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# A thermodynamic formulation of root water uptake

### A. Hildebrandt<sup>1,2</sup>, A. Kleidon<sup>2</sup>, and M. Bechmann<sup>1,2</sup>

<sup>1</sup>Friedrich-Schiller-Universität, Jena, Germany <sup>2</sup>Max-Planck-Institut für Biogeochemie, Jena, Germany

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#### Abstract

By extracting bound water from the soil and lifting it to the canopy, root systems of vegetation perform work. Here we describe how the energetics involved in root water uptake can be quantified. The illustration is done using a simple, four-box model of the

- soil-root system to represent heterogeneity and a parameterization in which root water uptake is driven by the xylem potential of the plant with a fixed flux boundary condition. We use this approach to evaluate the effects of soil moisture heterogeneity and root system properties on the dissipative losses and export of energy involved in root water uptake. For this, we derive an expression that relates the energy export at the root col-
- <sup>10</sup> Iar to a sum of terms that reflect all fluxes and storage changes along the flow path in thermodynamic terms. We conclude that such a thermodynamic evaluation of root water uptake conveniently provides insights into the impediments of different processes along the entire flow path and explicitly accounting not only for the resistances along the flow path and those imposed by soil drying but especially the role of heterograms
- soil water distribution. The results show that least energy needs to be exported dissipative losses are minimized by a root system if it extracts water uniformly from the soil. This has implications for plant water relations in forests where canopies generate heterogenous input patterns. Our diagnostic in the energy domain should be useful in future model applications for quantifying how plants can evolve towards greater effi-
- ciency in their structure and function, particularly in heterogenous soil environments. Generally, this approach may help to better describe heterogeneous processes in the soil in a simple, yet physically-based way.

#### 1 Introduction

Root water uptake is an important process, determining the transport of water between soil and atmosphere and influencing plant productivity and crop yield. A wealth of studies using both models and observations deals therefore with understanding root water

uptake, that is to, learn where plants take up water (Doussan et al., 2006; Javaux et al., 2008; Schneider et al., 2010), how root length and hydraulic properties affect uptake (Zwieniecki et al., 2003; Bechmann et al., 2014), how plant communities exploit heterogeneously distributed soil water (Lhomme, 1998; Couvreur et al., 2012; Guswa,

- <sup>5</sup> 2012), identifying efficient rooting depth (Guswa, 2010), learn how soil water storage is shared between plants (Ivanov et al., 2012; Hildebrandt and Eltahir, 2007) how plants may optimize water flow in order to prevent cavitation (Sperry et al., 1998; Johnson et al., 2014) and relations between root water uptake and stomatal control (Tuzet et al., 2003; Janott et al., 2011), as well as crop yield (Hammer et al., 2009).
- In order to evaluate the efficiency of root water uptake and learning how changes in root structure may improve it, we require some understanding of the impediment for water flow and how it is distributed along the soil-plant-atmosphere continuum, especially whether it lies within the plant or soil compartment (Draye et al., 2010). Much of our process understanding on the spatial distribution of water uptake and its evolution
- <sup>15</sup> in drying soil is based on physically based models of the root system (Dunbabin et al., 2013). Relying on the electrical analogue of water flow and mass balance (van den Honert, 1948; Lhomme, 1998), they mimic the flow of water over a chain of resistances along continuously dropping water potentials from the soil to the root, further up within the root xylem, sometimes up the canopy (Janott et al., 2011). At the same time, root
- water uptake depletes the soil reservoir leading to more negative soil hydraulic potentials which need to be overcome in order to maintain the necessary gradient between soil and atmosphere to allow for flow. 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.

In this paper we show that additional information about the system can be obtained from a thermodynamic perspective, specifically by combining the hydraulic potentials with mass fluxes, yielding fluxes of energy. This approach has the advantage that different processes, such as the change of soil water potential with decreasing soil water

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content as well as the transport of water along a resistance can be expressed in the same currency of energy fluxes and dissipation, with units of W  $(J s^{-1})$ .

While thermodynamics is most commonly associated with heat, its formulation is much more general and can be used to express the constraints and directions of energy

- <sup>5</sup> conversions of any form (Kondepudi and Prigogine, 1998; Kleidon, 2012). As soil water movement and uptake by plants involves changes in binding and gravitational energy, as expressed by the respective matric and gravitational potentials, the fluxes of water in the soil-vegetation-atmosphere system is associated with fluxes of energy, and we can compare which one of the processes in the uptake chain requires most energy, as
- well as quantifying the total energy expense of the uptake. Thus, the thermodynamic perspective allows us to evaluate the efficiency of different temporal dynamics of root water uptake and characterize more efficient from less efficient root systems.

