Towards understanding belowground resources acquisition: Applying data driven methods for deriving root water uptake profiles in grasslands of different diversity

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Für Franziska

„Müsset im Naturbetrachten

Immer eins wie alles achten.

Nichts ist drinnen, nichts ist draußen:

Denn was innen, das ist außen.“

- Johann Wolfgang von Goethe -

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Zusammenfassung

Sowohl für einzelne Pflanzen als auch auf der Ökosystemskale ist die Wasseraufnahme durch Pflanzenwurzeln eine wichtige Komponente im System Pflanze-Boden-Wasser. Bisher wurde bei Untersuchungen von Pflanzengesellschaften und deren Wassernutzung keine Abschätzung zur Wurzelwasseraufnahme vorgenommen. Um inter- und intraspezifische Wechselwirkungen von Pflanzen, wie beispielsweise „hydraulic lift“, Teilung von Ressourcen oder die Konkurrenz um Ressourcen und die Funktionsweise von Ökosystem, zu verstehen, ist jedoch die Kenntnis der Wurzelwasseraufnahme erforderlich. Deswegen bedarf es minimal-invasiver und einfacher Methoden um die Wurzelwasseraufnahme bestimmen zu können.

Im Rahmen dieser Dissertation wurde eine simple Methode ermittelt, die die Evapotranspiration und Wurzelwasseraufnahme von Bodenfeuchtemessungen ohne die vorherige Kenntnis von Wurzeleigenschaften ableitet. Diese wurde zur Untersuchung des Einflusses von Pflanzen-Biodiversität auf die Wurzelwasseraufnahme der gesamten Pflanzengemeinschaft herangezogen.

Im ersten Teil der Arbeit erfolgt eine Auswertung von vier verschiedenen Wasserbilanz Methoden unterschiedlicher Komplexität hinsichtlich ihrer Anwendbarkeit auf die ökohydrologische Thematik. In dieser Vergleichsstudie wird ein Experiment mit numerischen Simulationen für ein Graslandökosystem durchgeführt. Dabei werden die Methoden an Bodenfeuchten mit unterschiedlicher zeitlicher Auflösung und Unsicherheiten von Bodenfeuchtesensoren getestet. Als am besten geeigneter Ansatz für die Abschätzung der Wurzelwasseraufnahme stellte sich die Multi Step Multi Layer Regression (*msml*) heraus. Diese vergleichsweise einfache Methode nutzt den Tageszyklus von gemessenen Bodenfeuchten zur Ableitung der Wurzelwasseraufnahme.

Im zweiten Teil wird die Multi Step Multi Layer Regression einer zusätzlichen Genauigkeitsuntersuchung unterzogen, wobei speziell der Einfluss der Evapotranspirationrate, der Bodentextur und der Sensorungenauigkeit untersucht wird. Als Datengrundlage hierfür dienen unter anderem Bodenfeuchtemessungen von 12 wägbaren Lysimetern. Der Fokus hierbei liegt auf der Validierung der Methode sowie darin einen Überblick über Unsicherheiten und deren Ursachen in natürlichen Systemen zu erlangen. Die Ergebnisse verdeutlichen, dass die *msml*-Methode sensitiv auf die Größe der Evapotranspiration reagiert. Dies zeigt sich in höheren Ungenauigkeiten bei geringen Evapotranspirationsraten. Die Bodentextur hat dabei keinen Einfluss auf die Vorhersage der Wurzelwasseraufnahme. Um die Messungenauigkeiten der Bodenfeuchtesensoren in den Datenreihen zu reduzieren, wurde eine Filterroutine angewendet. Die Ergebnisse zeigen, dass der angewendete Filter die realen Daten ausreichend gut beschreibt.

Im dritten Teil der Arbeit wird der Einfluss von Pflanzen-Biodiversität auf die Wurzelwasseraufnahme der gesamten Pflanzengemeinschaft untersucht. Insbesondere wurde getestet, ob Pflanzengesellschaften mit höherem Artenreichtum das Bodenwasser effizienter nutzen können als Ökosysteme mit einer geringeren Diversität. Hierfür wurde die Multi Step Multi Layer Regression auf 12 Lysimeter eines Graslandexperimentes mit zwei unterschiedlichen Biodiversitätsstufen (4- und 16-Artenmischungen) angewendet. Das Neuartige dieser Arbeit ist die Analyse der abgeleiteten Wurzelwasseraufnahmeprofile in Kombination mit Messungen des Blattwasserpotential, der stomatären Leitfähigkeit und Wurzeleigenschaften. Die Ergebnisse zeigen, dass die untersuchten Pflanzengemeinschaften höherer Diversität ihre Wurzelwasseraufnahmestrategie so anpassen, dass der Wassernutzen des gesamten Systems optimiert wird. Die Struktur der jeweiligen Wurzelsysteme spielt dabei vermutlich eine entscheidende Rolle. Weiterhin zeigte sich, dass in diverseren Pflanzengemeinschaften die Wasseraufnahme gleichmäßiger über die Tiefe verteilt wird als in artenärmeren.

Diese Dissertation gibt einen ersten Einblick in die Prozesse der Wurzelwasseraufnahme von Pflanzengemeinschaften. Für ein tiefgründiges Verständnis der einzelnen Einflüsse auf die Wurzelwasseraufnahmestrategien bedarf es anknüpfender spezifischer Forschung. Beispielsweise ist die Untersuchung von Ökosystemen mit einem höheren Pflanzenartengradienten in den verschiedensten Umweltsituationen hierfür erforderlich. Die Kombination von hydrologischen und ökologischen Messungen erwies sich als zielführend für die Untersuchung des Systems Pflanze-Boden-Wasser. Interdisziplinäre Forschung ist daher notwendig um die Funktionsweise von Ökosystemen besser zu verstehen.

Executive Summary

Although root water uptake is an important component in the plant-soil-water relation for single plants and on ecosystem scale, studies investigating the effect of co-existing plant species on community water use have been conducted without estimating root water uptake profiles. However, knowledge of root water uptake is essential for understanding of intra- and interspecific interactions of plants, i.e. hydraulic lift, resource partitioning or competition and ecosystem functioning. For those reasons, minimal-invasive and easy to use methods for estimating root water uptake are inevitable.

Within this dissertation, an attempt has been made to identify a simple but sufficient accurate method for estimating evapotranspiration and root water uptake profiles from soil water content measurements without a priori information on root distribution parameters. Subsequently, this method was applied to investigate the effect of co-existing plant species on community root water uptake.

The first part of the thesis deals with the evaluation of four different complex water balance methods regarding their applicability on the ecohydrological issue. In this comparative study, a synthetic experiment with numerical simulations for a grassland ecosystem was conducted. The methods were tested for a range of measurement frequencies and soil moisture sensor uncertainties. The most suitable approach to estimate root water uptake was found to be the Multi Step Multi Layer Regression (*msml*). This simple method derives root water uptake from diurnal fluctuation of soil water content measurements.

In the second part of this PhD project, an additional accuracy assessment considering magnitudes of evapotranspiration, soil texture variability, and sensor uncertainty was carried out for the Multi Step Multi Layer Regression. Therefore, we employed measurements of soil moisture from 12 weighable lysimeters. The focus was here to validate the method and get an overview of the uncertainties and their sources occurring in natural applications. The results indicate that the *msml* method is sensitive regarding the magnitude of evapotranspiration. The uncertainty of the *msml* method decreases with increasing evapotranspiration respectively soil water depletion. Furthermore, soil texture was found to have no influence on the prediction quality of root water uptake. Additionally, we applied a filter routine to reduce the uncertainty of

sensor precision. The results proved that the proposed filter describes the real data sufficiently well.

The third part of this thesis deals with the investigation of the effect of co-existing plant species on the community root water uptake. Especially, it was examined whether diverse plant communities exploit soil water more efficiently than less diverse ones. Therefore, the Multi Step Multi Layer Regression was applied on a lysimeter setup hosting 12 experimental grasslands of contrasting species richness (4 and 16 sown species). Analysis of estimated root water uptake profiles were combined with measurements of leaf water potentials, stomatal conductance as well as root traits and constitutes the novelty of this thesis. The results indicate that the investigated communities with higher species richness are able to adjust their root water uptake strategy, based on the root system structure of single species, in a way that the water use of the entire community is optimized. Furthermore, we found that the water uptake in these communities is more equally distributed over depth.

This work provides a first glimpse on the processes associated with root water uptake in plant communities. However, for a thoroughly understanding of ecosystem functioning more research is yet required to disentangle the single impacts on root water uptake strategies. Particularly, similar investigations of more ecosystems with more different diverse plant communities and environmental situations are needed. In general, the combination of hydrological and ecological measurements was shown to be promising for investigating plant-soil-water relations. Hence, inter-disciplinary research is necessary towards a better understanding of ecosystem functioning.

Nomenclature

ANOVA	analysis of variance
BGBM	belowground biomass (g cm^{-2})
b	relative bias (%)
d_{T}	length of active transpiration period over a day (h)
$d_{\mathrm{z,i}}$	thickness of soil layer i (m)
d_{root}	average root diameter (cm)
DOY	day of year
e	difference in observed and estimated soil water content in the inverse model
E	evapotranspiration (mm h^{-1} or cm d^{-1})
E_{s}	bare soil evaporation (mm h^{-1})
E_{t}	transpiration (mm h^{-1})
$\tilde{E}$	estimated evapotranspiration (mm h^{-1})
FG	functional group identity
GR	grasses
g_s	stomatal conductance (mmol m^{-2} s^{-1})
h	soil matric potential (m)
i	soil layer index
im	Inverse Model
j	time step index
$K(h)$	hydraulic conductivity (m s^{-1})
K_{sat}	saturated hydraulic conductivity (m s^{-1})
LAI	leaf area index (cm^2 cm^{-2})
LAI_s	leaf area index per species (cm^2 cm^{-2})
LE	legumes
LWP	leaf water potential (MPa)
ldw	leaf dry weight (g cm^{-2})
m_{tot}	slope of fitted linear function on $\theta(t)$
m_{extr}	slope of fitted linear function on $\theta(t)$ due to sink term
m_{flow}	slope of fitted linear function on $\theta(t)$ due to vertical soil water flow
MC	Macrocosm
MLWP	Midday leaf water potential (MPa)
moi	moment of inertia (-)

$msml$	Multi Step Multi Layer Regression
n_{vG}	van Genuchten parameter (-)
NSE	Nash-Sutcliffe efficiency criterion
P	precipitation (mm h^{-1})
PLWP	predawn leaf water potential (MPa)
p	statistical significance
q	percolation (mm h^{-1})
R	correlation coefficient (-)
r	number of data points
RAI	root area index (cm^2 cm^{-2})
$RAI:LAI$	ratio between root area index and leaf area index (-)
RLD	root length density (cm cm^{-3})
RV	relative variability
S	sink term in Richards equation (s^{-1})
S_i	discretized sink term in the soil layer i (m s^{-1})
$\tilde{S}$	estimated sink term (m s^{-1})
SH	small herbs
SLA	specific leaf area (mm^2 mg^{-1})
s	standard deviation
sp	species
s_{res}	noise of volumetric soil water content measurements (-)
SR	species richness
$ssml$	Single Step Multi Layer Water Balance
$sssl$	Single Step Single Layer Water Balance
TDR	time-domain reflectometry
TH	tall herbs
t	time (s)
Δt	time step (h)
VPD	vapor pressure deficit (hPa)
v	iteration step number (-)
$\bar{x}$	mean value
x	observed (synthetic) value
$\tilde{x}$	estimated values
y	threshold value for moving average filter (-)
z	vertical coordinate (m)

z_r	active rooting depth (cm)
$z_{25\%}$	depth up to which 25 % of root water uptake occurs (cm)
$z_{50\%}$	depth up to which 50 % of root water uptake occurs (cm)
$z_{90\%}$	depth up to which 90 % of root water uptake occurs (cm)

α	van Genuchten parameter (m^{-1})
θ	Volumetric soil water content (m^3 m^{-3})
θ_r	residual volumetric soil water content (m^3 m^{-3})
θ_s	saturated volumetric soil water content (m^3 m^{-3})
$\tilde{\theta}$	estimated volumetric soil water content (m^3 m^{-3})
$\Delta\theta$	deviation in volumetric soil water content over time (m^3 m^{-3})
ε_{ZZ}	decision criterion for termination of the iteration process (Inverse Model from Zuo and Zhang (2002))
$\varepsilon_{GH,i}$	decision criterion for termination of the iteration process in the Inverse Model proposed here
ψ_g	gravimetric potential (m)
ψ_m	matric potential (m)
ψ_o	osmotic potential (m)
ψ_p	hydrostatic pressure (m)
ψ_w	water potential (m)
ψ_{RO}	water potential at the interface of root and soil (m)
ψ_{ws}	water potential in the bulk soil (m)
ψ_x	water potential in the xylem of roots (m)
ω_{RO}	resistance of water flow into the root xylem (s m^{-2})
ω_S	resistance to transport water out of the soil (s m^{-2})

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Chapter 1

General Introduction

1 General Introduction

1.1 Background

"No matter who we are, or where we live, our well-being depends on the way ecosystems work. Most obviously, ecosystems can provide us with material things that are essential for our daily lives, such as food, wood, wool and medicines. Although the other types of benefit we get from ecosystems are easily overlooked, they can, for example, also play an important role in regulating the environments in which we live. They can help ensure the flow of clean water and protect us from flooding or other hazards like soil erosion, land-slips and tsunamis. They can even contribute to our spiritual well-being, through their cultural or religious significance or the opportunities they provide for recreation or the enjoyment of nature."

(From Ecosystem Ecology: a new synthesis, R. Haines-Young & M. Potschin, 2009)

This quotation from Haines-Young and Potschin wonderfully condense the role of ecosystems for mankind and underlines the paramount importance of maintaining ecosystem functions. Additionally, as Schwartz et al. (2000) stated in their review, ecosystem functions are related to species richness and this is the most important argument for conservation of biodiversity to maintain ecosystem functions. Unfortunately, during the last five decades, economic interests of human society lead to increasing changes of ecosystems and biodiversity with a tremendous loss of species. The resulting benefits for a minority of the world's citizens are, however, only temporary, whereas the long-term consequences of biodiversity loss and the associated degradation of ecosystem functions are hard to assess. The contamination of groundwater and lakes due to the increased application of agro-chemicals, the reversible destruction of biotopes due to construction of streets and hydropower dams, or the increase of disruptive floods caused by land use changes, such as intensified agriculture or river regulation, are just a few consequences we have experienced yet (Hupet, 2003; Millennium Ecosystem Assessment, 2005). Beside these implications of ecosystem changes and biodiversity loss, a further one is the widely discussed climate change with increasing CO_2 in the atmosphere (Seneviratne et al., 2006; Bonan et al., 2008, Kumar, 2011). However, all the aforementioned processes interact together and not only at different time scales but also at local, regional and global scale. Thus, forecasts of long-term consequences are almost impossible and countermeasures are indispensable. Meanwhile, the awareness of governments and the public concerning protection of ecosystems and sustainable management increases substantially (Hupet, 2003). For example, the designation of conservation areas has doubled every decade since the 1990s to about 209.429, where a steep increase was recorded during the last ten years (Deguignet et al., 2014). Certainly, the Millennium Ecosystem Assessment (2005), the first global assessment which comprehensively investigated the implications of ecosystem changes, contributed to this tendency. Within this context, Haines-Young and Potschin (2009) further highlight, that sustainable management strategies respectively policies are inevitable for maintaining ecosystem functions. Though, therefore a clear understanding of ecological processes is crucial, especially the influence of biodiversity on ecosystem functions.

