A thermodynamic formulation of root water uptake

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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 root water uptake can be evaluated thermodynamically and demonstrate that this evaluation provides additional insights into the factors that impede root water uptake. We derive an expression that relates the energy export at the base of the root system to a sum of terms that reflect all fluxes and storage changes along the flow path in thermodynamic terms. We illustrate this thermodynamic formulation using an idealized setup of scenarios with a simple model. In these scenarios, we demonstrate why heterogeneity in soil water distribution and rooting properties affect the impediment of water flow even though the mean soil water content and rooting properties are the same across the scenarios. The effects of heterogeneity can clearly be identified in the thermodynamics of the system in terms of differences in dissipative losses and hydraulic energy, resulting in an earlier start of water limitation in the drying cycle. We conclude that this thermodynamic evaluation of root water uptake conveniently provides insights into the impediments of different processes along the entire flow path, which goes beyond resistances and also accounts for the role of heterogeneity in soil water distribution.

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 deal 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, 2012), how to identify efficient rooting depth (Guswa, 2010), 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 about 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 plants may regulate 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 the soil compartment (Draye et al., 2010; Vadez et al., 2014). Much of our process understanding on the spatial distribution of water uptake and its evolution 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, and 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 (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.
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 content as well as the transport of water over a resistance, can be expressed in the same currency of energy fluxes and dissipation, with units of joules per second (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 conversions of any form (Kondepudi and Prigogine, 1998; Kleidon, 2012). As soil water movement and uptake by plants involve 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 are 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 differentiate 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) and 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 impediments to root water uptake and the role of soil water heterogeneity, we illustrate them in a simplified process model, which is a conceptual four-box model for root water uptake.

2 Thermodynamics and soil hydrology

2.1 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 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 equilibrium 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 energies 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 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 stored water. As the remaining energy is converted into heat, this reduction to a minimum of Gibbs free energy corresponds to a maximum conversion into heat and thus 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 their respective potentials and how these forms of energy change during root water uptake and soil water redistribution. We state equations for discrete bulk soil compartments $V_{i}$ of sufficiently large size such that the porosity and the soil water retention curve are defined at that
scale. Soil properties are considered homogenous within but may vary between soil compartments. We thus use sums to integrate over the soil space in the following. The variable names used in this manuscript are summarized in Table 2.

2.2 Forms of energy associated with soil water content

Two types of energy are relevant for describing soil water states. We will refer to the sum of these as the total hydraulic energy (\(U_{wb}\), J) contained in a soil volume, which consists of the binding energy, \(U_{wb}\), and the gravitational energy, \(U_{wg}\), defined in each soil compartment \(i\) (with \(i = 1..n\)):

\[
U_{wb,i} = U_{wb,i} + U_{wg,i}.
\]  

(1)

For the total soil volume we have

\[
U_w = \sum_{i=1}^{n} U_{wb,i}.
\]  

(2)

The gravitational energy \(U_{wg,i}\) relates to the energy necessary to lift the water from a reference level up to the point where it is stored in the soil:

\[
U_{wg,i} = V_{s,i} \cdot \rho_w \cdot g \cdot \theta_i \cdot (z_i - z_r),
\]  

(3)

where \(\rho_w\) is the density of water (\(\rho_w = 1000 \text{ kg m}^{-3}\)), \(g\) is the gravitational acceleration (\(g = 9.81 \text{ m s}^{-1}\)), \(z_i\) is the elevation of the reference level, \(z_r\) the elevation of compartment \(i\), and \(\theta_i\) refers to the volumetric water content. This formulation neglects variations of gravitational energy within the compartment \(i\). More rigorously, the gravitational energy should be integrated over depth from the bottom to the top of the compartment. This requires information on the vertical distribution of soil water within the compartment, which is typically not available in model applications. If compartments are chosen to be shallow, the error associated with this simplification is small.