As will be shown in this paper, the thermodynamic formulations are comparatively simple, and straightforward to implement in models. Since the hydraulic potential is just

- the specific energy per mass (or volume), that is, the derivative of the Gibbs free energy to mass (or volume), the related soil energy content can be obtained by integration. The thermodynamic representation has, however, several advantages that are currently not well explored by the hydrological community. One of these advantages is, for example, related to describing the effects of soil heterogeneity. While soil water potential is an
- intensive property (i.e. a property that does not depend on the size of the system) that cannot meaningfully be averaged, the associated energy content is an extensive property (i.e. a property that depends on the size of the system), therefore is additive, and the total energy content in heterogenous soil can be calculated. As will be shown, the total energy content offers insights into the role of soil heterogeneity that cannot be derived when focussing only on the potential or the soil water content alone.

In the following, we will derive formulations for the energy contained in unsaturated soil as well as for the dissipation of energy for fluxes in unsaturated soil and along the root system. In order to illustrate how these fluxes can be interpreted to evaluate

efficiency of root water uptake and the role of soil water heterogeneity, we illustrate them in a conceptual four-box model for root water uptake, which we will introduce first.

#### 2 A conceptual model for root water uptake

- We consider a simple system as shown in Fig. 1. The system consists of four soil water reservoirs, from which water is extracted by root uptake. No water is added during the simulation. All soil reservoirs are assumed to be of equal volume,  $V_{\text{res}}$  (m<sup>3</sup>), and their water storage is described by the variables  $W_i = \theta_i V_{\text{res}}$  (in m<sup>3</sup>) with  $\theta_i$  being the volumetric soil water content (–) of the servoir *i*. Soil water is extracted by root water uptake with a collar xylem potential  $\varphi_x$  from all reservoirs. For simplicity, we assume
- that all reservoirs have an equally shallow depth, so that we can neglect differences in the gravitational potential between reservoirs. An overview of the variables including soil parameters used in this study is given in Table 1.

The mass balances of the reservoirs describe the temporal changes in  $W_i$  in terms of the root water uptake fluxes,  $J_{wr,i}$  (m<sup>3</sup>s<sup>-1</sup>) and soil moisture redistribution between the reservoirs,  $J_{w,ii}$  (m<sup>3</sup>s<sup>-1</sup>). They are expressed as

$$\frac{\mathrm{d}W_i}{\mathrm{d}t} = J_{\mathrm{wr},i} + J_{\mathrm{w},ij} \tag{1}$$

with both fluxes carrying negative signs when directed outward of the reservoir. The water flux  $(J_{w,ij}, m^3 s^{-1})$  between the neighboring reservoirs *i* and *j* is expressed by Darcy's law, being proportional to the difference in matric potentials ( $\psi_M = f(\theta)$ , m water):

$$J_{\mathbf{w},ij} = -K_{ij}(\psi_{\mathbf{M},i} - \psi_{\mathbf{M},j}) \tag{2}$$

where  $K_{ij}$  (m<sup>2</sup> s<sup>-1</sup>) is the effective unsaturated soil hydraulic conductivity between the adjacent compartments *i* and *j*.

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The total root water uptake  $(J_{wu}, m^3 s^{-1})$  is the sum of the uptake fluxes from each compartment, which are described in analogy to Darcy's law:

$$J_{\rm wu} = \sum_{i=1}^n J_{{\rm wr},i} \qquad \bigcirc$$

with

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<sup>5</sup> 
$$J_{\mathrm{wr},i} = -K_{\mathrm{r},i}(\psi_{\mathrm{M},i} - \psi_{\mathrm{x}})$$

where  $\psi_x$  (m water) is the xylem water potential which is taken to be equal throughout the entire root system. The conductivities  $(m^2 s^{-1})$  are effective conductivities representing the entire part of the root system and hydraulic conductivity of the flow path encompass the notion of active root length and hydraulic conductivity of the flow path from the bulk soil into the root xylem, all of which are positively related to  $K_r$ . In our

conceptual model, we will change the proportion of  $K_{r,i}/K_{r,j}$  to create heterogenous root water uptake from the different reservoirs (see below).

We obtain the uptake rates for each reservoir by solving the systems of equations with a prescribed boundary condition (total transpiration,  $J_{wr}$ ) for the unknown xylem water potential  $\psi_x$ . Water contents are then updated based on the root water uptake and soil water flow between reservoirs (if applicable). Initial conditions and root conductivities are varied as shown in the following.

We run the model for four scenarios, indicated in Table 2. In the scenarios we vary the distribution of initial soil water content and the implied root length (via changing to compartment root conductivity) to impose increasingly heterogenous conditions while keeping the average constant.

The first scenario is completely homogenous (initial soil water and root conductivity is the same in all compartments). The following three scenarios are all initialized with heterogenous initial soil water, and differ with regard to the heterogeneity of root conductivity. In all simulations the average initial soil water content is the same. In the

(3)

(4)

same way, the effective root conductivities ( $K_{r,i}$ ) were either homogeneously distributed or heterogenous with two compartments having more roots and two less than average. Working with four compartments allows us to combine the manipulation such that average root conductivity is equal between the dry and wet compartments and between all scenarios (see Table 2, Fig. 1).

