

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), 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 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 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

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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 illustrates 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 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 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 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 resulting 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 minimum 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.

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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
5 advantage of working in the “energy domain” constitutes the possibility to consider 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
10 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 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. Bechmann et al. (2014) have applied thermodynamics to root water uptake studies for discerning
15 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
20 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 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
5 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
10 in vascular networks 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
15 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
25 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

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

Symbol	Description	Value
n	Shape parameter	1.38
m	Shape parameter, $m = 1 + \frac{1}{n}$	0.275
α	Shape parameter	0.068 cm^{-1}
θ_{\min}	Lower integration boundary in Eq. (7)	0.07
θ_r	Residual soil water content	0.041
θ_s	Porosity	0.453

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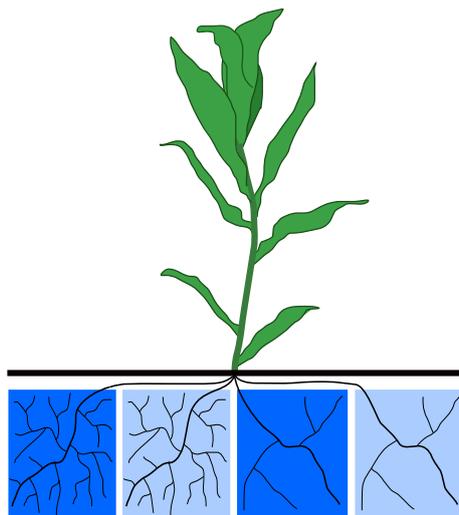


Figure 1. Schematic of the numerical split root experiment. The soil volume of each reservoir is explored by roots of a given root length thus changing the effective root conductivity. Reservoirs are paired with two reservoirs of high and low rooting density, and high and low initial water content each, while the evolution of average soil water content is the same in all simulations. Also, at the beginning of all simulations the average soil water content is the same in both reservoirs with high and low rooting density respectively.

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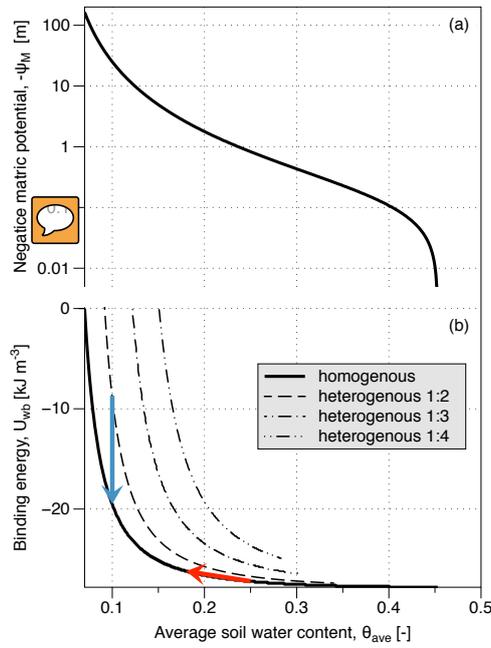


Figure 2. Example of the hydraulic and thermodynamic states of a sample soil (sandy loam): **(a)** water retention curve with logarithmic y axis, Parameters are given in Table B1, **(b)** for the same soil, binding energy, U_{wb} , as a function of soil water content, for homogenous and heterogenous soil water distribution in a total soil volume 1 m^3 . 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.

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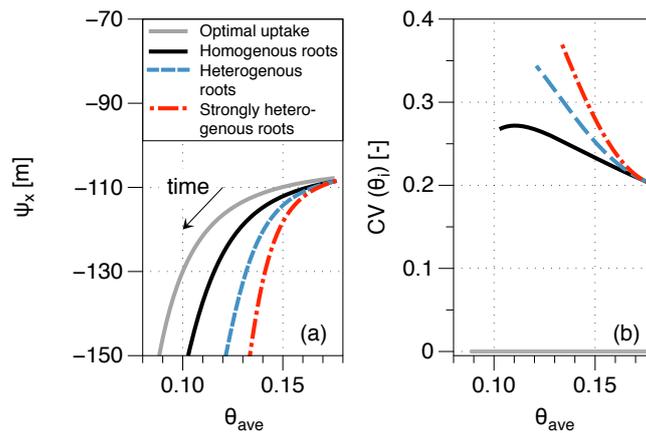


Figure 3. Model results of the simple model: **(a)** evolution of xylem potential over the course of root water uptake, **(b)** evolution of the coefficient of variation of soil water content during the simulation. Legend is the same as in Fig. 4. Average initial soil water content is the the same in all simulations. Only the unstressed uptake is shown. The time axis has been replaced by average volumetric soil water, which evolves parallel with time in this constant flux experiment.

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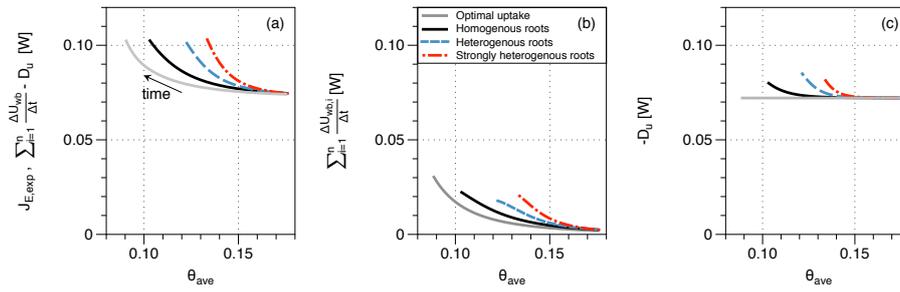


Figure 4. Exported energy and its components for the soil-plant-system over the course of a drying experiment and different root water uptake scenarios. As in Fig. 3, the time axis was replaced by the average soil water content. **(a)** Total energy exported from the system at the root collar. It is 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.