The binding energy \(U_{wb,i}\) 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 of each compartment \(i\):

\[
U_{wb,i} = U_{wb,i}(\theta_i) = V_{s,i} \cdot \rho_w \cdot g \cdot \int_{\theta_{min}}^{\theta_i} \psi_M(\theta') \cdot d\theta'.
\]  

(4)

Essentially, \(U_{wb,i}\) is the integral of the water retention curve (\(\psi_M(\theta)\)). The multiplication with \(\rho_w \cdot g\) serves to convert the units of the matric potential (\(\psi_M\)) from meter water to joule. An example for both \(\psi_M(\theta)\) and the related \(U_{wb}(\theta)\) is depicted in Fig. 1 for a sandy loam using the van Genuchten parameterization with parameters given in Table 1. The lower integration point \(\theta_{min}\) should refer to completely dry soil. However, some analytic formulations for the water retention function are not well defined in the very dry range (Rossi and Nimmo, 1994; Ciocca et al., 2014), and we therefore chose \(\theta_{min} > 0\). This has a great influence on the absolute values of binding energy in the soil, but, as will be shown below, the relative (i.e., temporal) differences in \(U_{wb,i}\) are of relevance. Therefore, the exact choice of \(\theta_{min}\) does not affect the results. We propose choosing a value just below the water content at the permanent wilting point, or another suitable value smaller than the water contents that will be reached in the desired application.

Figure 1b 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, \(U_{wb}\) 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 transferred to 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 along with the mass export of water from the soil system to the plant (with details described below).

When soil water potential is distributed heterogeneously, the binding energy increases (is less negative). Technically, this results from the strongly nonlinear water retention function. From a process perspective, this additional energy will drive water fluxes for equalizing the soil water gradients between compartments 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. 1b are steeper the greater the soil water heterogeneity. This illustrates that more energy has to be invested per decrease in total soil water content in heterogeneously compared to homogeneously wetted soils if water is to be extracted at an equal rate from the compartments.

2.3 Dissipation and energy export associated with soil water movement and root water uptake

Soil water fluxes lead to dissipation \( (D, \text{J} \text{s}^{-1}) \) of total hydraulic energy. Generally, dissipation of energy occurs when water flows over a resistance, and it is expressed as the product of the driving gradient and the water flow. Those fluxes may occur within the soil between compartments during redistribution of bulk soil water or at the small scale due to root water uptake, or further, within the plant tissue. The representation of fluxes in models differs according to model complexity, yet the dissipative nature of these fluxes should remain unaffected by how these are represented.

Energy dissipation due to soil water flow between compartments is written as

\[
D_{f,k} = \rho_w \cdot g \cdot (h_i - h_j) J_w,k
\]

and for the entire soil volume as

\[
D_t = \sum_{k=1}^{l} D_{f,k},
\]

where \( h \) refers is the soil hydraulic potential \( (h = \psi_M + (z_i - z_j), \text{m water}) \) of the neighboring compartments \( i \) and \( j \); \( J_w,k \) refers to the water flux between two neighboring compartments \( i \) and \( j \); \( D_{f,k} (\text{J} \text{s}^{-1}) \) refers to the respective dissipation of energy over the boundary \( k \) between those compartments; and \( D_t (\text{J} \text{s}^{-1}) \) refers to the total dissipation due to water fluxes within the total soil volume, i.e., over all interfaces between compartments \( l \). The dissipation is always negative, since it indicates a loss of hydraulic energy from the system, which is released in the form of a very small quantity of thermal energy.

The same applies to the dissipation of energy due to the small-scale radial root water uptake \( (D_{u,i}, \text{J} \text{s}^{-1}) \). The formulation depends a great deal on the complexity of the applied flow model. The flow may be represented over several steps, i.e., from bulk soil to the root surface, from root surface to the xylem, and within the xylem. Here, we represent the flow in a simple form, corresponding to the water uptake \( (J_{u,i}) \) of the water flow model presented in the next section (Eq. 15). Note that this may easily be adapted to more comprehensive formulations of water uptake. We write dissipation due to microscopic radial water uptake as

\[
D_{u,i} = \rho_w \cdot g \cdot (\psi_{M,i} - \psi_x) \cdot J_{u,i},
\]

with \( D_{u,i} (\text{J} \text{s}^{-1}) \) being the dissipation due to root water uptake in each reservoir \( i \) and \( \psi_x \) being the root xylem potential \( (\text{m}) \). The total dissipation \( D_u \) becomes

\[
D_u = \sum_{i=1}^{n} D_{u,i}.
\]

Lastly, the root water uptake constitutes an export of energy \( (J_{E,exp}, \text{J} \text{s}^{-1}) \) from the soil root system which is generally defined as the product of the potential at and the flow across the boundary. In our case, water leaves at the top of the root collar as total transpiration at the xylem water potential:

\[
J_{E,exp} = \rho_w \cdot g \cdot \psi_x \cdot J_{wu}.
\]

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 total hydraulic energy as the soil dries (compare Fig. 1). \( J_{E,exp} \) would be negative should water enter the system via the roots.