The plant-soil-water relation plays an important role within these processes and the understanding of this system is a major concern in ecohydrology. It’s not only that plants require water for nearly all physiological functions, for instance, as solvent, transport medium or to maintain the cell turgor (Silvertown et al., 2014). Water is also required for cooling the plants surface, which is enabled by transpiration of water stored in the soil. Thus, plants essentially link the water and the carbon cycle between soil and atmosphere (Feddes et al., 2001; Chapin et al., 2002; Feddes and Raats, 2004; Teuling et al., 2006b; Schneider et al., 2009; Seniveratne et al., 2010; Asbjornsen et al.,2011) and hence, the air temperature is indirectly linked to soil water content (Koster et al., 2006). Moreover, aboveground ecophysiological processes, which regulate the water and energy exchange to the atmosphere, are controlled by the dynamics of water flow from soil to plant roots (Bardgett and Wardle, 2010; Quijano et al., 2012; Kumar et al., 2013). Consequently, roots have a key function within the plant-soil-water relation as pathway for water from soil to atmosphere and by connecting the stock of the essential nutrients and water to the consuming organs of plants (Feddes and Raats, 2004).

This ability to acquire resources, especially water, through roots is crucial for plant productivity and survival, which is reflected in the various adaptions of water uptake strategies of plants to different environments (Feddes et al., 2001; Ho et al., 2004). However, ecosystems are characterized by the presence of different species which compete for the resources water or show a mutualistic relation, for instance hydraulic lift (Ludwig et al., 2003; Scott et al., 2008; Quijano et al., 2012). Thus, the monitoring and understanding of water uptake processes on the ecosystem level is even more challenging due to the variety of spatial and temporal water acquisition and partitioning strategies among the different plant species (McKane et al., 2002). At the same time, these different strategies prevent competition among plants due to occupation of different niches.

Niche complementarity is often used in ecology to explain coexistence and the positive relation of species richness and ecosystem functions, but it is at the same time a controversial issue (Silvertown et al., 1999; Hooper et al., 2005; Ashton et al., 2010; Silvertown et al., 2014). Nevertheless, a great deal of studies summarized by Araya et al. (2011) illustrate that availability of soil moisture, referred to as hydrological niche, is an important mechanism in a wide range of ecosystems from European grasslands to tropical forests. Silvertown et al. (2014) differentiated hydrological niches by segregation into the following characteristics: "(i) partitioning of space on fine-scale soil-moisture gradients, or (ii) partitioning of water as a resource through different strategies of water acquisition such as different phenologies or different rooting depths". A third strategy enabling co-existence is suggested as plasticity in resource use, which adapts to the spatial and temporal variance of soil water content (Casper and Jackson, 1997; Ashton et al., 2010; Silvertown et al., 2014). While the first two strategies can be grasped by measuring root distributions or capturing the space portioning as well as the pronounced phenologies, the latter one is more difficult to monitor since it is not possible to measure root water uptake directly. But, the statement of Ashton et al. (2010), who say that: "…plasticity could provide a general and important mechanism for resource partitioning, particularly for species that have broadly overlapping resource use patterns." underlines the relevance of an improved understanding of root water uptake particularly in diverse ecosystems. Furthermore, it illustrates the need for suitable methods to estimate root water uptake.

Recently developed imagine techniques enable the examination of water uptake from living roots (Garrigues et al., 2006; Pohlmeier et al., 2008; Zarebanadkouki et al., 2013). Even though these methods allow the monitoring and quantifying of water transport at high spatial and temporal resolution; they can only be applied on single plants. The same holds true for stable isotope analysis, which can be used to estimate the depths at which plants take up water (Ogle et al., 2004; Asbjornsen et al., 2006; Schwendenmann et al., 2014).

Beside these methods, researchers have developed different modelling approaches for indirect calculation of root water uptake within the last decades, which range from simple water balance methods to complex inverse model applications. Each method has its own assets and drawbacks. For instance, simple water balance methods neglects soil water fluxes and lead to substantial errors of estimated water uptake. In contrast, complex models do consider soil water fluxes, but require an extensive parametrization, i.e. of soil hydraulic properties and root distribution parameters. A comprehensive review of existing root water uptake models and approaches are given in Molz (1981), Hille (1998) and Feddes and Raats (2004).

The aforementioned points elucidate that knowledge of root water uptake is key to understanding plant-soil-water relations and thus ecosystem functioning, in particular efficient plant water use, storage keeping and competition in ecosystems. For those reasons, minimal-invasive and easy to use methods for estimating root water uptake are inevitable.

1.2 What is known about the process "root water uptake" and how to derive deeper insights in "ecosystem root water uptake"?

As already elucidated in Section 1.1, root water uptake is a substantial component of the soil water balance. In general, root water uptake is driven by a difference in hydraulic potential between the soil and the surface of roots. This potential gradient induces a convective flow of water towards the plant roots (Gardner, 1963; Moene and van Dam, 2014). The entire water transport in the plant from roots to leaves is caused by transpiration, which is a function of atmospheric demand and stomatal conductance (Jackson et al., 2000; Moene and van Dam, 2014). Willingen et al. (2005) described it as: "…purely physical process, a consequence of gradients in water potential in the path: bulk soil – soil/root interface – root – leaf – atmosphere." In this context, water potential (ψ_w) describes the water status of the bulk soil compartment and the plant water, and is commonly the sum of the osmotic potential (ψ_o), the gravimetric potential (ψ_g), and the hydrostatic pressure (ψ_p) or when considering the water potential in soils, the matric potential (ψ_m) (Lamberts, 2008),

$$\Psi_w = \Psi_o + \Psi_g + \Psi_p. \tag{1.1}$$

The water potential can be expressed as pressure units (MPa), when referred to a unit volume of water, or as the height of a water column (m), when referred to a unit weight of water (Hopmans and Bristow, 2002).

In general, soil and plant properties influence the water uptake at the single root scale (Garrigues et al., 2006). These are for instance soil texture and physical-chemical properties, which determine the strength with which water is adsorbed in soil pores and on surfaces of soil particles (Lamberts, 2008). When water is flowing into the root, it can enter via the cellular pathway (by root hairs of rhizodermis cells) or via the apoplastic pathway (by cells of the exodermis) (Moene and van Dam, 2014). Consequently, soil and plant properties introduce a resistance for water flow from bulk soil to soil-root interface and to root xylem, which is therefore mathematically often described in analogy to the Ohm's law:

$$Q = \frac{\Psi_{ws} - \Psi_{RO}}{\omega_s} = \frac{\Psi_{RO} - \Psi_x}{\omega_{RO}} \tag{1.2}$$

where Q is the flow (m^3 s^{-1}), Ψ_{ws} is the water potential in the bulk soil (m), Ψ_{RO} is the water potential at the interface of root and soil (m), Ψ_x is the water potential in the xylem of roots (m), ω_s describes the resistance to transport water out of the soil (s m^{-2}) and ω_{RO} describes the resistance of water flow into the root xylem (s m^{-2}) (Willingen et al., 2005). The soil resistance decreases with increasing soil water content, but the (radial) root resistance is assumed to be the highest resistance in the soil-root system (Willingen et al., 2005).

Commonly, Eq. (1.2) is used to describe water transport of a single root and is known as the "microscopic" approach (Hopmans and Bristow, 2002). This concept simply introduces the impact of soil resistances on water uptake and transpiration, while neglecting the osmotic potential and assumes resistances, which are constant and time-independent. However, it is not practical for application neither on an entire root system nor on plant communities, since transpiration rate influences the plant resistance, the plant itself is much more intricate, and water flow in the soil-root-plant-atmosphere system is highly dynamic (Hopmans and Bristow, 2002). Moreover, root system architecture and xylem anatomy have a substantial impact on transpiration and water uptake (Jackson et al., 2000). Plants, for instance, take up water from upper soil layers, where the main body of roots is concentrated, as long as there is sufficient water stored. With increasing desiccation of the soil, the water uptake shifts to deeper wet layers (Lamberts, 2008). This can only be conducted with deep root systems (Jackson et al., 2000).

In summary, water uptake at single root scale occurs on a micro scale within a vicinity of about 6 mm of the root and depends on hydraulic continuity and conductivity (Lamberts, 2008). The sum and interactions of these small scale processes drive the water uptake at root system and community level. In turn, this is influenced by transpiration and root properties like root hydraulics and root architecture (Garrigues et al., 2006). However, understanding the small scale processes on the single root scale does not necessary lead to understanding of root water uptake at the ecosystem scale. Therefore we have to consider the entire system where a bunch of intra- and interspecific plant interactions shape the water use of the community. For instance, hydraulic lift, resource partitioning, or competition increase the complexity of ecosystem root water uptake. For those reasons, assumptions on the water uptake patterns, root properties and root parametrization, which are normally implemented in water uptake models, are notoriously uncertain and their application is questionable (Hamblin and Tennant, 1987; Lai and Katul, 2000; Li et al., 2002; Doussan et al., 2006; Garrigues et al., 2006; Schneider et al., 2009). Yet, only little is known about the processes of root water uptake at ecosystems scale. Therefore, methods for estimating root water uptake are suggested to have a minimal requirement of (model) parameters and are applicable on the ecosystem scale. Moreover, the technical implementation of direct measurements and real time observation of root water uptake is difficult to realize. The main obstacles for deriving and monitoring ecosystem root water uptake might be the scale at which this takes place. Nevertheless, in this work we assume that the “small” scale of soil water content measurements contain a great deal of information on root water uptake.

1.3 Aims and research questions

The main focus was to identify a simple but sufficient accurate method for estimating water uptake from soil water content measurements and their application on the eco-hydrological question, whether there is an effect of co-existing plant species on community root water uptake.

Following the need for a suitable method for estimating root water uptake, Chapter 2 of this thesis deals with the examination of four different complex water balance methods on a numerical experiment regarding their applicability. In general, these should be methods, which meet the following demands:

- Easy implementation;
- Applicable on standard measurements, such as volumetric soil water contents;
- Minimal-invasive regarding estimation of required input data;
- Minimal computation effort;
- Minimal requirement of model parameters;
- Insensitive towards measurement errors.

Such a method suggests for application by non-hydrologists respectively researcher, who are not familiar in the field of modelling.

In particular, the following issues are addressed in this part of the thesis:

1. *Which data-driven method can be adopted to obtain accurate estimates of evapotranspiration and root water uptake from standard volumetric soil water content measurements?*
2. *Which impact has the measurement frequency on the prediction of evapotranspiration and root water uptake?*
3. *How are the estimates of evapotranspiration and root water uptake influenced by sensor uncertainties?*

This comparative study was aimed on the determination of the most suitable method for application on ecological research questions. Since the investigations in Chapter 2 were done with synthetic soil moisture data, an evaluation of the successful Multi Step Multi Layer Regression (*msml*) on lysimeter data followed in Chapter 3. The specific issues in this part of the thesis are:

4. *How does the magnitude of evapotranspiration influence the prediction of evapotranspiration and root water uptake?*
5. *Is the method restricted by soil texture variability?*
6. *How to deal with real sensor uncertainties?*

To date, the studies investigating the relations between species richness and water use have been limited and were conducted without estimating root water uptake profiles. Considering this research gap, the main aim of this thesis is to improve our understanding on the effect of co-existing plant species on the community root water uptake. Therefore, the thoroughly evaluated *msml* method was applied on lysimeters with soil-vegetation monoliths of a long-term grassland biodiversity experiment (Jena Biodiversity Experiment) to answer the following questions (Chapter 4):

7. *Is root water uptake in diverse plant communities achieved by exploiting greater depths (spatial complementarity)?*
8. *Is there a vertical belowground niche separation due to different rooting distributions between two diversity levels?*
9. *How do root traits of the involved species influence community root water uptake patterns?*

1.4 Outline of the thesis

The results of this PhD thesis are presented in three main chapters. Chapters 2 to 4 are structured around the objectives and research questions presented in section 1.2. Two chapters (2 to 3) are devoted to the evaluation of the chosen water balance methods; one (Chapter 4) to the estimation of root water uptake of twelve grassland communities with 4 and 16 species and the investigation of their uptake strategies.

In Chapter 2, theoretical and practical aspects of estimation of evapotranspiration and root water uptake are reviewed. Further, we describe the compared methods, the generation of the synthetic soil water content and root water uptake profiles as well as the introduced soil moisture sensor uncertainty. An evaluation of each method considering the evapotranspiration and root water uptake for a range of measurement frequencies and soil moisture sensor uncertainties was conducted.

Based on the results of Chapter 2, the most suitable method (Multi Step Multi Layer Regression) was chosen and tested on a lysimeter study conducted in the CNRS Ecotron Montpellier. The results are described in Chapter 3. Here, we also provide an introduction of the long-term grassland biodiversity experiment (Jena Biodiversity Experiment) from where the lysimeters originated as well as the infrastructure of the CNRS Ecotron. In a first part, we derived root water uptake profiles and evapotranspiration from soil water content measurements. Further, we performed an accuracy assessment considering the influence of magnitudes of evapotranspiration, soil texture variability, and sensor uncertainty on estimation of evapotranspiration. In a second part, water uptake profiles estimated with the Multi Step Multi Layer Regression were compared with data from stable isotope measurements. The results corroborate the findings from Chapter 2 that the Multi Step Multi Layer Regression is a sufficient accurate method for estimating water uptake from soil water content measurements, whereas best predictions could be reached on days with high evapotranspiration.

In Chapter 4, root water uptake estimated in Chapter 3 are used to compare root water uptake patterns with measured leaf water potentials, stomatal conductance and root traits in order to investigate how root water uptake strategies differ between plant communities. The results indicate that the investigated communities with higher species richness are able to adjust their root water uptake strategy, based on the root system structure of single species, in a way that the water use of the entire community is optimized. Furthermore, we found that in these communities the water uptake is more equally distributed over depth.

