: Exported energy and its components for the soil-plant-system over the course of a drying experiment and different root water uptake scenarios. Results from a transient model. As in Fig. S01(b), the time axis was replaced by the average soil water content. (a) Total energy exported from the system at the root collar. It is the sum of the two components given in the other subplots, (b) Component due to decrease of soil binding energy, which is due to both soil drying and enhanced heterogeneity (compare Fig. S02b), (c) Component due to energy dissipation by water flow from the soil into the root.