For matters of simplicity, we present only results for periods where the soil does not limit uptake. We somewhat arbitrarily assume that soil water becomes limiting when the water demand cannot be satisfied when the root xylem potential falls somewhat below the permanent wilting point (-150 m). When this point is reached, we fix  $\psi_x = -150$  m.

To derive soil hydraulic properties, we use a soil with parameters given in Table B1. The conceptual model serves for demonstration purposes, while realistic modeling of root water uptake is not the primary goal for its application here. However, the thermodynamics we wish to illustrate can (and we hope will) be applied to more complex models with larger number of compartments and using realistic formulations for root water uptake and water flow. 15

## 3 Thermodynamics and soil hydrology

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#### 3.1 Thermodynamic background

Thermodynamics is a general theory of physics that describes the rules for energy conversions. The first law of thermodynamics ensures energy conservation and formulates

- that the internal changes in energy are balanced with external additions or removals 20 and internal conversions between different forms. The second law describes that with every conversion of energy, energy is increasingly dispersed, which is described by entropy as a physical quantity. It is the second law that sets the natural direction of processes to deplete their driving gradients and that is, for instance, reflected in soil water
- movement depleting gradients in soil water potential. The state of thermodynamic equi-

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librium is then described as a state of maximum entropy and represents a state in which no driving gradients are present within the system.

To describe soil water movement in thermodynamic terms, it needs to be formulated in terms of the energies involved and it needs to be associated with entropy. The en-

- ergies involved consist of the binding energies associated with capillary and adhesive forces, gravitational energy, and heat. The first two forms of energy are directly relevant to soil water movement. Their formulation in energetic terms is straightforward as these are directly related to the matric and gravitational potentials. These potentials are formally defined as chemical potentials (Edlefsen and Anderson, 1943; Kondepudi
- and Prigogine, 1998), i.e. defined as the change in Gibbs free energy resulting from an 10 incremental change in mass.

The use of heat is important as it is required to ensure energy conservation within the soil when the other forms of energy change, and because heat is directly linked to the entropy of the system. When water is redistributed within the soil due to gradients in soil

- water potential, this results in a reduction of the binding and gravitational energy, with the reduced energy being released as heat of immersion (see also below). The state of thermodynamic equilibrium is reached when there is no gradient in soil water potential. This state corresponds to a state of minimum Gibbs free energy, i.e. the binding and gravitational energy is minimized for a given amount of water. As the remaining energy
- is converted into heat, this reduction to a minimum of Gibbs free energy corresponds 20 to a maximum conversion into heat and thereby a maximization of entropy that can be achieved by soil water redistribution. This is despite the fact that the actual amounts of heat involved are rather small compared to the heat fluxes involved in heat diffusion in the soil.
- Next, we describe how these forms of energies are determined quantitatively from 25 their respective potentials, and how these forms of energy change during root water uptake and soil water redistribution.

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#### 3.2 Forms of energy associated with soil water content

Two types of energy are relevant for describing soil water states. We will refer to this sum as the total hydraulic energy ( $U_w$ , J) contained in a soil volume, which consists of the binding energy,  $U_{wb}$  (Jm<sup>-3</sup>), and the gravitational energy,  $U_{wg}$  (Jm<sup>-3</sup>):

$$= \int_{V} (U_{wb} + U_{wg}) dV.$$
(5)

The gravitational energy ( $U_{wg}$ , m<sup>-3</sup>) relates to the energy necessary to lift the water from a reference level up to the point where it is stored in the soil:

$$U_{\rm wg} = \rho_{\rm w} \cdot g \cdot \theta(z) \cdot (z_{\rm r} - z)$$

where  $\rho_w$  is the density of water ( $\rho_w = 1000 \text{ kg m}^{-3}$ ), g is the gravitational acceleration,

 $z_r$  is the elevation of the reference level, *z* the vertical coordinate, while  $\theta(z)$  refers to the volumetric water content at level *z*. Equation (6) is only given for completeness, but has no effect in the simple model presented. In the conceptual model described above, all reservoirs are of the same elevation and therefore temporal changes in water content or its distribution between reservoirs do not reflect on changes of the gravitational energy of the system.

The binding energy  $(U_{wb}, Jm^{-3})$  relates to the capillary forces in the soil pores. With the soil matric potential being the change of Gibbs free energy per change of mass, the related energy can be found by integration. We obtain it here by integration of soil water volume:

<sup>20</sup> 
$$U_{wb}(\theta) = \rho_w \cdot g \cdot \int_{\theta_{min}}^{\sigma} \psi_M(\theta') \cdot d\theta'$$

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Essentially,  $U_{wb}$  is the integral of the water retention curve  $(\psi_M(\theta))$ . The multiplication with  $\rho_w \cdot g$  serves for converting the units of  $\psi_M$  from meter water to Joule. An example for both  $\psi_M(\theta)$  and the related  $U_{wb}(\theta)$  is depicted in Fig. 2 for a sandy loam. The lower integration point has a great influence on the absolute values of the integral of binding energy in the soil, but as will be shown in the next paragraph, the relative differences in  $U_{wb}$  are of relevance. Therefore, the exact choice of  $\theta_{min}$  does not affect the results. We chose a value just below the water content at the permanent wilting point, in other words, a value smaller than the water contents that will be reached in our simulations.