Finally, in Chapter 5, the main findings of the thesis are summarized and discussed as well as an outlook on their potential future implications is given.

Each main chapter (2 to 4) comprises its own introduction as well as material and method section, since these chapters are dealing with different aspects and objectives. Furthermore, these chapters correspond to the form of complete papers for submission to international peer-reviewed journals. This might lead to some repetitions of the introductory material. To date, Chapter 2 was published as research paper in Hydrology and Earth System Sciences. Chapter 4 is in preparation for submission to a peer-reviewed journal.

Chapter 2

Using measured soil water contents to estimate evapotranspiration and root water uptake profiles – a comparative study

2 Using measured soil water contents to estimate evapotranspiration and root water uptake profiles – a comparative study

Abstract

Understanding the role of plants for soil water relations, and thus ecosystem functioning, requires information about root water uptake. We evaluated four different complex water balance methods to estimate sink term patterns and evapotranspiration directly from soil moisture measurements. We tested four methods: The first two take the difference between two measurement intervals as evapotranspiration, thus neglecting vertical flow. The third uses regression on the soil water content time series and differences between day and night to account for vertical flow. The fourth accounts for vertical flow using a numerical model and iteratively solves for the sink term. None of these methods requires any a priori information of root distribution parameters or evapotranspiration, which is an advantage, compared to common root water uptake models. To test the methods, a synthetic experiment with numerical simulations for a grassland ecosystem was conducted. Additionally, the time series were perturbed to simulate common sensor errors, like those due to measurement precision and inaccurate sensor calibration. We tested each method for a range of measurement frequencies and applied performance criteria to evaluate the suitability of each method. In general, we show that methods accounting for vertical flow predict evapotranspiration and the sink term distribution more accurately than the simpler approaches. Under consideration of possible measurement uncertainties, the method based on regression and differentiating between day and night cycles leads to the best and most robust estimation of sink term patterns. It is thus an alternative to more complex inverse numerical methods. This study demonstrates that highly resolved (temporally and spatially) soil water content measurements may be used to estimate the sink term profiles when the appropriate approach is used.

2.1 Introduction

Plants play a key role in the Earth system by linking the water and the carbon cycle between soil and atmosphere (Feddes et al., 2001; Chapin et al., 2002; Feddes and Raats, 2004; Teuling et al., 2006b; Schneider et al., 2009; Seniveratne et al., 2010; Asbjornsen et al., 2011). Knowledge of evapotranspiration and especially root water uptake profiles is key to understanding plant-soil-water relations and thus ecosystem functioning, in particular efficient plant water use, storage keeping and competition in ecosystems (Davis and Mooney, 1986; Le Roux et al., 1995; Jackson et al., 1996; Hildebrandt and Eltahir, 2007;Arnold et al., 2009; Schwendenmann et al., 2014).

For estimation of root water uptake, models are prevalent in many disciplines. Most commonly, root water uptake is applied as a sink term *S*, incorporated in the 1D soil water flow equation (Richards equation, Eq. 2.1),

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right] - S(z,t) \tag{2.1}$$

where θ is the volumetric soil water content, *t* is time, z is the vertical coordinate, *h* is the soil matric potential, *K*(*h*) is the unsaturated soil hydraulic conductivity and *S*(z, *t*) is the sink term (water extraction by roots, evaporation etc.). The sink term profile *S*(z, *t*) depends on root activity, which has to be known previously. Often root activity is assumed to be related to rooting profiles, represented by power laws (Gale and Grigal, 1987; Jackson et al., 1996; Schenk, 2008; Kuhlmann et al., 2012). The parameters of those rooting profile functions are cumbersome to measure in the field, and the relevance for root water uptake distribution is uncertain (Hamblin and Tennant, 1987; Lai and Katul, 2000; Li et al., 2002; Doussan et al., 2006; Garrigues et al., 2006; Schneider et al., 2009). Therefore, assumptions have to be made in order to determine the sink term for root water uptake in soil water flow models. The lack of an adequate description of root water uptake parameters was mentioned by Gardner (1983) and is currently still an issue (Lai and Katul, 2000; Hupet et al., 2002; Teuling et al., 2006a; Teuling et al., 2006b). For those reasons, methods for estimating root water uptake are a paramount requirement.

Standard measurements, for instance of soil water content profiles, are recommend to be used for estimation of evapotranspiration and root water uptake at low cost, since the evolution of soil moisture in space and time is expected to contain information on root water uptake (Musters and Bouten, 2000; Hupet et al., 2002; Zuo and Zhang, 2002; Teuling et al., 2006a). Methods using these measurements are, for instance, simple water balance approaches, which estimate evapotranspiration (Wilson et al., 2001; Schume et al., 2005; Kosugi and Katsuyama, 2007; Breña Naranjo et al., 2011) and root water uptake (Green and Clothier, 1995; Coelho and Or, 1996; Hupet et al., 2002) by calculating the difference in soil water storage between two different observation times. The advantages of these simple water balance methods are the small amount of information required and the simple methodology. However, a disadvantage is that the depletion of soil water is assumed to occur only by root water uptake and soil evaporation, and soil water fluxes are negligible (Hupet et al., 2002). This is only the case during long dry periods with high atmospheric demand (Hupet et al., 2002).

A possible alternative which allows for the consideration of vertical soil water fluxes is the inverse use of numerical soil water flow models (Musters and Bouten, 1999; Musters et al, 2000; Vrugt et al., 2001; Hupet et al., 2002; Zuo and Zhang, 2002). In those models, root water uptake or parameters on the root water uptake function are estimated by minimizing the differences between measured soil water contents and the corresponding model results by an objective function (Hupet et al., 2002). However, the quality of the estimation depends, on the one hand, strongly on system boundary conditions (e.g., incoming flux, drainage flux or location of the groundwater table) and soil parameters (e.g., hydraulic conductivity), which are on the other hand notoriously uncertain under natural conditions (Musters and Bouten, 2000; Kollet 2009). Another problem is that the applied models for soil water flow potentially ignore biotic processes. For example Musters et al. (2000) and Hupet et al. (2002) attempted to fit parameters for root distributions in a model determining uptake profiles from water availability, whereas empirical and modeling studies suggest that adjustment of root water uptake distribution may also be from physiological adaptations (Jackson et al., 2000; Zwieniecki et al., 2003; Bechmann et al., 2014). In order to avoid this problem, Zuo and Zhang (2002) coupled a water balance approach to a soil water model, which enabled them to estimate root water uptake without the a priori estimation of root water uptake parameters.

A second option for accounting for vertical soil water flow in a water balance approach is to analyze the soil moisture fluctuation between day and night (Li et al., 2002). In comparatively dry soil, Li et al. (2002) fitted third-order polynomials to the daytime- and nighttime-measured soil water content time series and calculated vertical soil water flow using the first derivative of the fitted polynomials during the nighttime.

Up to now, little effort has been made to compare those different data-driven methods for estimating evapotranspiration and root water uptake profiles in temperate climates. In this paper, we compare those water balance methods we are aware of that do not require any a priori information of root distribution parameters. We used artificial data of soil moisture and sink term profiles to compare the quality of the estimates of the different methods. Furthermore, we investigated the influence of sensor errors on the outcomes, as these uncertainties can have a significant impact on both data-driven approaches and soil hydrological models (Spank et al., 2013). For this, we artificially introduced measurement errors to the synthetic soil moisture time series that are typical for soil water content measurements: sensor calibration error and limited precision.

Our results indicate that highly resolved soil water content measurements can provide reliable predictions of the sink term or root water uptake profile when the appropriate approach is used.

2.2 Material and Methods

2.2.1 Target variable and general procedure

The evapotranspiration E consists of soil evaporation E_s and the plant transpiration E_t (Eq. 2.2)

$$E = (E_s + E_t). \tag{2.2}$$

The distinction between soil evaporation and combined transpiration is not possible for any of the applied water balance methods. Therefore, the water extraction from soil by plant roots and soil evaporation is referred to as the sink term profile in the rest of the paper. The integrated sink term over the entire soil profile results in the total evapotranspiration (Eq. 2.3),

$$E(t) = \int_{z=z_r}^{0} S(t,z)dz \rightarrow E_j = \sum_{\mathrm{i}=1}^{n} S_{i,j} \cdot d_{z,i} \tag{2.3}$$

where z is the soil depth, $d_{\mathrm{z,i}}$ is the thickness of the soil layer i, t is time and j is the time step. For matters of simplicity we will drop the index j when introducing the estimation methods in the following.

In this study, synthetic time series of volumetric soil water content generated by a soil water flow model coupled with a root water uptake model (section 2.2.3) were treated as measured data and are used as the basis for all methods (section 2.2) estimating the sink term $\widetilde{S}\,(z)$ and total evapotranspiration $\widetilde{E}$. In order to investigate the influence of sensor errors, the generated time series were systematically disturbed, as shown in section 2.4. Based on these estimations we evaluate the data-driven methods on predicting evapotranspiration $\widetilde{E}$ and sink term profiles using the quality criteria given in section 2.5. As the depth at which a given fraction of root water uptake occurred is often interesting in ecological studies (e.g., Green and Clothier, 1999; Plamboeck et al., 1999; Ogle et al., 2004), estimated sink term profiles were compared accordingly. Specifically, we determined up to which depths 25 %, 50 % and 90 % ($z_{25\%}$, $z_{50\%}$ and $z_{90\%}$) of water extraction takes place.

2.2.2 Investigated data-driven methods for estimation of the sink term profile

In the following we introduce the four investigated methods, which are summarized in Table 2.1.

Table 2.1 Overview of the four applied data-driven methods, the acronym of the methods for further use and the required input data.

Acronym	Method	Method short description	Input data
sssl	*S*ingle *S*tep *S*ingle *L*ayer Water Balance	Water balance (Breña Naranjo et al., 2011)	Volumetric soil water content at a single depth Precipitation
ssml	*S*ingle *S*tep *M*ulti *L*ayer Water Balance	Water balance over entire soil profile (Green and Clothier, 1995; Coelho and Or, 1996; Hupet et al., 2002)	Volumetric soil water content at several depths Precipitation
msml	*M*ulti *S*tep *M*ulti *L*ayer Regression	Approach to use the short term fluctuations of soil moisture (Li et al., 2002)	Volumetric soil water content at several depths Precipitation
im	*I*nverse *M*odel	Water balance solved iteratively with a numerical soil water flow model (Zuo and Zhang, 2002; Ross, 2003)	Soil hydraulic parameters Volumetric soil water content at several depths Precipitation

Single Step Single Layer (*sssl*) Water Balance

Breña Naranjo et al. (2011) derived the sink term using time series of rainfall and changes of soil water content between two observation times (*s*ingle *s*tep), based on measurements at one single soil depth (*s*ingle *l*ayer). The complete water balance equation for this single layer method is

$$\widetilde{E}_{sssl} = P - q - z_r \frac{\Delta\theta}{\Delta t} , \tag{2.4}$$

where z_r is the active rooting depth, which is also the depth of the single soil layer, and is taken equal to the measurement depth of volumetric soil water content, θ. Δt indicates the length of the considered single time step. P is the rainfall and q the percolation out of the soil layer during the same time step. When rainfall occurs, infiltration as well as soil water flow takes place. It is assumed that percolation occurs only during this time and persists only up to several hours after the rainfall event (Breña Naranjo et al., 2011). Since the percolation flux is unknown, the methods cannot be applied during these wet times. During dry periods, q is set to zero and Eq. (2.4) simplifies to Eq. (2.5) (Breña Naranjo et al., 2011)

$$\widetilde{E}_{sssl} = z_r \frac{\Delta\theta}{\Delta t} . \tag{2.5}$$

We applied Eq. (2.5) to estimate evaporation (in the single layer method equal to the sink term) from artificial soil water contents at 30 cm. Required input information is thus only time series of soil water content and active rooting depth z_r. Additionally, rainfall measurements are required to select dry periods, where no percolation occurs. These could start several hours up to several days after a rainfall event (Breña Naranjo et al., 2011), and the exact timing depends on the amount of rainfall and the site-location parameters like soil type and vegetation. In this study we waited until 24 hours after the end of the precipitation event before applying the model.

Single Step Multi Layer (*ssml*) Water Balance

This method is similar to the *sssl* method introduced above. It calculates the sink term based on two observation times (*s*ingle *s*tep), but is extended to several measurement depths (*m*ulti *l*ayer). The water balance during dry periods of each layer is the same as in Eq. (2.5) and uptake in individual layers is calculated by neglecting vertical soil water fluxes and therefore assuming that the change in soil water content is only caused by root water uptake (Hupet et al., 2002)

$$\tilde{S}_{ssml,i} = d_{z,i}\frac{\Delta\theta_i}{\Delta t}, \tag{2.6}$$

where $\tilde{S}_{\mathrm{ssml},i}$ is the estimated sink term in soil layer i, $\Delta\theta_i$ is the change in soil water content in the soil layer i over the single time step (Δt) and $d_{z,i}$ is the thickness of the soil layer i. Actual evapotranspiration (E_{ssml}) is calculated by summing up $\tilde{S}_{\mathrm{ssml},i}$ over all depths in accordance with (Eq. 2.3). The application of the *ssml* method is restricted to dry periods. It requires time series of volumetric soil water content and rainfall measurements as input to select dry periods.

Multi Step Multi Layer (*msml*) Regression

The third method derives actual evapotranspiration and sink term profiles from diurnal fluctuation of soil water contents (Li et al., 2002). It uses a regression over multiple time steps (*m*ulti *s*tep) and can be applied at several measurement depths (*m*ulti *l*ayer).

During daytime, evapotranspiration leads to a decrease in volumetric soil water content. This extraction of soil water extends over the entire active rooting depth. Additionally, soil water flow occurs both at night and during the daytime (Khalil et al., 2003; Verhoef et al., 2006; Chanzy et al., 2012), following potential gradients in the soil profile. Thus, during dry weather conditions, the time series of soil water content shows a clear day–night signal (Fig. 2.1). We split up the time series by fitting a linear function to each day and night branch of the time series. The onset of transpiration is mainly defined by opening and closure of plant stomata, which is according to the supply of solar energy (Loheide, 2008; Maruyama and Kuwagata, 2008; Sánchez et al., 2013), usually 1 or 2 h after sunrise or before sunset (Lee, 2009).