Although the dissipation terms \( (D_t, D_u) \) 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, \( J_{E,exp} \) is an energy flux (energy transported) across the system boundary. Note, however, that in general this flux also depletes a gradient (between the soil and the atmosphere), but this gradient is not described in our simple soil–root model explicitly.

2.4 Energy balance equation

The energy balance for the soil–root system can be written as the sum of the changes in total hydraulic energy over all compartments, the dissipation terms, and the energy export:

\[
\sum_{i=1}^{n} \frac{dU_{w,i}}{dr} = \sum_{k=1}^{l} D_{f,k} + \sum_{i=1}^{n} D_{u,i} + J_{E,exp}.
\]
Some properties of this equation are noteworthy. First, rearranging Eq. (10) yields an expression that relates the characteristics at the outlet of the system to a series of internal processes:

\[ J_{\text{E,exp}} = \rho_w \cdot g \cdot \psi_x \cdot J_{\text{wu}} \]

\[ = \sum_{i=1}^{n} \frac{dU_{\text{wu},i}}{dr} - \sum_{k=1}^{l} D_{t,k} - \sum_{i=1}^{n} D_{w,i}. \]  

(11)

The units in all terms of Eq. (11) are joules per second (J s\(^{-1}\)), as they all indicate rates of energy flux and changes of energy content with time. More practically, \( J_{\text{E,exp}} \), as the product of root collar xylem potential and transpirational flux, is influenced by several processes, and Eq. (11) shows that they act as a sum (remember that all dissipative terms have negative signs). For a given water flux, Eq. (11) shows that the collar xylem potential has to be more negative when water has to be moved within the soil (thus decreasing \( D_{t,k} \)), 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 \( U_{\text{wb}} \), as shown in Fig. 1). For model applications, comparison of the magnitude of the separate terms of the sum in Eq. (11) provides a tool to assess which of the successive pathways involved in root water uptake most strongly impedes water flow.

3 Conceptual root water uptake model

The thermodynamic evaluation introduced in the last section is meant to be applied to a water flow model (process model). We illustrate the application using a simple model system as shown in Fig. 2. 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, \( V_{s,i} \) (m\(^3\)), and their water storage is described by the variables \( W_i = \theta_i \cdot V_{s,i} \) (in m\(^3\)), with \( \theta_i \) being the volumetric soil water content (–) of the reservoir \( i \). Soil water is extracted from the soil reservoirs by root water uptake. In the model scenarios presented below, we will assume that soil compartments are isolated; hence no flow between compartments takes place. However, in order to formulate all terms in the energy balance, we also state the corresponding flow equations for bulk water flow between compartments for reference.

The mass balances of the reservoirs describing the temporal changes in \( W_i \) in terms of the root water uptake fluxes, \( J_{\text{wt},i} \) (m\(^3\) s\(^{-1}\)) and soil water flow between the reservoirs, \( J_{w,k} \) (m\(^3\) s\(^{-1}\)), are expressed as

\[ \frac{dW_i}{dt} = J_{\text{wt},i} + \sum_{k=1}^{m} J_{w,k}. \]  

(12)

with both fluxes carrying negative signs when directed outward of the reservoir. Here, \( m \) describes the total number of neighbors of cell \( i \). The water flux (\( J_{w,k} \), m\(^3\) s\(^{-1}\)) from the neighboring reservoirs is expressed by Darcy’s law, being proportional to the difference in hydraulic potentials (\( h_i = \psi_M+(z_i-z_r) \), m water). For any two neighboring cells \( i \) and \( j \), it is given as

\[ J_{w,k} = -K_{ij}(h_i - h_j), \]  

(13)

where \( K_{ij} \) (m\(^2\) s\(^{-1}\)) is the effective unsaturated soil hydraulic conductivity between adjacent compartments \( i \) and \( j \). For convenience the spatial scale is factored into the effective conductivity \( K_{ij} \).