Figure 2b shows the binding energy of the soil water as a function of the volumetric soil water content both for homogeneously and heterogeneously wetted soil. Like the soil matric potential *II* is pagative, reaching the lowest values at soil saturation. The

- soil matric potential, *U*<sub>wb</sub> is negative, reaching the lowest values at soil saturation. The negative sign relates to the fact that energy is released (in form of a very small amount of heat), when water attaches to the pore walls ("heat of immersion", Edlefsen and Anderson, 1943; Hillel, 1998). The same amount of energy has to be replaced in the soil when water is removed from the pores, and hence the bond between the water
- and the pore wall is broken. Thus, decreasing the water content via root water uptake constitutes an export of negative energy to the soil system.

When soil water is distributed heterogeneously, the binding energy increases (is less negative). Technically, this results from the strongly non-linear water retention function, and combining Eqs. (5) and (7). From a process perspective, this additional energy will drive water fluxes for equalizing the internal gradients, and will during this process eventually dissipate this amount of energy by conversion into heat.

During root water uptake, a given amount of energy has to be invested to take up a certain volume of water over time. Hence differential changes of binding energy per change in water content are relevant. Note that the slopes on the curves in Fig. 2b are steeper the greater the soil water heterogeneity. This implies that more energy has to be invested per decrease in total soil water content in heterogenously compared to homogeneously wetted soils.

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#### 3.3 Dissipation and energy export associated with soil water movement and root water uptake

Soil water fluxes lead to dissipation  $(D, Js^{-1} = W)$  of total hydraulic energy. Those fluxes may occur between compartments during redistribution of bulk soil water or at the small scale due to root water uptake. For our simple model, energy dissipation due to soil water flow between compartments is written as:

$$D_{\mathbf{f},k} = \rho_{\mathbf{w}} \cdot g \cdot (\psi_{\mathbf{M},i} - \psi_{\mathbf{M},i}) \cdot J_{\mathbf{w},ij}$$

$$\tag{8}$$

with

$$D_{\rm f} = \sum_{k=1}^{l} D_{\rm f,k} \tag{9}$$

where  $J_{w,ii}$  refers to the water flux between the neighboring compartments *i* and *j*,  $D_{t,k}$  (J s<sup>-1</sup>) to the respective dissipation of energy over the boundary k between those compartments and  $D_{\rm f}$  (J s<sup>-1</sup>) to the total dissipation due to water fluxes within the total soil volume. The dissipation is always negative, since it indicates a loss of hydraulic energy from the system, which is released in form of a very small quantity of thermal energy. 15

The same applies to the dissipation of energy due to the small-scale radial root water uptake  $(D_u, J s^{-1})$ , which is written for our simple model as:

$$D_{u,i} = \rho_{w} \cdot g \cdot (\psi_{M,i} - \psi_{x}) \cdot J_{wr,i}$$
(10)

with  $D_{u,i}$  (Js<sup>-1</sup>) being the dissipation due to root water uptake in each reservoir *i*, and  $_{20}$   $D_{II}$  becomes

$$D_{\rm u} = \sum_{i=1}^{n} D_{{\rm u},i}.$$
 (11)

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Lastly, the root water uptake constitutes an export of energy  $(J_{E,exp}, Js^{-1})$  from the soil root system, which is defined as

$$J_{\mathsf{E},\mathsf{exp}} = \rho_{\mathsf{w}} \cdot g \cdot \psi_{\mathsf{x}} \cdot J_{\mathsf{wu}}.$$

The sign of  $J_{E,exp}$  is positive since in our case, water leaves the system (a negative flux) over the root collar at negative hydraulic potential. Correspondingly, this increases the internal hydraulic energy as the soil dries (compare Fig. 2).  $J_{\rm E,exp}$  would be negative, should water enter the system via the roots.

Although the dissipation  $(D_f, D_u)$  and energy fluxes  $(J_{E,exp})$  carry the same units, their difference is noteworthy. Dissipative fluxes refer to internal processes within the thermodynamic system. They are irreversible. In our example they reflect the heat dissipated when water fluxes degrade the gradients in soil water potential. On the other hand,  $J_{\rm E,exp}$  is an energy flux (energy transported) across the system boundary, as defined in this model. Note, however, that in general also this flux depletes a gradient

(between the soil and the atmosphere), but this gradient is not described in our simple soil-root model explicitly.