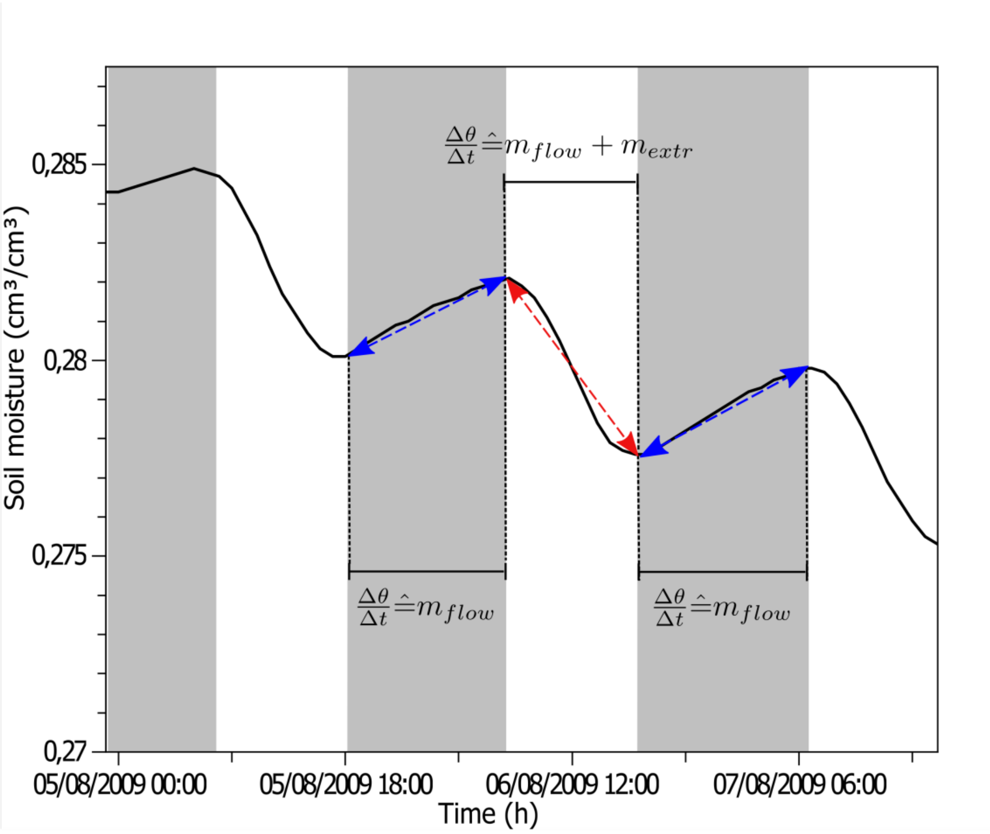


Figure 2.1 Short-term fluctuations in soil moisture in 15 cm depth during August 2009, showing the rewetting of soil at nighttime (blue line) and the water extraction during the day (red line); dashed lines depict the change between times with soil water extraction (grey) and rewetting of soil (white).

Here, the basic assumption is that the soil water flow does not change significantly between day and night (Fig. A.1). The slope of the fitted linear functions gives the rate of root water extraction and vertical flow. This can also be shown mathematically by disassembling the Richards' equation (Eq. 2.1) in vertical flow (subscript flow) and sink term (subscript extr) (Eq. 2.7), whereas the change of soil water content over time $(\partial\theta\ /\partial t)$ integrates both fluxes:

$$\frac{\partial\theta}{\partial t} = \frac{\partial\theta}{\partial t}\Big|_{\text{flow}} + \frac{\partial\theta}{\partial t}\Big|_{\text{extr}} = m_{tot}\ , \tag{2.7}$$

where m_{tot} corresponds to the slope of the fitted linear function for the day or night branch. Assuming that evapotranspiration during the night is negligible; the slope for the night branch is entirely due to soil water flow. During the day, uptake processes and soil water flow act in parallel:

day: $$m_{tot} = m_{\text{flow}} + m_{\text{extr}}\ , \tag{2.8a}$$

night: $m_{tot} = m_{\text{flow}}$, (2.8b)

The sink term can be calculated from Eq. (2.8a), assuming that m_{flow} can be estimated from Eq. (2.8b) and using the average of the antecedent and the preceding night. A similar procedure has previously been applied in diurnal groundwater table fluctuations (Loheide, 2008). Also with Loheide's method, the extraction will be overestimated if day and night fluxes are not separately considered. With the soil layer thickness of the respective layer i ($d_{z,i}$) taken into account, the mean daily sink term of soil layer i ($\tilde{S}_{msml,i}$) is obtained:

$$\tilde{S}_{\mathrm{msm},i} = (\mathrm{m}_{\mathrm{tot},i} - \overline{m}_{\mathrm{flow},i}) \cdot \mathrm{d}_{\mathrm{z},i}. \tag{2.9}$$

Since a diurnal cycle of soil moisture is only identifiable up to a time interval of 12 hours, the regression method is limited to minimum measurement frequency of 12 hours. Furthermore, as rainfall causes changes of soil water content and blurs the diurnal signal, the *msml* regression is only applicable during dry periods. Time series of soil water content and rainfall measurements to select dry periods are required as input.

Inverse Model (im)

The fourth approach is the most complex. The *i*nverse *m*odel (*im*) estimates the average root water uptake by solving the Richards equation (Eq. 2.1) and iteratively searching for the sink term profile which produces the best fit between the numerical solution and measured values of soil moisture content (Zuo and Zhang, 2002). The advantage of this method is the estimation of root water uptake without the a priori estimation of rooting profile function parameters, since they are highly uncertain, as elucidated in the Introduction. We implemented the inverse water balance approach after Zuo and Zhang (2002) with the Fast Richard's solver (Ross, 2003), which is available as Fortran 90 code. We modified the original method by changing the convergence criterion. In the following section, we first introduce the iterative procedure as proposed by Zuo and Zhang (2002) and then explain the modification which we made.

The iterative procedure by Zuo and Zhang (2002) runs the numerical model over a given time step (Δt) in order to estimate the soil water content profile $\tilde{\theta}_i^{(v=0)}$ at the end of the time step, and assuming that the sink term ($\tilde{S}_{im,i}^{(v=0)}$) is zero over the entire profile. Here ~ depicts the estimated values at the respective soil layer *i*, and *v* indicates the iteration step. Next, the sink term profile $\tilde{S}_{im,i}^{(v=1)}$ is set equal to the difference between previous approximation $\tilde{\theta}_i^{(v=0)}$ and measurements θ_i while accounting for soil layer thickness and length of the time step for units.

In the following iterations, $\tilde{S}_{im,i}^{(v)}$ is used with the Richards equation to calculate the new soil water contents $\tilde{\theta}_i^{(v)}$. The new average sink term $\tilde{S}_{im,i}^{(v+1)}$ is then determined with Eq. (2.10).

$$\tilde{S}_{im,\mathrm{i}}^{(v+1)} = \tilde{S}_{im,\mathrm{i}}^{(v)} + \frac{\tilde{\theta}_i^{(v)} - \theta_i}{\Delta t} \cdot d_{z,i} \,. \tag{2.10}$$

This iteration process continues until a specified decision criterion ε_{ZZ} is reached:

$$\varepsilon_{ZZ} \geq \frac{1}{n} \sum_{i=1}^{n} \left[\frac{\tilde{\theta}_i^{(v)} - \theta_i}{\theta_i} \right]^2 \quad , \tag{2.11}$$

where *n* is the number of soil layers in the soil column.

Since ε_{zz} is a normalized root-mean-square error over depth, good and poor estimations cancel between layers. This leads to termination of the iterative procedure even if the estimation of the sink term is very poor in several layers. We therefore propose a slightly adapted termination process, which applies to separate soil layers as follows. The estimation of the sink term in general is applied as proposed by Zuo and Zhang (2002):

(1) Calculate the difference between the estimated and measured soil water content (Eq. 2.12) and compare the change in this difference to the difference of the previous iteration (Eq. 2.13):

$$e_i^{(v)} = \left| \theta_i - \tilde{\theta}_i^{(v)} \right| \tag{2.12}$$

$$\varepsilon_{GH,\mathrm{i}}^{(v)} = e_i^{(v-1)} - e_i^{(v)} \tag{2.13}$$

(2) In soil layers where $\varepsilon_{GH}^{(v)} < 0$, set the root water uptake rate back to the value of the previous iteration ($\tilde{S}_{im,\mathrm{i}}^{(v+1)} = \tilde{S}_{im,\mathrm{i}}^{(v-1)}$), since the current iteration was no improvement. Only if $\varepsilon_{GH,\mathrm{i}}^{(v)} \geq 0$, go to step (3). This prevents acceptance of the estimated sink term $\tilde{S}_{im,\mathrm{i}}^{(v)}$ even if it leads to a worse fit than the previous iteration.

(3) If $e_{\mathrm{i}}^{(v)} > 1.0e^{-4}$, calculate $\tilde{S}_{im,\mathrm{i}}^{(v+1)}$ according Eq. (2.10); otherwise the current iteration sink term ($\tilde{S}_{im,\mathrm{i}}^{(v+1)} = \tilde{S}_{im,\mathrm{i}}^{(v)}$) is retained, as it results in a good fit between estimated and measured soil water contents.

The iteration process continues until the convergence criterion $\varepsilon_{GH}^{(v)}$ (Eq. 2.13) no longer changes between iterations (i.e., all layers have reached a satisfactory fit), or after a specified number of iterations (we chose 3000).
Besides the soil water content measurements and the rainfall, the input information required is the soil hydraulic parameters.

2.2.3 Generation of synthetic reference data

We used synthetic time series of volumetric soil water content with a measurement frequency of 1h, 3h, 6h, 12h and 24h. The time series of soil water content as well as the sink term profiles were generated with a soil water flow model (Fast Richards Solver, Ross, 2003, same as used in section 2.2.2 for the *im*). These were treated as measured data and are used as the basis for all methods. The synthetic data are based on meteorological and soil data from the Jena Biodiversity Experiment (Roscher et al., 2011). Root water uptake was calculated using a simple macroscopic root water uptake model which uses an exponential root distribution with water stress compensation (Li et al., 2001). Soil evaporation is taken as 20% of total evapotranspiration.

The soil profile is based on the Jena Experiment, both in terms of measurement design and soil properties. The model was set up for a one-dimensional homogeneous soil profile 220 cm deep. Measurement points were set at depths of 15 cm, 30 cm, 60 cm, 100 cm, 140 cm, 180 cm and 220 cm. The spatial resolution of the soil model is according to the measurement points 15-15-30-40-40-40-40 cm. The advantage of the applied soil water flow model is that the water fluxes are calculated with the matrix flux potential (Kirchhoff transformation), which allows for spatial discretization with large nodal spacing (Ross, 2006). We used a maximum rooting depth of 140 cm, with 60% of root length density located in the top 15 cm of the root zone, which corresponds to mean values measured on the field site (Ravenek et al., 2014). We used van Genuchten soil hydraulic parameters (van Genuchten, 1980) derived from the program ROSETTA (Schaap et al., 2001) based on the texture of a silty loam: $\theta_s = 0.409$ (cm^3 cm^{-3}), $\theta_r = 0.069$ (cm^3 cm^{-3}), $K_{sat} = 1.43\text{e-}6$ (m s^{-1}), $\alpha = 0.6$ (m^{-1}) and $n_{vG} = 1.619$ (-).

Upper boundary conditions are derived from measured precipitation and potential evapotranspiration calculated after Penman-Monteith (Allen et al., 1998) from measurements of the climate station at the experimental site (Weather Station Saaleaue, Max Planck Institute for Biogeochemistry - http://www.bgc-jena.mpg.de/wetter/). The weather data used have a measurement resolution of 10 minutes. Before applying evapotranspiration and rainfall as input data to generate the synthetic reference soil moisture and root water uptake data, both data sets were aggregated to the temporal resolutions applied for the reference run (1 hour). Soil moisture and root water uptake were generated with the same temporal resolution. When translating the evapotranspiration into sink term profiles (four-digit precision), rounding errors introduce a small inaccuracy. Thus, the sum of the sink term in the reference run deviates by 0.02% compared to the original evapotranspiration.

The lower boundary is given by the groundwater table, which fluctuates around -200 cm at the field site, but was set to constant head for simplification. Initial conditions are taken as the equilibrium (no flow) hydraulic potential profile in the soil.

We run the model with precipitation data from the field site for the year 2009, starting on 1 January to calculate time series of soil water content and the root water uptake up to September 2009. The atmospheric boundary conditions during the growing season are shown in Fig. 2.2 (a) as daily values. For testing the methods, we used the period from 26 July to 28 August 2009, which covers a dry period with little rainfall (Fig. 2.2, black-outlined area). The times were chosen to cover a representative but dry period during the growing season and to guarantee a warm-up phase for the soil model.

The described forward simulation produces time series of soil water contents and root water uptake. Soil water content time series were used instead of measured data (synthetic measurements) as input for the investigated methods, while evapotranspiration and sink term profiles were used to evaluate them, based on the quality criteria described in section 2.2.5.

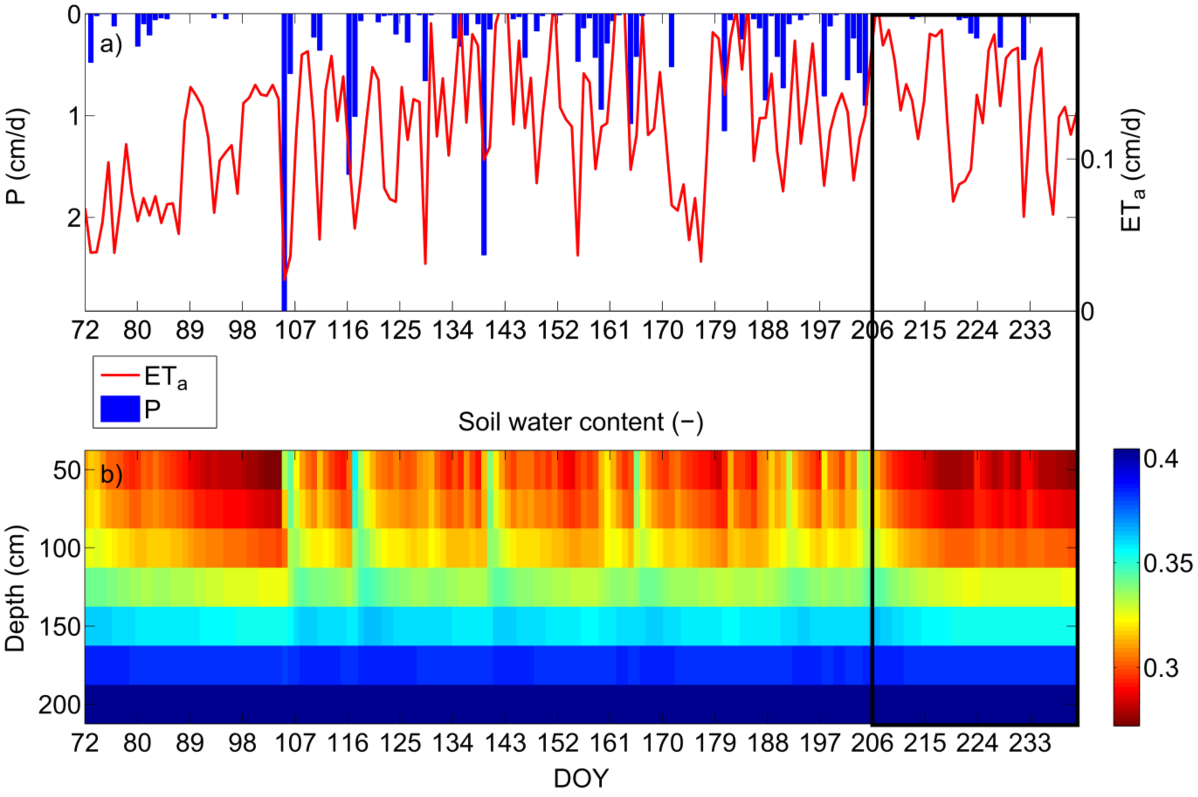


Figure 2.2 Actual evapotranspiration (ET$_a$) and precipitation (P) (cm day^{-1}) in the growing season (from March 2009 to September 2009) (a) and synthetic time series of soil water content (b) with daily resolution.