The total root water uptake (\( J_{\text{wu}} \), m\(^3\) s\(^{-1}\)) is the sum of the uptake fluxes from each compartment:

\[ J_{\text{wu}} = \sum_{i} J_{\text{wt},i}, \]  

(14)

which are described in analogy to Darcy’s law:

\[ J_{\text{wt},i} = -K_{r,i}(\psi_{M,i} - \psi_x), \]  

(15)

where \( \psi_x \) (m) is the xylem water potential which is taken to be equal throughout the entire root system and the index \( i \) runs over the number of compartments. The conductivities \( K_{r,i} \) (m\(^2\) s\(^{-1}\)) are effective radial conductivities of active compartments.
roots in compartment $i$. They 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 $K_{i,i}/K_r$ to create heterogenous root water uptake from the different reservoirs (see below). As mentioned above, root water uptake may be represented more comprehensively. We keep it simple here to better support the purpose of demonstrating the thermodynamic diagnostics.

For the purpose of demonstration, we keep the model simulations deliberately simple. All soil compartments are arranged horizontally, so that differences in gravitational energy do not play a role and all changes in hydraulic energy will be due to changes in water content. Also, we model a split-root experiment, where no water flow between compartments is possible and all changes in soil water content are due to root water uptake. This enables us to increase the heterogeneity in the soil water content and demonstrate its effect on the energy balance, xylem potential, and uptake dynamics. In this simplified setup we solve Eqs. (14) and (15) with a prescribed boundary condition (total transpiration, $J_{wu}$) for the unknown xylem water potential $\psi_x$ as follows:

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

(16)

For each time step ($\Delta t$), Eq. (16) yields the xylem water potential, based on the current water contents in the compartments. Next, we obtain the water uptake for the same time step using Eqs. (12) and (15). Water contents are then updated for the next time step based on the root water uptake. Initial soil water contents and root conductivities are applied as shown in Table 1. For purposes of simplicity, we run the model until soil water limits uptake. We somewhat arbitrarily assume that soil water becomes limiting 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.

Additional scenarios with diurnal fluctuations of transpirational forcing and other soil hydraulic properties are given as a reference in the Supplement. They yield similar results.

4 Scenarios

We run the model for four scenarios, as shown in Table 1. In the scenarios we vary the distribution of initial soil water content and the implied root length by changing to compartment root conductivity to impose increasingly heterogenous conditions while keeping the average constant.

The first scenario is completely homogenous with a uniform initial soil water content and root conductivity across compartments. Three additional scenarios are 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 same way, the effective root conductivities ($K_{i,i}$) 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 1, Fig. 2).

The model is representative of a plant having access to a soil volume of $0.5 \text{ m}^3$, consisting of a soil monolith of $0.5 \text{ m}$ depth and a surface area of $1 \text{ m}^2$. Each of the compartments is the same volume ($0.125 \text{ m}^3$). The transpiration rate is indicative of a hot summer day in Germany, with $6 \text{ mm d}^{-1}$. Effective root conductivities correspond to roots with radial conductivity of $3 \times 10^{-6} \text{ m s}^{-1} \text{ MPa}^{-1}$, which is on the upper end of the values summarized in Draye et al. (2010), and total root length densities in the compartments varying between $1 \text{ cm cm}^{-3}$ (most densely rooted), $0.5 \text{ cm cm}^{-3}$ (average), and $0.1 \text{ cm cm}^{-3}$ (least densely rooted). This is