The energy balance for the soil-root-system can thus be written as follows for the general case:

$$\frac{\mathrm{d}U_{\mathrm{w}}}{\mathrm{d}t} = \int_{V} \frac{\mathrm{d}(U_{\mathrm{wb}} + U_{\mathrm{wg}})}{\mathrm{d}t} \mathrm{d}V = \int_{V} D_{\mathrm{f}} + \int_{V} D_{\mathrm{u}} + J_{\mathrm{E,exp}}.$$
(13)

For a model with bulk soil compartments, like the simple model used as an example here, the volume integral is replaced by summation over all compartments and the time differential becomes a difference notation. Thus Eq. (13) becomes

$$\sum_{i=1}^{n} \frac{\Delta(U_{\text{wb},i} + U_{\text{wg},i})}{\Delta t} = \sum_{k=1}^{l} D_{\text{f},k} + \sum_{i=1}^{n} D_{\text{u},i} + J_{\text{E,exp}}.$$
(14)
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(12)

Some properties of this equation are noteworthy. First, re-arranging Eq. (14) yields an expression that relates the characteristics at the outlet of the system to a series of internal processes:

$$J_{\mathsf{E},\mathsf{exp}} = \rho_{\mathsf{w}} \cdot g \cdot \psi_{\mathsf{x}} \cdot J_{\mathsf{wu}}$$
$$= \sum_{i=1}^{n} \frac{\Delta U_{\mathsf{w},i}}{\Delta t} - \sum_{k=1}^{l} D_{\mathsf{f},k} - \sum_{i=1}^{n} D_{\mathsf{u},i}.$$

The units in all terms of Eq. (15) are  $J s^{-1}$  or W, as they all indicate rates of energy flux and changes of energy content with time. More practically,  $J_{E,exp}$ , as the product of root collar xylem potential and transpirational flux, is influenced by several processes and Eq. (15) shows that they act as a sum (remember that all dissipative terms have

- <sup>10</sup> negative signs). For a constant water flux, Eq. (15) shows that the collar xylem potential would have to be more negative when water has to be moved within the soil (thus decreasing  $D_{\rm f}$ ), when water is taken up in drier soil at more negative soil water potentials, and also when soil water potentials are more heterogeneously distributed (both increasing  $U_{\rm wb}$ , as shown in Fig. 2). For model applications, comparison of the
- <sup>15</sup> magnitude of the separate terms of the sum in Eq. (15) provides a tool to assess which of the successive pathways involved in root water uptake most strongly impedes water flow.

#### 4 Results

We present a model run of the simple model to demonstrate how the thermodynamic concepts explained above can be applied to separate the impediments to root water uptake, and thus provide a better process understanding of the model results. For matters of simplicity, we ignore soil water redistribution in our model, and thus changes in water content are due to root water uptake alone. Also, we only consider times with

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unstressed transpiration, which ensures a constant flux boundary condition, while root water uptake and average soil water contents at a given time is equal in all scenarios.

- Figure 3 shows the evolution of the root collar potential over the course of the water uptake and the associated creation of heterogeneity of soil water contents (coefficient of variation). Shown are the results of all scenarios given in Table 2. Remember that the difference between scenarios is only with regard to the prescribed heterogeneity. The average initial water contents, root conductivities and root water uptake is the same in all simulations. 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 as it minimizes dissipation. It is obvious from the evolution of the root collar potential that, despite everything relating to the overall water balance being the same in all scenarios, the homogenous (optimal) scenario is the one where limiting xylem potentials are reached at the lowest average soil water content and longest time after beginning of the experiment. The limiting xylem potential is reached earlier the more
- <sup>15</sup> heterogenous the distribution of root water uptake and soil water contents. Also, it is shown analytically in the Appendix that uptake from homogeneously distributed soil water minimizes (i.e. optimizes from the plants point of view) the dissipative losses due to root water uptake.

Based on the output of the root water uptake model, we applied Eq. (15) to diagnose

- <sup>20</sup> the impediments to root water uptake. The individual terms of Eq. (15) (except dissipation to soil water flow, which was not modeled) are plotted separately in Fig. 4: on the left the total export of energy ( $J_{\rm E,exp}$ ), which proves to be composed of the change of binding energy in the soil ( $\Delta U_{\rm wb}/\Delta t$ , middle) and dissipation due to root water uptake ( $-D_{\rm u}$ , right). All individual terms ( $\Delta U_{\rm wb}/\Delta t$ ,  $D_{\rm u}$  and  $J_{\rm E,exp}$ ) were calculated separately,
- applying Eqs. (7), (10) and (12). Thus, Fig. 4 provides a proof of concept for the correct derivation of Eq. (15).

The energy export ( $J_{E,exp}$ ) corresponds closely to the evolution of the root xylem potential (Fig. 3, left panel), because the transpirational flux is prescribed as constant.  $J_{E,exp}$  increases continuously as the soil dries in order to maintain the constant rate of

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(15)

uptake. The decomposition of the energy export informs about the impediments to root water uptake in this model. The greatest contribution in wet soil is from the dissipation when water flows from the soil into the root, which constitutes about 97 % of the energy export. When the soil dries out, it becomes increasingly more costly to detach water

from the soil matrix, and the change of the binding energy makes up a somewhat more substantial proportion of the total energy exported from the system (17–22%, depending on the scenario).