2.2.4 Influence of soil moisture sensor uncertainty

Data-driven methods are as good as their input data. Therefore, we investigate and quantify the influence of common uncertainties of soil moisture sensor measurements on the estimation of sink term profiles. Sensor performance is usually characterized by three criteria, namely: the accuracy, the precision and the resolution. The correctness of a measurement is described by the accuracy and for water content sensors depends greatly on the soil-specific calibration. Repeatability of many single measurements is referred to as precision, while the resolution describes the fineness of a measurement.

In this paper, we investigated the uncertainty of the applied methods stemming from calibration error (accuracy) and precision. For this we superimposed the original synthetic soil water content measurements generated in section 2.2.3 with artificial errors. Three types of errors were implemented, as follows (i) Precision error: the time series for each soil layer were perturbed with Gaussian noise of zero mean and standard deviation of 0.067 vol.% corresponding to a precision of 0.2 vol.%; (ii) calibration error: the perturbed time series were realigned along a new slope, which pivoted around a random point within the measurement range and a random intercept within ± 1.0 vol.%; (iii) calibration and precision: perturbed series were created as a random combination of (i) and (ii), which is a common case in field studies (Spank et al., 2013). Errors were applied independently to all soil depths, and 100 new time series were created for each of the error types. We determined the quality of the estimation methods using the median of 100 ensemble simulations with the 100 perturbed input time series. The values for the applied calibration uncertainty and precision are taken from the technical manual of the IMKO TRIME©-PICO32 soil moisture sensor (http://www.imko.de/en/products/soilmoisture/soil-moisture-sensors /trimepico32).

A common procedure with environmental measurements for dealing with precision errors is smoothing of the measured time series (Li et al., 2002; Peters et al., 2013), which we also reproduced by additionally applying a moving average filter on the disturbed soil moisture time series.

2.2.5 Evaluation criteria

A successful model should be able to reproduce the first and second moment of the distribution of the observed values (Gupta et al., 2009), and we used a similar approach to assess the quality of the methods for estimating the total evapotranspiration and the sink term profiles. The first and the second moment refer to the mean and the standard deviation. Additionally, the correlation coefficient evaluates whether the model is able to reproduce the timing and the shape of observed time series. To compare the applicability and the quality of the four methods we use three performance criteria suggested by Gupta et al. (2009): (i) the correlation coefficient (R), (ii) the relative variability measure (RV) and (iii) the bias (b), which are described in this section. The comparison is based on daily values.

First, we use R to estimate the strength of the linear correlation between estimated (~) and synthetic values:

$$R = \frac{\mathrm{Cov}(\tilde{x},x)}{s_x \cdot s_{\tilde{x}}}, \qquad (2.14)$$

where “Cov” is the covariance of estimated and observed (synthetic) values, and s_x and $s_{\tilde{x}}$ are the standard deviations of synthetic and estimated values, respectively. The variable x stands for any of the variables of interest, such as total evapotranspiration or $z_{25\%}$. R ranges between -1 and +1. The closer R is to 1, the better the estimate.

Second, we use the relative variability in estimated and synthetic data (RV) to determine the ability of the particular method to reproduce the observed variance (Gupta et al., 2009):

$$\mathrm{RV} = \frac{s_{\tilde{x}}}{s_x}. \qquad (2.15)$$

RV values around 1 indicate a good estimation procedure.
Third, we use the relative bias (b) to describe the mean systematic deviation between estimated (~) and observed (synthetic) values, which is not captured by *R:*

$$b = \frac{\bar{\tilde{x}} - \bar{x}}{\bar{x}} \cdot 100 \ (\%) \ , \qquad (2.16)$$

where $\bar{\tilde{x}}$ and $\bar{x}$ are the means of the estimated and synthetic data, respectively. The best model performance is reached if the bias is close to zero.

2.3 Results

In total, we compared synthetic evapotranspiration rates from 33 consecutive days in July/August 2009. Evapotranspiration could not be estimated for days with rainfall using either the *sssl* or *ssml* method, nor with the *msml* regression. Therefore, we excluded all days with rainfall from the analysis for all considered methods. In sections 2.3.1 and 2.3.2 we first consider the performance of the estimation methods on undisturbed synthetic time series, i.e., we ignore measurement errors or assume they do not exist. The influence of measurement errors is investigated in section 2.3.3.

2.3.1 Evapotranspiration derived by soil water content measurements

The performance of the data-driven methods depends strongly on the complexity of the respective method, which substantially increases with a higher degree of complexity. However, the influence of the measurement frequency differs considerably among the four methods.

The *im* predicted the daily evapotranspiration for a measurement frequency of 12 h with a very small relative bias of 0.89 %, which is the best value of all investigated methods. Additionally, the *im* reaches the best R value ($R = 0.99$) for all measurement frequencies (Tab. 2.2), and closely follows the 1:1 line between synthetic and estimated evapotranspiration (Fig. 2.3a, b). However, the RV and the relative bias indicate better prediction with decreasing measurement frequency.

Table 2.2 Comparison of the model performance of the four data-driven methods for reproducing daily evapotranspiration for the particular time resolution of soil moisture measurements. The model performance is expressed as correlation coefficient *R*, relative variability in simulated and reference values (RV), and relative bias (*b*) for the period 25 July to 26 August 2009. Days on which rainfall occurs were excluded for the data analysis.

	Single Step Single Layer Water Balance			Single Step Multi Layer Water Balance			Multi Step Multi Layer Regression			Inverse Model		
Δt (h)	*R*	RV	*b* (%)	*R*	RV	*b* (%)	*R*	RV	*b* (%)	*R*	RV	*b* (%)
1	0.77	1.51	-38.6	0.64	3.32	54.2	0.58	1.54	-22.9	0.99	0.78	-41.5
3	0.75	1.54	-38.6	0.66	3.37	46.8	0.71	1.03	20.3	0.99	0.97	-18.2
6	0.75	1.69	-35.9	0.67	3.52	36.4	0.78	1.87	86.5	0.99	1.03	-7.6
12	0.75	1.44	-38.6	0.70	3.49	37.1	0.85	4.22	202.4	0.99	1.04	0.89
24	0.58	1.76	-37.3	0.53	3.72	26.4	-	-	-	0.99	1.11	3.5

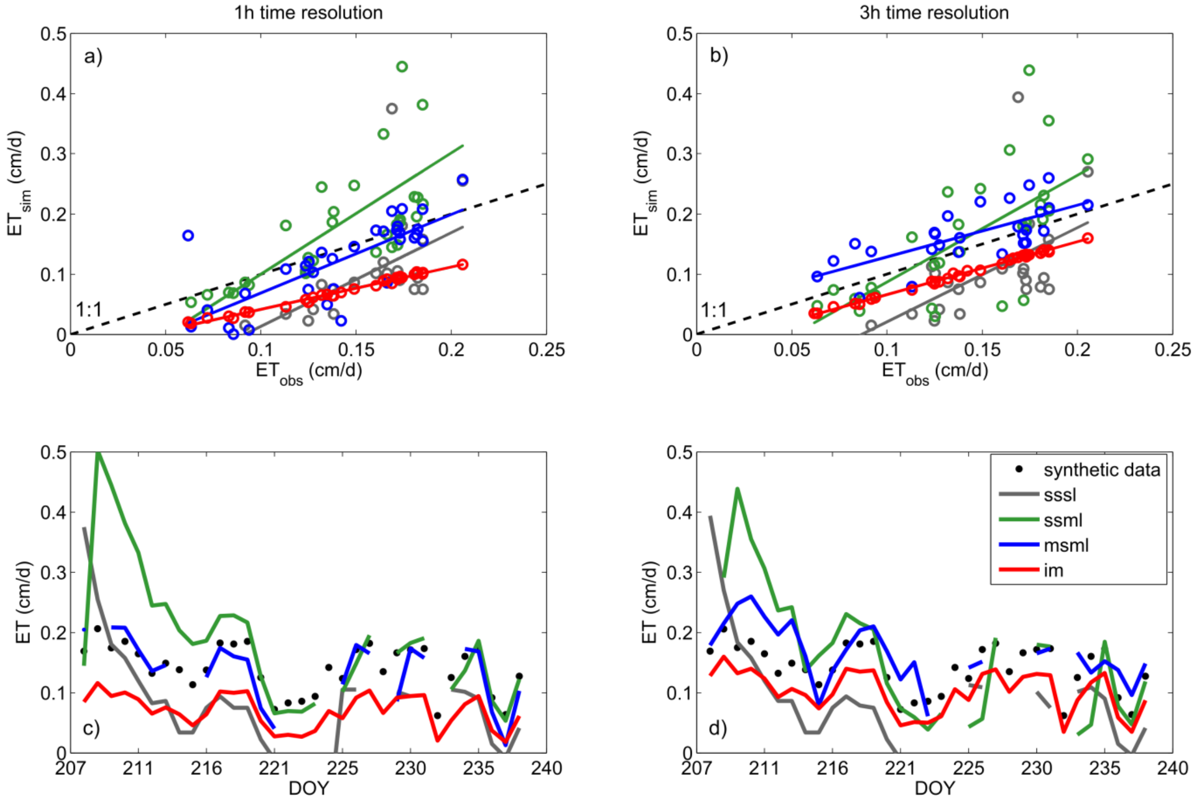


Figure 2.3 Top: comparison of synthetic (ET_{obs}) and estimated (ET_{sim}) values of daily evapotranspiration for hourly (a) and 3-hourly (b) observation intervals of soil water content measurements. Bottom: comparison of synthetic and estimated time series of daily evapotranspiration (ET) for hourly (c) and 3-hourly (d) observation intervals of soil water content measurements (25 July to 26 August 2009). Missing values are times when rainfall and percolation appeared. An estimation of evapotranspiration was not possible with the Single Step Single Layer Water Balance (sssl), the Single Step Multi Layer Water Balance (ssml) and the Multi Step Multi Layer Regression (msml) at these days.

The second-best method is the *msml* regression, in particular when applied for high temporal resolution measurements (1 and 3 hours). There, the bias is comparatively small (± 20%) and the correlation between synthetic (observed) and estimated values is relatively high ($R = 0.58$ and $R = 0.71$ for 1h and 3h resolution, respectively). Also, the *msml* results match the 1:1 line well between synthetic and estimated evapotranspiration (Fig. 2.3a, b).

The *sssl* and *ssml* methods show a weaker performance compared to the more complex *im* and *msml* methods. Neither of them follows the 1:1 line well between synthetic and estimated evapotranspiration (Fig. 2.3a, b). Regardless, they could reproduce the synthetic evapotranspiration with a relatively high linear correlation (Tab. 2.2), and comparable bias to the regression method, in particular for the range of intermediate measurement frequencies. However, values for the RV are comparatively large, in particular for the *ssml* method. Interestingly, the model performance criteria of the simpler *sssl* method show only minor differences between the particular temporal resolutions, and overall the *sssl* method performs better than *ssml* method. Note that both water balance methods (*sssl* and *ssml*) overestimate the evapotranspiration at the beginning of the study period (Fig. 2.3c and 2.3d), which was marked by greater vertical flow between top soil and deeper soil due to preceding rainfall events.

Our results also show that less complex data-driven methods, also perform better at higher temporal resolution (1 and 3 h), except for the *ssml* method. In contrast, the *im* is better in predicting evapotranspiration when a coarse measurement frequency is used. Further, the results indicate that the estimated actual evapotranspiration becomes more accurate with increasing model intricacy, and with vertical flow accounted for.

2.3.2 Root water uptake profiles estimated with three different data-driven methods

The *ssml*, *msml* and *im* method are appropriate for determining root water uptake profiles by inclusion of all available measurements over depth. Table 2.3 summarizes the model applicability to estimate the depths at which 25 %, 50 % and 90 % of water extraction occurs (later stated as $z_{25\%}$, $z_{50\%}$ and $z_{90\%}$). Here, we used the standard deviation $s_{\tilde{x}}$ instead of the relative variability to evaluate the observed variance. This criterion was chosen because the standard deviation of the synthetic reference values is approximately zero and thus the RV is increasing, which is not practical for the method evaluation. The criteria are shown for the respective best achieved model performance (1h – *ssml* and *msml*; 24h – *im*).

Again, the quality of predicting the sink term distribution depends on the method complexity and increases with increasing complexity. The most complex *im* delivers the best prediction of sink term distribution for a temporal resolution of 24 hours. The depths up to which 50 % of water extraction occurs ($z_{50\%}$) could be predicted with a bias of less than 2 % (Tab. 2.3) and for $z_{90\%}$; the relative bias increased only slightly to approximately 3 %. Indeed, these comparatively accurate results are to be expected due to the two intrinsic assumptions: (1) the required soil hydraulic parameters for the implemented soil water flow model are exactly known, and (2) the measurement uncertainty of the soil sensors is zero.

The regression method (*msml*) also delivers good estimations of sink term profiles over the entire soil column (Tab. 2.3 and Fig. 2.4), although it manages without any intrinsic assumptions. Figure 2.4 shows that the *msml* regression overestimates the sink term at the intermediate depths. The maximum relative bias is about -21% at $z_{50\%}$. Overall, the *msml* is applicable for determining the mean sink term distribution with an acceptable accuracy.

The *ssml*-estimated sink terms correspond only weakly to the synthetic ones, and the relative bias is lowest for $z_{25\%}$ with 33 % but increases strongly for $z_{50\%}$ and $z_{90\%}$ (Tab. 2.3). Moreover, the standard deviations of the predictions are substantial at most measurement depths (Tab. 2.3, Fig. 2.4). Because of these large variations in sink term distribution, the prediction of sink term profiles becomes imprecise. Thus, for the chosen simulation experiment, the *ssml* method is not applicable for deriving the sink term from soil water content measurements.