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

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Variable</th>
<th>$i = 1$</th>
<th>$i = 2$</th>
<th>$i = 3$</th>
<th>$i = 4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>All</td>
<td>$V_{z,i}$ (m$^2$)</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
</tr>
<tr>
<td>(1) optimal case: soil and roots homogenous</td>
<td>Initial soil water $\theta_{init,i}$ (–)</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
</tr>
<tr>
<td></td>
<td>Root abundance</td>
<td>Average</td>
<td>Average</td>
<td>Average</td>
<td>Average</td>
</tr>
<tr>
<td></td>
<td>$K_{r,i}$ (m$^2$ s$^{-1}$)</td>
<td>$5.0 \times 10^{-6}$</td>
<td>$5.0 \times 10^{-6}$</td>
<td>$5.0 \times 10^{-6}$</td>
<td>$5.0 \times 10^{-6}$</td>
</tr>
<tr>
<td>Heterogenous soil cases</td>
<td>Initial soil water</td>
<td>Dry</td>
<td>Dry</td>
<td>Wet</td>
<td>Wet</td>
</tr>
<tr>
<td>(2) homogenous roots</td>
<td>Root abundance</td>
<td>Average</td>
<td>Average</td>
<td>Average</td>
<td>Average</td>
</tr>
<tr>
<td></td>
<td>$K_{r,i}$ (m$^2$ s$^{-1}$)</td>
<td>$5.0 \times 10^{-6}$</td>
<td>$5.0 \times 10^{-6}$</td>
<td>$5.0 \times 10^{-6}$</td>
<td>$5.0 \times 10^{-6}$</td>
</tr>
<tr>
<td>(3) heterogenous roots</td>
<td>Root abundance</td>
<td>Many</td>
<td>Few</td>
<td>Many</td>
<td>Few</td>
</tr>
<tr>
<td></td>
<td>$K_{r,i}$ (m$^2$ s$^{-1}$)</td>
<td>$7.5 \times 10^{-6}$</td>
<td>$2.5 \times 10^{-6}$</td>
<td>$7.5 \times 10^{-6}$</td>
<td>$2.5 \times 10^{-6}$</td>
</tr>
<tr>
<td>(4) strongly heterogenous roots</td>
<td>Root conductivity</td>
<td>9.0 $\times 10^{-6}$</td>
<td>1.0 $\times 10^{-6}$</td>
<td>9.0 $\times 10^{-6}$</td>
<td>1.0 $\times 10^{-6}$</td>
</tr>
</tbody>
</table>
Table 2. Variables used in this study.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Variable</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_T$</td>
<td>Dissipation due to soil water flow</td>
<td>J s$^{-1}$ or W</td>
</tr>
<tr>
<td>$D_u$</td>
<td>Dissipation due to root water uptake</td>
<td>J s$^{-1}$ or W</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration</td>
<td>9.81 m s$^{-2}$</td>
</tr>
<tr>
<td>$h$</td>
<td>Soil hydraulic potential</td>
<td>m</td>
</tr>
<tr>
<td>$i, j$</td>
<td>Soil compartment indices</td>
<td>–</td>
</tr>
<tr>
<td>$J_{E,exp}$</td>
<td>Export of energy from the soil–root system through the root collar</td>
<td>J s$^{-1}$ or W</td>
</tr>
<tr>
<td>$J_{w_u}$</td>
<td>Total root water uptake</td>
<td>m$^3$ s$^{-1}$</td>
</tr>
<tr>
<td>$J_{w,k}$</td>
<td>Soil water redistribution between compartments over the interface $k$</td>
<td>m$^3$ s$^{-1}$</td>
</tr>
<tr>
<td>$J_{wt,i}$</td>
<td>Water flux from bulk soil into the root compartments</td>
<td>m$^3$ s$^{-1}$</td>
</tr>
<tr>
<td>$k$</td>
<td>Index for interfaces between compartments</td>
<td>–</td>
</tr>
<tr>
<td>$l$</td>
<td>Number of interfaces between compartments</td>
<td>–</td>
</tr>
<tr>
<td>$K_{ij}$</td>
<td>Soil hydraulic conductivity between compartments $i$ and $j$</td>
<td>m$^2$ s$^{-1}$</td>
</tr>
<tr>
<td>$K_{r,i}$</td>
<td>Effective radial conductivity of the active roots in compartment $i$</td>
<td>m$^2$ s$^{-1}$</td>
</tr>
<tr>
<td>$n$</td>
<td>Number of soil compartments</td>
<td>4</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
<td>s</td>
</tr>
<tr>
<td>$U_w$</td>
<td>Total hydraulic energy</td>
<td>J</td>
</tr>
<tr>
<td>$U_{wb}$</td>
<td>Binding energy</td>
<td>J</td>
</tr>
<tr>
<td>$U_{wg}$</td>
<td>Gravitational energy</td>
<td>J</td>
</tr>
<tr>
<td>$W_i$</td>
<td>Total soil water storage</td>
<td>m$^3$</td>
</tr>
<tr>
<td>$V$</td>
<td>Volume</td>
<td>m$^3$</td>
</tr>
<tr>
<td>$V_{s,i}$</td>
<td>Volume of the model compartments</td>
<td>m$^3$</td>
</tr>
<tr>
<td>$z$</td>
<td>Elevation</td>
<td>m</td>
</tr>
<tr>
<td>$z_e$</td>
<td>Elevation of the reference level</td>
<td>m</td>
</tr>
<tr>
<td>$\psi_M$</td>
<td>Soil matric potential</td>
<td>m</td>
</tr>
<tr>
<td>$\psi_x$</td>
<td>Xylem water potential</td>
<td>m</td>
</tr>
<tr>
<td>$\rho_w$</td>
<td>Density of water</td>
<td>1000 kg m$^{-3}$</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Volumetric soil water content</td>
<td>–</td>
</tr>
<tr>
<td>$\theta_{ave}$</td>
<td>Average volumetric soil water content</td>
<td>–</td>
</tr>
<tr>
<td>$\theta_{min}$</td>
<td>Lower integration boundary for $U_{wb}$</td>
<td>–</td>
</tr>
</tbody>
</table>