The optimal case (grey solid line) is the one with the least possible expenditure in  $\Delta U_{wb}/\Delta t$ , and the difference between the solid grey curve and the other curves illus-

- trates the impact of soil water heterogeneity on the water uptake at each time step. At the same average soil water content, differences in  $\Delta U_{wb}/\Delta t$  between scenarios are entirely due to heterogenous soil water distribution. When comparing the optimal scenario and the one with strongly heterogenous roots at  $\theta_{ave} = 0.15$ , we observe that less than half of the investment in detaching water is due to soil drying and the re-
- <sup>15</sup> maining part is due to the heterogenous distribution of the soil water. The effect of soil heterogeneity increases further after this point.

At the same time, in heterogenous soils the impediment to uptake due to water flow over the root resistance increases, since uptake occurs preferentially in a limited part of the root system (the compartment with greatest root length that was initialized as wet, data not shown). However, this dissipation effect is less dynamic over time as the one related to soil drying in this modeling exercise.

#### 5 Discussion

We have applied a very simple model for root water uptake, and the main purpose was to illustrate the power of diagnosing the results by applying thermodynamics to this

<sup>25</sup> process. The same concepts can easily be implemented in more complex models of root water uptake and will then be more useful with regard to interpreting the individual processes impeding root water uptake. However, the main results of this paper are

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independent of the model complexity. First, the energy export at the root collar is the sum of a series of dissipative fluxes and changes in total hydraulic energy storage along the uptake path. Second, creating heterogeneity in soil water decreases the efficiency of root water uptake. The latter process may become less important in extended root

- networks, where dissipation along the lateral pathway within the root is substantial. Application of thermodynamics as proposed in this paper may help to identify and understand the effects of heterogeneity in more realistic models of root water uptake. In our thermodynamic description of the soil-plant system, we have not considered the changes of soil temperature, which should be induced particularly when latent heat
- is generated as water attaches to the soil. We have done this, because the related changes of temperature are so small that they would not affect the water flow and generally small compared to changes of temperature due to radiative soil heating.

We have also deliberately limited our model scenarios to situations where roots do not grow and root length does not depend on water availability. In contrast, we made sure that root abundance and water availability were arranged like in a factorial design.

Again, the goal of the specific scenarios was to illustrate the thermodynamic diagnostics, not to investigate uptake strategies with this simple model.

Finally, we have assumed in this derivation that the soil water retention function is known and is non-hysteretic. The latter may have considerable influence on the result-

<sup>20</sup> ing trajectory of  $\Delta U_{wb}/\Delta t$ . Generally, hysteresis can be included in the framework to investigate this effect further in the future. In combination with soil water content, the total hydraulic energy provides a mini-

mum description that captures heterogeneity in soil water distribution. Neither the soil matric potential nor water content carry this information. The soil can assume only one

value of average saturation, regardless of whether moisture is heterogenous or homogeneously distributed in the soil. In contrast, the total hydraulic energy takes different values in soils where soil moisture is distributed at the equilibrium (minimum energy) compared to heterogenous, non-equilibrium distribution. In the latter case, the extra energy is available to drive the fluxes that act to equalize gradients. Discussion Paper

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The water potentials, the derivative of the Gibbs free energy per mass, are an intensive property of the system and in heterogenous systems, they cannot be meaningfully averaged. The Gibbs free energy itself is an extensive property, can be averaged and hence allows to describe efficiently states also in heterogenous systems. An additional

- advantage of working in the "energy domain" constitutes the possibility to consider 5 both the influence of the water retention function, heterogeneous soil water distribution and the various resistances along the flow path in the same realm and using the same units. In particular, heterogeneity of soil water increases the total hydraulic energy, which necessarily implies that xylem water potentials have to be more negative to
- transpire at the same rate and same average soil water content. Thus, plants rooted in heterogeneously wetted soils are expected to reach water limitation earlier. This phenomenon has already been observed in models dealing with spatially heterogenous infiltration patterns caused by forest canopies (Guswa and Spence, 2011).
- We have given equations for our simple system, but the concept can easily be ex-15 tended to more complex systems, for example three dimensional models of root water uptake (Doussan et al., 2006; Javaux et al., 2008; Kalbacher et al., 2011) which include more process details, particularly more complex description of water flow within the root system or any other process models describing root water uptake. Bechmann et al. (2014) have applied thermodynamics to root water uptake studies for discerning
- efficient root parameterizations from less efficient ones by minimizing the time average of  $J_{E,exp}$ . More practically, measurements of leaf water potential and transpiration are used to assess plant water relations, and Eq. (15) informs about the processes involved. Thus, when information on potentials and flux along the flow path are available, the formulations can also be implemented in experimental studies, while imposed system boundaries can be adapted to fit the specific setup. 25

At the more general level, this study adds to the thermodynamic formulation of hydrologic processes and the application of thermodynamic optimality approaches (Kleidon and Schymanski, 2008; Porada et al., 2011; Kleidon et al., 2013; Zehe et al., 2013). What we described here focused on reducing dissipative losses to a minimum, rather