Table 2.3 Comparison of model performance for reproducing the sink term profile (Single Step Multi Layer Water Balance, Multi Step Multi Layer Regression and Inverse Model). Depths where 25, 50 and 90 % water extraction occurs were regarded. Mean synthetic (syn.) depth and mean estimated (est.) depth describe the mean depth over 33 days, where water extraction occurs. b is the relative bias and $\tilde{s}$ is the standard deviation of the estimated values. Larger width of the black arrow denotes higher accuracy of the model results.

Time resolution of measurements	Single Step Multi Layer Water Balance			Multi Step Multi Layer Regression			Inverse Model		
	1h			1h			24h		
Criterion	$z_{25\%}$	$z_{50\%}$	$z_{90\%}$	$z_{25\%}$	$z_{50\%}$	$z_{90\%}$	$z_{25\%}$	$z_{50\%}$	$z_{90\%}$
Mean syn. depth (cm)	8.1	17.1	55.6	8.1	17.1	55.6	8.1	17.1	55.6
Mean est. depth (cm)	10.8	28.5	101.9	9.7	13.9	63.8	8.2	17.3	57.3
b (%)	33	74	83	-14	-21	15	0.75	1.05	2.97
$\tilde{s}$	4.07	12.31	57.89	1.69	4.01	25.83	1.81	4.08	68.26

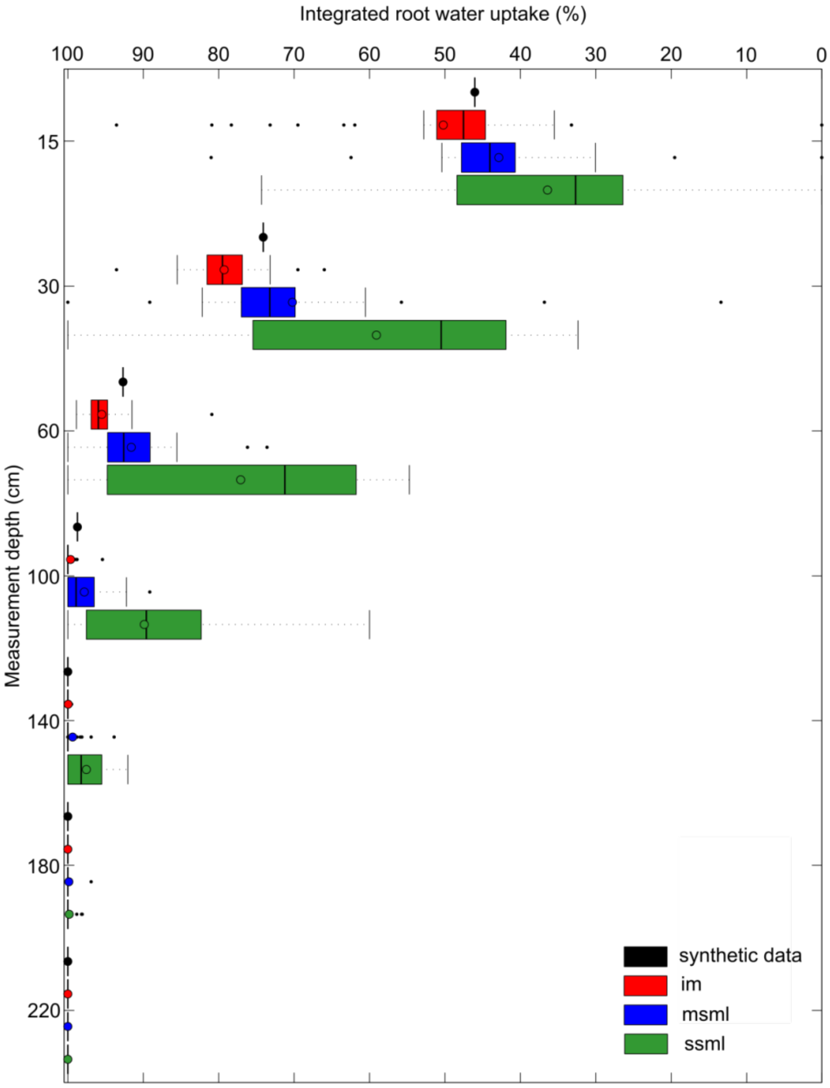


Figure 2.4 Box plots of the estimated daily percentage of integrated sink term. Colors are assigned as follows: synthetic values are black, the im is red, the msml is blue and the ssml water balance is green. The percentage of integrated sink term is shown for all measurement locations over the soil column. The circles show the mean values; the vertical line depicts the median and the 25% and 75% percentile. Values are given for the respective underlying time resolution which achieved the best results according to Table 3 (ssml - 1h; msml - 1h; im - 24h).

2.3.3 Influence of soil moisture sensor uncertainty on root water uptake estimation

We only evaluated the influence of measurement errors for two methods (*msml* and *im*). The single layer approach was omitted since it does not allow for estimation of the sink term profile and *ssml* was omitted, since the estimation of the sink term profile was already inappropriate when ignoring measurement errors (see section 2.3.2).

The influences of soil moisture sensor uncertainties differ considerably among the investigated methods. The *msml* method predicted the median daily evapotranspiration with precision uncertainty, calibration uncertainty and a combination of both reasonably well (Fig. 2.5). For all three types of uncertainty, the correlation between synthetic (observed) and estimated values is relatively high (around $R = 0.9$, Table 2.4). Also, with respect to the median relative bias (%) the three cases differ only marginally ($|\mathrm{b}| = 7\%$, Tab. 2.4). Interestingly, the calibration uncertainty showed the lowest impact on the predicted evapotranspiration with a median bias of about -5% for the respective 100 ensemble calculations (Fig. 2.5).

Additionally, the bias is also used to compare the predicted relative water extraction depths ($z_{25\%}$, $z_{50\%}$ and $z_{90\%}$) (Fig. 2.6). The uncertainty caused by the calibration of the sensor shows the least differences to the observed values below 10%. These results are similar to those from simulations with soil moisture without any introduced measurement uncertainty. Further, the uncertainties caused by the precision of the sensors have the highest impact on predicted root water uptake patterns. It turns out that the relative uncertainty increases with increasing depth (decreasing sink term or rather water extraction, Fig. 2.6a).

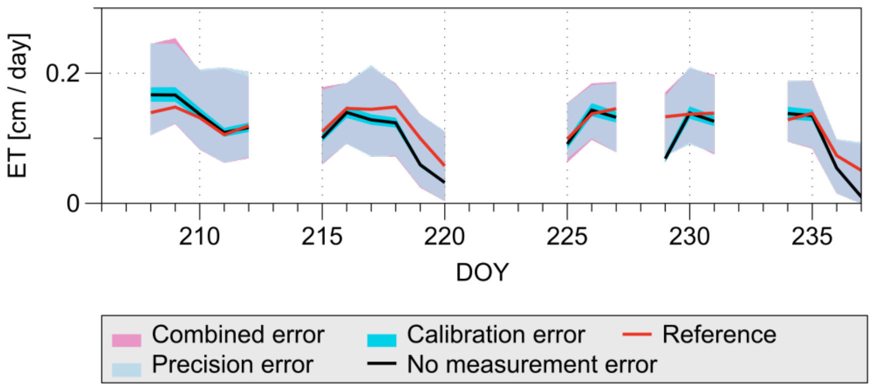
Interestingly, the *im* shows worse model performances than the *msml* regression for all three types of uncertainty. Although, the predicted evapotranspiration from soil moisture with precision uncertainty is close to the observed values (Fig. 2.5), it differs around days when rainfall occurs (DOY 225, 230 and 234). This results in underestimation of evapotranspiration during these times with a weak correlation (Tab. 2.4), but an acceptable relative bias of about -10%. In contrast, for the calibration uncertainty it is the other way around. Here, the correlation is relatively high ($R = 0.85$) but evapotranspiration is greatly overestimated ($b = 498\%$). A combination of both uncertainty sources does not further increase the overall error, but does combine both weaknesses to an overall poor estimation (Tab. 2.4).

Table 2.4 Comparison of the model performance with considering soil moisture measurement uncertainties for the msml regression and the im for reproducing daily evapotranspiration and the mean depths where 25 %, 50 % and 90 % water extraction occurs. The model performance is expressed as correlation coefficient (R), relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. The precision uncertainty is abbreviated as prec err, the calibration uncertainty as cali err and the combined uncertainty by com err. The relative bias for reproducing evapotranspiration is abbreviated with b_{ET}, and is abbreviated as $b_{25\%}$, $b_{50\%}$ and $b_{90\%}$ for reproducing mean depths where 25, 50 and 90 % water extraction occurs respectively.

Time resolution of measurements	Multi Step Multi Layer Regression 1h			Invese Model 24h		
Criterion	prec err	cali err	com err	prec err	cali err	com err
R	0.90	0.89	0.91	-0.027	0.847	-0.054
RV	1.35	1.50	1.35	1.51	1.25	1.85
Median bias b_{ET} (%)	-6.2	-4.9	-6.1	-10.3	498.1	483.3
Median bias $b_{25\%}$ (%)	19.6	3.6	19.5	25.2	531.1	405.1
Median bias $b_{50\%}$ (%)	28.0	5.4	27.7	42.0	622.4	659.1
Median bias $b_{90\%}$ (%)	80.8	27.7	84.7	128.5	757.6	569.0

The sensitivity to the type of uncertainty concerning prediction of sink term patterns is shown in Fig. 2.6b and Table 2.4. Similar to the *msml* regression, the *im* is able to handle uncertainties in sensor precision to predict root water uptake depths whereas uncalibrated sensors lead to considerable increases in relative bias. Overall, the simpler *msml* regression method shows a higher robustness against measurement uncertainties than the more complex *im.*

(a) Regression Model (msml)



(b) Inverse Model (im)

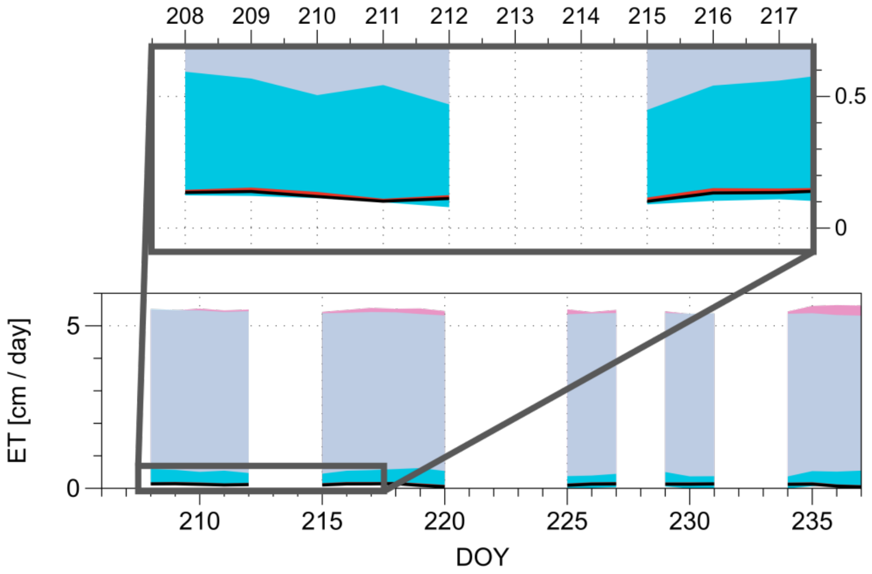


Figure 2.5 Influence of soil moisture uncertainty on evapotranspiration estimated with the Multi Step Multi Layer Regression (Regression Model - *msml*) (a) and the Inverse Model (*im*) (b). The red line is the evapotransiration from the synthetic data (Reference). The colored bands indicate the 95% confidence intervals.

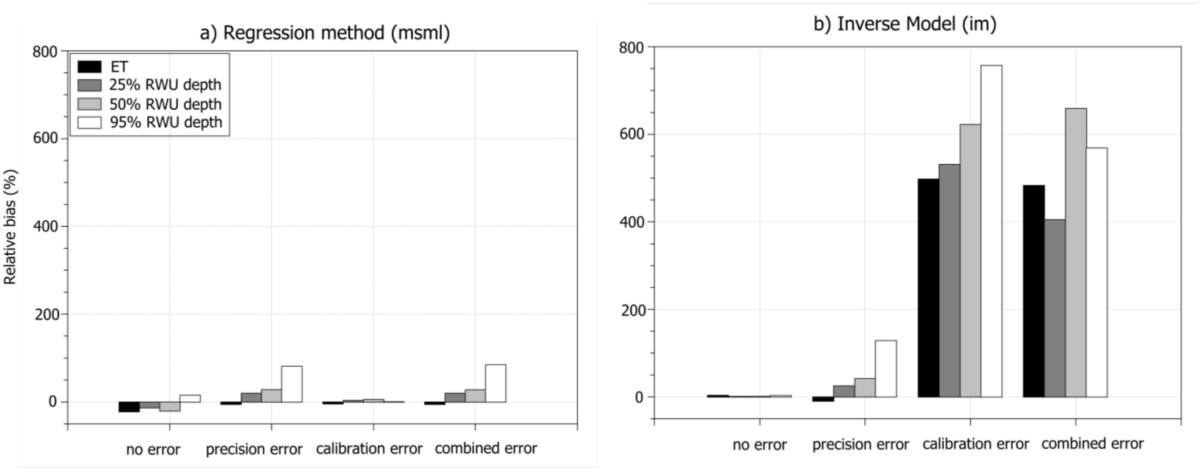


Figure 2.6 Comparison of the mean relative bias between synthetic and predicted values of evapotranspiration and the mean depths where 25, 50, 90% of water extraction occurs for soil moisture time series: without uncertainty (no error), precision uncertainty (precision error), calibration uncertainty (calibration error) and precision & calibration uncertainty (combined error) for the Multi Step Multi Layer Regression (Regression method - *msmsl*) (a) and the Inverse Model (*im*) (b).

2.4 Discussion

We tested the application of several methods deriving based on the soil water balance, how much water was extracted from the soil by evapotranspiration and how the extraction profile (sink term profile) changed with soil depth. The bases for all methods are time series of volumetric soil water content derived from measurements, although some methods require more information on soil properties, in particular the Inverse Model (*im*). None of the methods relies on a priori information on the shape of the sink term profile, nor do make any assumptions on it being constant with time. This is the great advantage of these methods over others (Dardanelli et al., 2004; McIntyre et al., 1995; Hopmans and Bristow, 2002; Zuo et al., 2002). Since only changes in soil water content are considered, none of the investigated methods distinguish between soil evaporation and root water uptake. For the same reason, none of the water balance methods can be applied during times of fast soil water flow, for example during or after a rainfall event.