within the range of observed root length densities for maize (Kuchenbuch et al., 2009).

The soil hydraulic properties are equal in all compartments and derived using van Genuchten (1980) with parameters for a sandy loam (Rawls et al., 1993) given in Table B1. Starting from the initial condition, we model a dry-down event until limiting soil water xylem potential is reached. In each simulation, first root water uptake and the resulting temporal evolution of soil water content were explicitly solved for each compartment. Second, the thermodynamic evaluation was applied a posteriori based on the results of the root water uptake model.

5 Results

Figure 3 shows the evolution of the root collar potential obtained from the process model over the course of the drying cycle and the associated creation of heterogeneity of soil water contents (as reflected in the coefficient of variation). Shown are the results of all scenarios given in Table 1. 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 are 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 from a plant’s point of view, as it minimizes dissipation, which keeps the xylem potentials less negative and delays time to water stress. 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 the beginning of the experiment. The limiting xylem potential is reached earlier the more heterogeneous the distribution of root water uptake and soil water contents is. Also, Appendix A shows analytically that uptake from homogeneously distributed soil water minimizes (i.e., optimizes from the plant’s point of view) the dissipative losses due to root water uptake in a situation in which soil hydraulic properties are homogeneous.

Based on the output of the root water uptake model, we applied Eq. (11) to diagnose the impediments to root water uptake. The individual terms of Eq. (11) (except dissipation to soil water flow, which was not modeled) are plotted separately in Fig. 4: on the left the total export of energy ($J_{E,exp}$), which proves to be composed of the change of binding energy in the soil ($dU_{wb}/dt$, middle) and dissipation due to root water uptake ($-D_u$, right). All individual terms ($dU_{wb}/dt$, $D_u$ and $J_{E,exp}$) were calculated separately, applying Eqs. (4),
The energy export \( J_{E,\text{exp}} \) corresponds closely to the evolution of the root xylem potential (Fig. 3, left), because the transpirational flux is prescribed as constant. \( J_{E,\text{exp}} \) increases continuously as the soil dries in order to maintain the constant rate of uptake. The decomposition of the energy export provides information about the impediments to root water uptake in the different scenarios. For example, the greatest contribution to \( J_{E,\text{exp}} \) in wet soil in our setup originates 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 \( dU_{wb}/dt \), and the difference between the solid grey curve and the other curves illustrates the impact of soil water heterogeneity on the water uptake at each time step. At the same average soil water content, differences in \( dU_{wb}/dt \) between our scenarios are entirely due to heterogenous soil water distribution. When comparing the optimal scenario and the one with strongly heterogenous roots at \( \theta_{\text{ave}} = 0.15 \), we observe that less than half of the investment in detaching water is due to soil drying and the remaining 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 than the one related to soil drying in this modeling exercise.

6 Discussion

We used thermodynamics to evaluate the dynamics of a very simple process model for root water uptake to demonstrate that besides fluxes and potentials there is more relevant information in the system that relates to change of hydraulic energy and dissipative losses of water uptake. The main contribution of the paper lies in providing a tool for assessing where the impediments to root water uptake lie along the flow path between soil and atmosphere. For this the thermodynamic formulations are applied a posteriori to water fluxes and changes of soil water contents calculated with the hydrological model. The relative contribution of each of the impediments can then be quantified, by evaluation of the relative contribution of each process to the total energy export. At the same time, the calculations with the simple model serve as a proof of concept: the energy balance is closed; i.e., the sum of change in hydraulic energy and dissipation equal the energy export.