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than the maximization of dissipation, or entropy production, as suggested by some previous studies (Kleidon and Schymanski, 2008; Zehe et al., 2013). This is, however, not a contradiction. A reduction of dissipative losses in a system allows to maintain greater fluxes for the same forcing gradient, which may then result in a greater depletion of the

- driving gradients. In our study, we did not consider this effect on the driving gradients, which in the case of root systems are the difference in chemical potential between soil moisture and the water vapor in the near-surface atmosphere. The minimization of internal dissipation was already applied in hydrology in characterization of river network structure (Rinaldo et al., 1996, 2014). Notably, it was also used as the starting point
- in vascular networks to derive scaling laws and the fractal nature of plant branching 10 systems (West et al., 1997). It would seem that our study fits very well into the scope of this previous study and extends it to include the transport of soil water towards the vascular network of the rooting system. In a further step, this transport would need to be linked into the whole soil-vegetation-atmosphere system along with its driving
- gradient to fully explore the thermodynamic implications of an optimized root system. Such extensions could form the scope of future research. The thermodynamic formulation of root water uptake as described here provides the necessary basis to test the applicability of thermodynamic optimality approaches to root system functioning.

#### 6 Summary and conclusions

- 20 Systems approaches and modeling will certainly be tools to investigate plant water relations and efficient rooting strategies in the future (Lobet et al., 2014). In this paper we give a description of how root water uptake can be expressed in terms of changes of total energy in the system, and be used to quantify the contribution of individual processes to root water uptake. It also sheds new light on some impediments not yet
- accounted for, like heterogeneity in soil water. This is a slightly different and potentially complementary approach to describing flow resistances over potential gradients. Our derivation shows that the product of xylem water potential and transpiration flux carries

a great deal of information, as it can be partitioned into the sum of individual processes impeding water flow in the soil-plant-system. Particularly in process models on root water uptake (Doussan et al., 2006; Kalbacher et al., 2011; Couvreur et al., 2012), the changes of total hydraulic energy and energy dissipation provide the opportunity to

evaluate which processes dominate the impedance to root water uptake at given times, and shed light on whether those are of biotic (within the plant) or abiotic (within the soil) origin.

#### Appendix: Analytical derivations

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It can be shown analytically that a homogeneous soil water distribution result in the least dissipation associated with root water uptake (as shown in Fig. 4c). Such a minimization of dissipation then results in a lower decrease  $dU_w/dt$  and/or in a lower export  $J_{\rm E,exp}$ , as expressed in Eq. (13). To show this minimum analytically, we consider a simplified setup of only two reservoirs, *a* and *b*, yet use the same formulations as in the main text and the same boundary condition of a prescribed flux of root water uptake,  $J_{wu}$ . Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper

We consider the case of a uniform root system (i.e.  $K_{r,a} = K_{r,b} = K_r$ ) that takes up water from the two soil reservoirs. The distribution of soil water is described by matric potentials  $\psi_{M,a} = \psi_M - \Delta \psi$  and  $\psi_{M,b} = \psi_M + \Delta \psi$ . When  $\Delta \psi$  is relatively small, then the water retention curve is approximately linear with the soil water content, so that this

formulation represents a case in which the total soil water of the two reservoirs is the same, and it is only the distribution across the two reservoirs that differs, as described by  $\Delta \psi$ . With this formulation, the prescribed boundary condition in terms of the root water uptake  $J_{wu}$  results in a constraint of the form

$$J_{wu} = -K_r(\psi_M - \Delta \psi_M - \psi_x) - K_r(\psi_M + \Delta \psi_M - \psi_x)$$
  
=  $-2K_r(\psi_M - \psi_x)$  (A1)

so that  $\psi_x = \psi_M + J_{wu}/(2K_r)$ . The dissipation,  $D_u$ , associated with root water uptake then becomes

$$D_{\rm u} = D_{{\rm u},a} + D_{{\rm u},b} = -\rho_{\rm w}g \cdot \kappa_{\rm r} \left[ 2\left(\frac{J_{\rm wu}}{2\kappa_{\rm r}}\right)^2 + 2\Delta\psi_{\rm M}^2 \right]. \tag{A2}$$

It is easy to see in this expression that the minimum is reached when  $\Delta \psi_{\rm M} = 0$  (which can also be derived analytically by  $\partial D_{\rm u}/\partial \Delta \psi_{\rm M} = 0$ ). In other words, for a uniform root system, dissipation associated with root water uptake is at a minimum when moisture is distributed homogeneously in the soil.

In principle, one can also show that a uniform root system results in a minimum of dissipation. This requires an integration over time, which makes an analytical treatment

<sup>10</sup> more complex so that it is easier illustrated by the numerical simulations done in the main text.

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Table 1. Variables used in this study.