We used synthetic soil water content “observations” to validate the model results. This procedure has the great advantage that the “true” water flow and sink term profiles are perfectly known, including the nature of data uncertainty with regard to calibration error and sensor precision. However, our model only accounts for vertical matrix flow, notably neglecting horizontal heterogeneity, which may be an additional challenge for deriving evapotranspiration in real-world situations. Thus, additional tests of the methods in controlled field conditions, like with large lysimeters, and comparison with additional data, like isotope profiles, are necessary to confirm our results.

In the first part of the paper, we investigated how well all methods reproduced the sink term profile and total evapotranspiration when assuming that the measurements of soil water content were free of measurement errors, i.e., they were well calibrated and measured precisely. Even in this idealistic setting, the investigated methods performed very differently, most prominently depending on whether or not vertical flow could be accounted for by the method. The methods showing the greatest deviation between the “observed” (synthetic) evapotranspiration and sink term profiles were those not accounting for vertical flow within the soil (*sssl* and *ssml* methods). In those simpler soil water balance methods, any change in soil moisture is assigned only to root water uptake (Rasiah et al., 1992; Musters et al., 2000; Hupet et al., 2002). However, even several days after a rainfall event, the vertical matrix flow within the soil can be similar in magnitude to the root water uptake (Schwärzel et al., 2009), and this leads to considerable overestimation of the sink term when soil water flow is not accounted for. This error adds up, when the sink term is integrated over depth and leads to a substantial bias in the evapotranspiration estimate, which is the case for the *ssml* method.

This distinction between vertical soil water flow and water extraction is the major challenge when applying water balance methods, because these fluxes occur concurrently during daytime (Gardner, 1983; Feddes and Raats, 2004). The regression method (*msml*) avoids this problem by considering vertical soil water fluxes, estimated from change in soil water content during nighttime. Li et al. (2002) used a similar approach to derive transpiration and root water uptake patterns from soil moisture changes between different times of the day. This direct attribution of nighttime change in soil water content to soil water flow inherently assumes that both nighttime evapotranspiration and hydraulic redistribution are negligible. Li et al. (2002) measured nocturnal sap flow in order to ascertain that nighttime transpiration was insignificant. Also, in lysimeters, the weight changes can be used to validate the assumption. This assumption is the main drawback of this method, which in contrast to the large great advantage that it requires very limited input data, especially no a priori information on soil properties. In contrast, the *im* approach inferred evapotranspiration and sink term patterns with greater quality when soil water content measurements were free of error.

However, because our analysis uses model-generated time series of soil water content in order to mimic measurements, the soil properties of the original "experiment" are completely known, which is not usually the case in natural conditions. Usually, soil hydraulic parameters have to be estimated by means of a calibration procedure. This process is non-trivial and limited by the non-uniqueness of the calibrated parameters (Hupet et al., 2003), which results in uncertainties in simulated soil water fluxes and root water uptake rates (Duan et al., 1992; Musters and Bouten, 2000; Musters et al., 2000; Hupet et al., 2002; Hupet et al., 2003). This reliance of the *im* approach on precise knowledge of the soil environment is the main drawback of that approach.

Several studies on estimation of root water uptake profiles focused on uncertainties related to calibrated parameters of soil and the root water uptake models (Musters and Bouten, 2000; Musters et al., 2000; Hupet et al., 2002; Hupet et al., 2003). When data and models are used, uncertainties arise not from soil parameter uncertainty alone but in fact already evolve during the measurement process of the environmental data (Spank et al., 2013). Thus, in the second part of this paper, we investigated how measurement noise (precision), wrong sensor calibration (accuracy) and their combination reflect on the derivation of evapotranspiration and sink term patterns from soil water content measurements. We only performed this analysis for the two methods which performed satisfactorily without sensor errors: the *msml* regression method and *im*. In this more realistic setting, the simpler regression method (*msml*) performed much better than the *im*. The latter was strongly affected by inaccurate or lack of site-specific calibration. This "calibration error" renders the evolution of the vertical potential gradients and soil moisture profile inconsistent with the evolution of the vertical sink term distribution, and thus introduces forbidding overestimation of root water uptake and evapotranspiration for the considered time steps (Fig. A.2). Generally, the prediction of the *im* improves when longer evaluation periods are considered (cf. Zuo and Zhang, 2002) and therefore the calibration error may become less prominent when considering time steps of several days as done in Zuo and Zhang (2002). Compared to the effect of calibration, the sensor precision had a much smaller effect. Thus, the *im* may be applicable and should be tested in situations where all sensors in the profile are well calibrated. A further improvement of the *im* could be achieved by smoothing the measured soil water content profiles via a polynomial function to get an accurate and continuous distribution of soil water contents as done in Li et al. (2002) and Zuo and Zhang (2002).

The *msml* regression method was overall more robust towards the investigated measurement errors. It was barely affected by calibration error but was somewhat affected by sensor precision. This is expected, since the sensor calibration only improves the absolute values of the measurements, and does not affect the course of the soil moisture desiccation. The case is different for uncertainty due to sensor precision, which results in higher deviations between observed and predicted sink term uptake patterns (Fig. 2.6). As this method uses linear regression on the temporal evolution of soil water contents, the quantity of root water uptake depends on the gradient of the slopes. Those slopes are strongly influenced by the random scatter of data points, which is characteristic for sensor noise. Using the smallest time step of 1h, we could estimate the relative depth where 50% of water extraction occurs with a bias less than 30%. Using higher time resolution with several measurements per hour or several minutes and noise-reducing filters (Li et al., 2002; Peters et al., 2013) would likely further improve this result. This method should be further evaluated with lysimeters in order to test its application in controlled but more realistic environments.

Furthermore, our study demonstrates that measured soil moisture time series already include information on evapotranspiration and root water uptake patterns. This has already been stated by Musters and Bouten (2002) as well as Zuo and Zhang (2002). Contrary to these studies, where only temporal resolutions of 1 day or more are investigated, we additionally looked at measurement time intervals in the range of hours. Our results confirm that different methods require measurements with different temporal resolutions. The more simple *msml* regression method showed better applicability for measurements taken with an interval less than 6 hours. These results are similar to Breña Naranjo et al. (2011) for a water balance method. The higher time resolution better reflects the temporal change in evapotranspiration, which may be considerable over the course of a day (Jackson et al., 1973). Conversely, the *im* works better for coarser temporal resolution for the case that soil water content measurements are error-free. If a possible measurement error is considered, coarser temporal resolutions are also better suitable to estimate evapotranspiration and root water uptake. With a higher temporal resolution (here 1 day instead of several hours) the total evapotranspiration and sink term also increases (integrated over the entire time). Therefore, the iteration of the *im* procedure could determine the sink term with a higher accuracy.

Another important prerequisite besides temporal resolution of the soil moisture time series is the adequate number of soil moisture measurements over the entire soil column to well capture the very nonlinear depth profile of water removal from the soil. This becomes most obvious when comparing the results from the simple single layer water balance method (*sssl*) with the multi layer (*ssml*) one. The prediction of the single layer model is dominated by the specific depth at which the single sensor is located, and how much it is affected by root water uptake. In the presented case it strongly underestimated overall evapotranspiration because it observes only one part of the sink term profile, and omits both the much more elevated uptake in the top soil and the deep uptake below the measurement depth. In contrast to that, the multi-layer method reproduces better the time series of evapotranspiration, because it samples the uptake profiles more holistically. Similarly, Schwärzel et al. (2009) and Clausnitzer et al. (2011) also found that high spatial resolution of water content sensors allow for a more reliable determination of evapotranspiration. Important consideration should be given to the very shallow soil depths, representative of the pure soil evaporation process ($z < 5$ cm), which are notoriously undersampled due to technical limitations. This may lead to underestimation of evaporation and therefore evapotranspiration in all investigated water balance applications.

Our results show that water balance methods have potential to be applied for derivation of water extraction profiles, but they also suggest that their application may be challenging in realistic conditions. In particular, the *im* has great potential, in theory, but obtaining information of the soil environment with sufficient accuracy may be unrealistic. The *msml* regression method is particularly promising, as it requires little input and is comparably robust towards measurement errors. Further tests in controlled environments and ideally in concert with isotope studies should be conducted to further test the application of these methods in real-world conditions.

The great advantage of all considered methods is that they do not require a priori information about total evapotranspiration or the shape of the root water uptake profiles. Root water uptake moves up or down depending on soil water status (Lai and Katul, 1998; Li et al., 2002, Doussan et al., 2006; Garrigues et al., 2006), and many existing approaches are unable to account for this dynamic of root water uptake. Root water extraction profiles are central topics in ecological and ecohydrological research on resource partitioning (e.g., Ogle et al., 2004; Leimer et al, 2014; Schwendenmann et al., 2014) and drivers for ecosystem structure (Arnold et al., 2010). Water balance methods are potential tools for comparing those extraction profiles between sites and thus contributing to ecohydrological process understanding.

2.5 Conclusions

The aim of this study was to evaluate four water balance methods of differing complexity to estimate sink term profiles and evapotranspiration from volumetric soil water content measurements. These methods do not require any a priori information of root distribution parameters, which is the advantage compared to common root water uptake models. We used artificial data of soil moisture and sink term profiles to compare the quality of the estimates of those four methods. Our overall comparison involve the examination of the impact of measurement frequency, and model intricacy as well as the uncertainties of soil moisture sensors on predicting sink term profiles. For the selected dry period of 33 days and under consideration of possible measurement uncertainties the Multi Step Multi Layer Regression (*msml*) obtained the best estimation of sink term patterns. In general, the predictions with the four data-driven methods show that these methods have different requirements on the measurement frequency of soil moisture time series and on additional input data like precipitation and soil hydraulic parameters. Further, we were able to show that the more complex methods like the *msml* regression and the Inverse Model (*im*) predict evapotranspiration and the sink term distribution more accurately than the simpler Single Step Single Layer Water Balance (*sssl*) and the Single Step Multi Layer Water Balance (*ssml*).

Unfortunately, the estimations of the *im* are strongly influenced by the uncertainty of measurements. Moreover, numerical soil water flow models like the *im* require a large amount of prior information (e.g., boundary conditions, soil hydraulic parameters) which is usually not available in sufficient quality. For example, the soil hydraulic parameters have to be calibrated before use, which introduces additional uncertainties in the parameter sets. It is important to keep this in mind while comparing the *im* with the *msml* regression method, especially in light of the influence of measurement uncertainties.

Our results show that highly resolved (temporal and spatial) soil water content measurements contain a great deal of information, which can be used to estimate the sink term when the appropriate approach is used. However, we acknowledge that this study using numerical simulations is only a first step towards the application on real field measurements. The *msml* regression method has to be tested with real field data, especially with lysimeter experiments. Lysimeters allow for closing of the water balance and validation with measured evapotranspiration, while soil water content measurements can be conducted in a similar way to field experiments. With such experiments, the proposed method can be evaluated in an enhanced manner.

Chapter 3

Evaluation of the *msml* method on a lysimeter study

3 Evaluation of the Multi Step Multi Layer Water Balance on a lysimeter study

Abstract

Root water uptake is an important component in the soil water balance and it is essential in various research disciplines, especially in eco-hydrology to understand plant-soil water relations and ecosystem functioning. The Multi Step Multi Layer Regression (*msml*) proposed in Chapter 2 is a simple and straightforward method for estimating water uptake profiles and evapotranspiration based on volumetric soil water content measurements without a priori information on root distribution properties. Since the *msml* was only tested on a numerical study, we conducted an additional accuracy assessment on lysimeter experiments to verify the functioning of the method on a long-term grassland biodiversity experiment (Jena Experiment). Therefore, we employed measurements of soil moisture from 12 weighable lysimeters. Additionally, we used stable water isotope measurements to double-check the water uptake profiles estimated with the *msml* method. Our results showed that about 79 % of the measured evapotranspiration could be explained by the *msml* method. Best predictions could be reached on days with high evapotranspiration respectively soil water depletion. We found that the *msml* method is insensitive to different soil textures. Furthermore, sensor imprecision has no effect on the quality of predictions when an adequate filter routine is applied on the raw soil moisture measurements. This demonstrates that the *msml* method can be applied on real field data, especially for the comparison of root water uptake profiles of different ecosystems.

3.1 Introduction

Root water uptake is an important component in the soil water balance and thus together with evapotranspiration (*E*) one of the major components in the hydrological cycle (Hupet, 2003; Nachabe et al., 2005; Willingen et al., 2005). Consequently, both processes are important in various research disciplines like meteorology, hydrology, ecology and especially in eco-hydrology, in particular to understand plant-soil water relations and ecosystem functioning (Davis and Mooney, 1986; Le Roux et al., 1995; Jackson et al., 1996; Wilson et al., 2001; Hildebrandt and Eltahir, 2007; Arnold et al., 2009; Schwendenmann et al., 2014; Guderle and Hildebrandt, 2015). Hence, a wide range of methodologies exist for estimating root water uptake and actual evapotranspiration, each of them operating across different spatial and temporal scales and with different accuracies (Wilson et al., 2001; Drexler et al., 2004; Fahle et al., 2014; Guderle and Hildebrandt, 2015). An overview was already given in Chapter 2.

Methods like the soil water balance are frequently used since they are simple and straightforward (e.g. Wilson et al., 2001; Hupet et al., 2002; Schume et al., 2005; Willingen et al., 2005 among others) and they only require measurements of volumetric soil water content (Hupet 2003). Here, evapotranspiration and root water uptake are calculated by the soil water storage difference between two observation times (Hupet et al., 2002; Willingen et al., 2005; Guderle and Hildebrandt, 2015). One major drawback of the soil water balance method is the neglect of soil water fluxes (Hupet et al., 2002; Guderle and Hildebrandt, 2015). An alternative are methods like the Multi Step Multi Layer Regression (*msml*) introduced in Chapter 2 since they are as simple as the soil water balance but are able to decouple soil water fluxes from evapotranspiration. This is possible due to the assumption that soil water fluxes are constant over a 24h-period and thus, they can be estimated during nighttime where evapotranspiration is assumed to be zero (Li et al., 2002; Nachabe et al., 2005; Guderle and Hildebrandt, 2015).