In our thermodynamic description of the soil–plant system, we have not considered the changes of soil temperature, which should be induced particularly when 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.

Also, 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 resulting trajectory of \( dU_{wb}/dt \). Generally, hysteresis can be included in the framework to investigate this effect further in the future.
Finally, we have also deliberately limited our model scenarios to situations where roots do not grow and where root length does not depend on water availability, and we have not allowed for redistribution of water between compartments. This way, we artificially maintained heterogeneity, which was done in order to demonstrate in the separate scenarios how heterogeneity alone affects uptake and its thermodynamics.

An important advantage of evaluating the process model output in the energy domain lies in the possibility for evaluating the role of heterogenous soil water potentials. 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 states in heterogenous systems to be efficiently described. An additional advantage of working in the “energy domain” is the possibility to consider the influence of the water retention function, the 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 if root systems are equally distributed. Thus, with everything else being equal and independent of soil water potential distribution, 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). At the same time heterogeneous soil water retention properties may induce root growth that alleviates water stress, and root systems are likely adapted to such conditions. This reasoning may be further extended to understanding horizontal and vertical distribution of root systems and uptake in adapting to their environment (Adiku et al., 2000; van der Ploeg et al., 2008) also in terms of reducing their dissipative losses.

We have given equations for our simple system, but the concept can easily be extended 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. 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. Furthermore, a thermodynamic evaluation may be applied to investigate the effects of dynamic root growth, aquaporin and stomatal regulation (Aroca et al., 2012; Vadez et al., 2014), or mucilage (Carminati et al., 2011) on the impediments of the whole plant root water uptake. Bechmann et al. (2014) have applied thermodynamics to root water uptake studies in order to differentiate efficient root parameterizations from less efficient ones by minimizing the time average of \( J_{E,\text{exp}} \). More practically, measurements of leaf water potential and transpiration are used to assess plant water relations, and Eq. (11) elucidates 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.

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 is more targeted towards reduction in dissipative losses, rather 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 greater fluxes for the same forcing gradient to be maintained, which may then result in a greater depletion of the driving gradients, thus maintaining low xylem potentials and delaying the onset of water stress or cavitation. 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 has already been applied in hydrology for characterization of river network structure (Rinaldo et al., 1996, 2014) and vertical root water uptake (Adiku et al., 2000). Notably, it has also been used in vascular networks as the starting point to derive scaling laws and the fractal nature of plant branching 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 upon which to test the applicability of thermodynamic optimality approaches to root system functioning.

7 Summary and conclusions

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 relates to changes of total energy in the system, which can be used to quantify the contribution of individual processes to impeding 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 A: Analytical derivations

It can be shown analytically that a homogeneous soil water distribution results 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 $J_{E,exp}$, as expressed in Eq. (11). 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, $J_{wu}$.

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

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

(A1)

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

$$D_u = D_{u,a} + D_{u,b} = -\rho_w g \cdot K_r \left[ 2 \left( \frac{J_{wu}}{2K_r} \right)^2 + 2\Delta \psi_M^2 \right].$$

(A2)

It is easy to see in this expression that the minimum is reached when $\Delta \psi_M = 0$ (which can also be derived analytically by $\partial D_u/\partial \Delta \psi_M = 0$). 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 more complex so that it is more easily illustrated by the numerical simulations done in the main text.
Appendix B: Soil parameters

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

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$</td>
<td>Shape parameter</td>
<td>1.38</td>
</tr>
<tr>
<td>$m$</td>
<td>Shape parameter, $m = 1 + \frac{1}{n}$</td>
<td>0.275</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Shape parameter</td>
<td>0.068 cm$^{-1}$</td>
</tr>
<tr>
<td>$\theta_{\text{min}}$</td>
<td>Lower integration boundary in Eq. (4)</td>
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<tr>
<td>$\theta_r$</td>
<td>Residual soil water content</td>
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<tr>
<td>$\theta_s$</td>
<td>Porosity</td>
<td>0.453</td>
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