Symbol	Variable	Units
$D_{\rm f}$	Dissipation due to soil water flow	W, J s <sup>-1</sup>
Du	Dissipation due to root water uptake	W, J s <sup>-1</sup>
g	Gravitational acceleration	9.81 m s <sup>-2</sup>
ī, j	soil compartment indices	-
J <sub>E.exp</sub>	Export of energy from the soil-root-	W, J s <sup>-1</sup>
-,+	system through the root collar	
$J_{wu}$	Total root water uptake	m <sup>3</sup> s <sup>-1</sup>
J., , ,	Soil water redistribution between	m <sup>3</sup> s <sup>-1</sup>
w,,,,	compartments <i>i</i> and <i>j</i>	
J <sub>wr</sub> i	Water flux from reservoir to root system	m <sup>3</sup> s <sup>-1</sup>
k	Index for interfaces between	-
	compartments	
1	Number of interfaces between	-
	compartments	
$K_{ii}$	Soil hydraulic conductivity between	m <sup>2</sup> s <sup>-1</sup>
	compartments <i>i</i> and <i>j</i>	
$K_{\mathrm{r},i}$	Effective conductivity of the	m <sup>2</sup> s <sup>-1</sup>
	root system in compartment i	
n	Number of soil compartments	4
t	Time	S
$U_{\rm w}$	Total hydraulic energy	J
U <sub>wb</sub>	Binding energy	Jm <sup>-3</sup>
U <sub>wg</sub>	Gravitational energy	Jm <sup>-3</sup>
$W_i$	Total soil water storage	m <sup>3</sup>
V	Volume	m <sup>3</sup>
$V_{\rm res}$	Volume of the model reservoirs	0.25 m <sup>-2</sup>
Z	Vertical coordinate	m
Zr	Elevation of the reference level	m
$\psi_{M}$	Soil matric potential	m
$\psi_{x}$	Xylem water potential	m
$ ho_{ m w}$	Density of water	1000 kg m <sup>-3</sup>
θ	Volumetric soil water content	-
$\theta_{\text{ave}}$	Average volumetric soil water content	-
$\theta_{min}$	Lower integration boundary for $U_{\rm ub}$	-



**Table 2.** Parameters and initial conditions applied for each of the scenarios in the conceptual model for the compartments (i = 1...4). Given are the differences between scenarios in words and the corresponding manipulations in initial states and parameters.

Scenario	Variable	<i>i</i> = 1	<i>i</i> = 2	i = 3	<i>i</i> = 4
all	$V_{\text{res},i}$ (m <sup>3</sup> )	0.125	0.125	0.125	0.125
<ul><li>(1) optimal case</li><li>= soil and roots homogenous</li></ul>	initial soil water $\theta_{init,i}$ (-) root abundance $K_{r,i}$ (m s <sup>-1</sup> )	average 0.18 average 5.0 × 10 <sup>-6</sup>			
heterogenous soil cases	initial soil water θ <sub>init i</sub> (–)	dry 0.15	dry 0.15	wet 0.21	wet 0.21
(2) homogenous roots	root abundance $K_{r,i}$ (m s <sup>-1</sup> )	average $5.0 \times 10^{-6}$	average 5.0 × 10 <sup>-6</sup>	average $5.0 \times 10^{-6}$	average $5.0 \times 10^{-6}$
(3) heterogenous roots	root abundance $K_{r,i}$ (m s <sup>-1</sup> )	many 7.5 × 10 <sup>-6</sup>	few 2.5 × 10 <sup>-6</sup>	many 7.5 × 10 <sup>-6</sup>	few 2.5 × 10 <sup>-6</sup>
(4) strongly heterogenous roots	$K_{r,i} (m s^{-1})$	$9.0 \times 10^{-6}$	$1.0 \times 10^{-6}$	$9.0 \times 10^{-6}$	$1.0 \times 10^{-6}$

**Table B1.** Parameters used for calculation of soil hydraulic properties using van Genuchten(1980).

Symbol	Description	Value
n	Shape parameter	1.38
т	Shape parameter, $m = 1 + \frac{1}{n}$	0.275
α	Shape parameter	0.068 cm <sup>-1</sup>
$\theta_{min}$	Lower integration boundary in Eq. (7)	0.07
$\theta_{\rm r}$	Residual soil water content	0.041
$\theta_{s}$	Porosity	0.453

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**Figure 1.** 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 mater content is the same in both reservoirs with high and low rooting density respectively.



Figure 2. Example of the hydraulic and thermodynamic states of a sample soil (sandy loam): (a) water retention curve with logarithmic y axis, Parameters are given in Table B1, (b) for the same soil, binding energy,  $U_{\rm wb}$ , as a function of soil water content, for homogenous and heterogenous soil water distribution in a total soil volume 1 m<sup>3</sup>. The ratio indicated in the legend corresponds to the ratio of soil water contents in two compartments of equal size but different soil water content. The blue arrow indicates how much energy is available for driving fluxes to equalize the gradients in water potentials between compartments. The red arrow along the solid curve indicates (homogenous) root water uptake.









**Figure 4.** Exported energy and its components for the soil-plant-system over the course of a drying experiment and different root water uptake scenarios. As in Fig. 3, 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. 3), (c) component due to energy dissipation by water flow from the soil into the root.

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