Nevertheless, a rigorous accuracy assessment is necessary to validate the method and to get an overview of the uncertainties as well as their sources occurring in natural applications. Nachabe et al. (2005) compared a similar approach (*TSM* - Total Soil Moisture method) with estimates from pan evapotranspiration and found a good agreement characterized by a R^2 of 0.78. In contrast, Li et al. (2002) derived root water uptake rates of corn, which matched very closely hourly sap flow rates. A more detailed examination was done by Guderle and Hildebrandt (2015) using synthetic data where the influence of measurement frequencies and sensor uncertainties on the estimated evapotranspiration and water uptake profiles was investigated. It was shown that the *msml* has great potential for predicting the evapotranspiration and root water uptake during periods without rainfall. However, the results were obtained based on a numerical study and a validation with experimental data was still missing. Whereas the water flow, evapotranspiration and water uptake profiles are known in numerical studies, these components are notoriously unknown under field conditions. To close the gap between numerical and field experiments, weighable lysimeters are well suited to calibrate and evaluate water balance methods and water transport models (Durner et al., 2008; Schelle et al., 2012) since they deliver a precise and realistic measure of evapotranspiration by registration of weight changes (Meissner et al., 2008; von Unhold and Fank, 2008; Allen et al., 2010; Peters et al., 2013).

A further source of uncertainty is related to the upscaling of estimated evapotranspiration based on soil moisture measurements to the field-scale, as they cover only a few dm^2 compared to an entire ecosystem (Hupet, 2003). Therefore, due to their transpiring surface area up to two m^2 and the registration of the evapotranspiration rate from this particular surface, lysimeter measurements are ideally suited to test for upscaling as well. Thus, project frameworks like the TERENO-SoilCan project with more than 120 lysimeters at different sites (Pütz et al., 2011; Schelle et al., 2012) or the Jena-Ecotron project with 12 lysimeters from different diverse grassland ecosystems (Milcu et al., 2014) enable the investigation of the influence of soil texture and sensor uncertainties on soil moisture measurement based methods like the *msml*.

The objective of this Chapter is to evaluate the *msml* method for predicting evapotranspiration and water uptake profiles on real field data. Following up on the analysis of Chapter 2 an accuracy assessment considering texture variability, sensor uncertainty, magnitudes of evapotranspiration and implicitly upscaling is carried out. Therefore, we employed measurements of soil moisture from 12 weighable lysimeters from the Jena-Ecotron project and verify them with measured evapotranspiration data. Additionally, we use stable water isotope measurements to double-check the water uptake profiles estimated with the *msml* method.

3.2 Material and Methods

3.2.1 Lysimeter set up in the CNRS Ecotron facility

Twelve lysimeter (2 m^2, diameter of 1.6 m, 2 m height with a weight of 7-8 tonnes) were excavated at the Jena Experiment field site in Dezember 2011. The lysimeters were buried to the top edge near the experimental field, before being transported to the Ecotron facility in March 2012. This allowed recovering after excavation disturbances (Milcu et al., 2014). The Jena Experiment is a long-term grassland biodiversity experiment located on the floodplain of the Saale River in Jena, Germany (50° 55´ N, 11° 35´ E, 130 m above sea level). Mean annual precipitation is 587 mm and mean annual temperature is 9.3 °C (Kluge and Müller-Westermeier, 2000). The experiment was established in 2002 and the site was previously used as arable land. The experiment consists of 82 plots (20x20 m), which are subdivided in four blocks according to the variation of soil texture from sandy loam near the river to silty clay with increasing distance from the river. The 82 plots consist of different plant species richness varying from 1-60 species and four functional groups (grasses, tall and small herbs and legumes) typically for the local *Arrhenatherion* grasslands (Roscher et al., 2004). The lysimeter were taken from plots equally distributed across the Jena Experiment to consider the differences in the soil texture.

The Montpellier European Ecotron is a new experimental infrastructure developed by the Centre National de la Recherche Scientifique (CNRS, France) to study the response of ecosystems to global change (Milcu et al., 2014). For this experiment we took advantage of the Macrocosm platform, which consist of 12 controlled environment units (30 m^3 dome), each exposed to natural light and UV radiation owing to the 250 µm thick Teflon-FEP film (DuPont, USA) which covers each lysimeter (Milcu et al., 2014). A simplified schematic of one Ecotron dome and the lysimeter setup is shown in Fig. (3.1). The domes enable the controlling of air temperature, CO_2 concentration and humidity while the plant canopy and soil surface is still exposed to natural sunlight. Each lysimeter system consists of a soil monolith based on a balance (4 CMI-C3 shear beam load cells, Precia-Molen, Privas, France; accuracy: ± 300 g) and is equipped with soil moisture sensors (design is described in Section 3.2.3) and a soil temperature control system. Further, a constant groundwater table was adjusted by a Mariott's bottle and controlled by two T8 tensiometer (UMS Munich, Germany) installed in 165 cm and 180 cm below ground (Fig. 3.1). For the vegetative growing season 2012, beginning in end of March, the lysimeters were kept under controlled conditions. The experiment was terminated end of July by a destructive harvest. The adjusted climate was similar to the average climatic conditions at the Jena Experiment field site in 2007. As there are differences in incoming solar radiation between Jena and Montpellier (37 % lower in Jena), the radiation was reduced by a black shading mesh by 44 %, which was installed in each dome. Additional information on the experimental design and the Ecotron facility are given in Milcu et al. (2014).

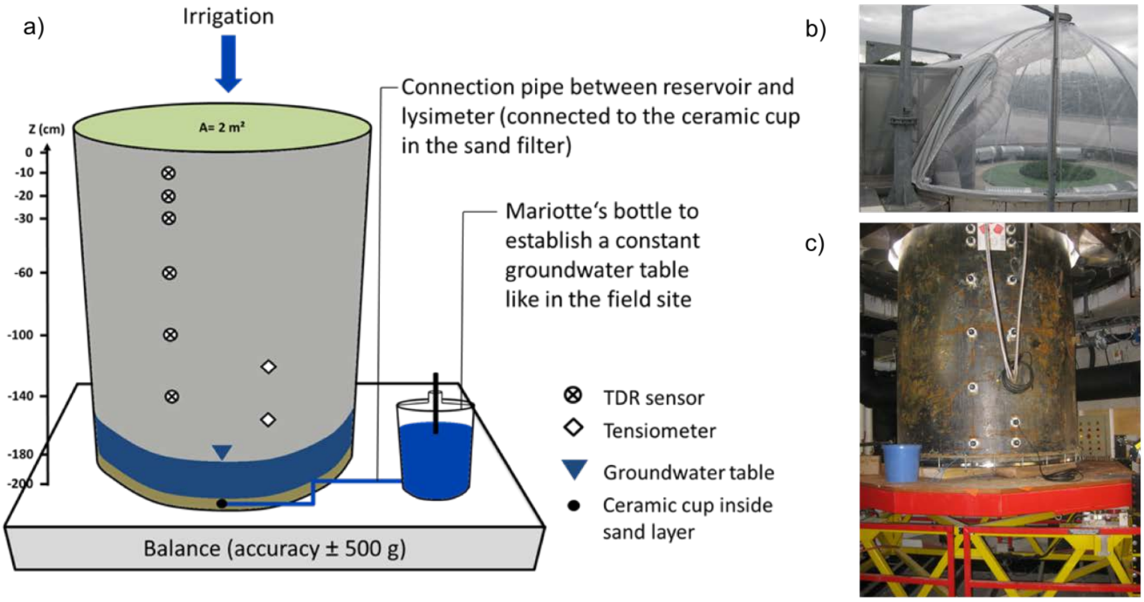


Figure 3.1 Schematic diagram of the experimental setup and the instrumentation of the lysimeters in the CNRS Ecotron (a), the UV radiation and light transparent Teflon-FEP dome (b) and one representative lysimeter chamber during sensor installation (c).

3.2.2 Multi Step Multi Layer Regression (msml)

The Multi Step Multi Layer Regression (*msml*) was used to estimate evapotranspiration (E_{msml}) and sink term profiles from diurnal fluctuation of soil water content measurements (Li et al., 2002; Guderle and Hildebrandt, 2015) (Fig. 3.2 a). It applies a regression over multiple time steps on soil moisture time series of each measurement depth. Here we used measurements in 10 cm, 20 cm, 30 cm and 60 cm as we found no changes in soil moisture due to transpiration in the deeper soil layers and these depths are consistent with the measurement depths of stable isotopes (Section

3.2.6). The transpirational time is defined by the activity of plant stomata or rather by their opening and closure, which is driven by the supply of solar energy (Loheide, 2008; Maruyama and Kuwagata, 2008; Sánchez et al., 2013). We defined the transpirational time between 05:00 am until 06:30 pm. The major assumption of the *msml* is that the soil water fluxes do not change significantly between day and night. As in several nights the lysimeters registered evapotranspiration, we excluded these nights for estimation of soil water fluxes, which entails that the depletion of soil moisture during daytime is assumed to be caused by evapotranspiration only. Furthermore, we assume that the estimated evapotranspiration represents evapotranspiration from a surface of one m^2 and thus multiplied the results by the factor two for upscaling to the surface of the lysimeters of two m^2. As irrigation causes rapid changes of soil water contents the *msml* is only applied during dry periods (Fig. 3.2 b). A detailed description and method evaluation can be found in Section 2.2.2 and in Guderle and Hildebrandt (2015).

3.2.3 Soil water content measurements

Volumetric soil water content was measured with the TDR (Time Domain Reflectometry) sensor TRIME®-PICO 32 (IMKO Micromodultechnik GmbH, Germany) in six depths (10 cm, 20 cm, 30 cm, 60 cm, 100 cm, and 140 cm) below ground. Since soil water contents below 60 cm did not change, they were not included in this study. The measurements were taken from mid of June to end of July 2012 with a temporal measurement resolution of one minute. The sensors were installed in such a way that each of the sensor rods had a distance of 22 cm to the edge of the steel cylinder of the lysimeter. To reduce measurement errors due to the precision uncertainty of the TDR sensors, we processed the raw data with two filter routines. First, we applied a moving average with a window width of 30 minutes to eliminate all values, which are greater or smaller than a given threshold y

$$y_j = \bar{x}_j \pm 1.5 \cdot s_j, \tag{3.1}$$

where $\bar{x}$ is the mean value of volumetric soil water content within the respective window width, s is the standard deviation within the respective window width and j is the time step. This filter routine enables the removing of outliers in the time series of measured soil moisture. Subsequently, we applied a second filter routine to reduce the common measurement noise of the TDR sensors. For this, we used a Savitzky-Golay FIR smoothing filter of third order over 241 minutes for 10 cm and 20 cm depth and additionally a moving average over 721 minutes for 30 cm and 60 cm. The latter procedure was necessary because soil moisture changes over one day were small in these depths and thus precision uncertainty has a higher influence on the applied msml method for estimating root water uptake profiles (Chapter 2; Guderle and Hildebrandt, 2015). Furthermore, the measurements of soil water content in the lysimeters showed unclear abnormalities/disturbances in their course like jumps over several time steps (some hours up to one day), which occurred over all measurement depths (Fig. 3.2 c & d). Hence, these days where excluded for the application of the *msml* method since these disturbances could be hardly adjusted by smoothing functions (Fig. 3.2 c) and lead to errors in estimated root water uptake rate. Thus only an unequal amount of days within the monoliths were available for the analysis.

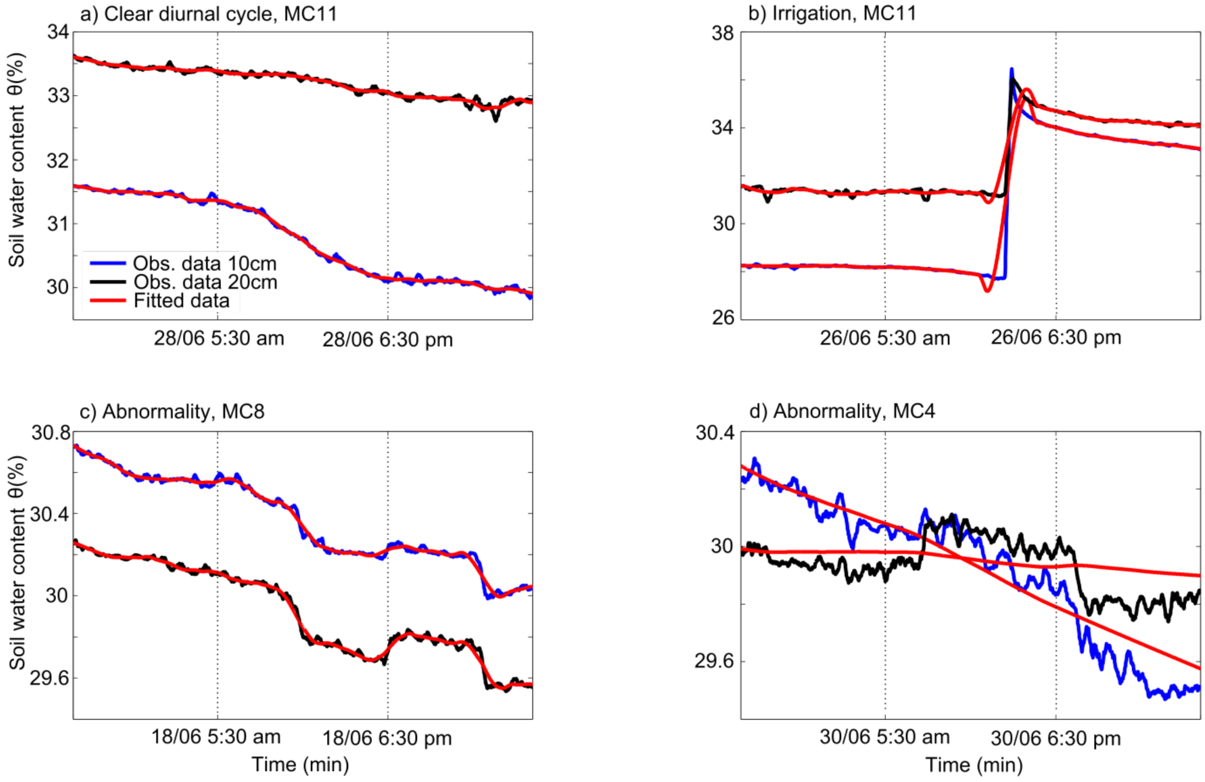


Figure 3.2 Comparison of the daily course of soil water content in 10 cm and 20 cm depth with different data quality, which are a clear diurnal cycle (a), increasing soil water content due to irrigation (b), and jumps in data from unclear origin (c and d). Note the different lysimeters (MC) shown, the different times and the different y-axis of the figures.

3.2.4 Measures for signal noise, soil water depletion and texture

The aim of this method evaluation was to investigate which factors influence the estimates of the *msml* method. The influence of uncertainties of soil moisture sensor measurements on the estimation of evapotranspiration was already discussed in Chapter 2. Nevertheless, as the used soil water content measurements in this lysimeter study are afflicted by real sensor uncertainty, we applied an additional measure for the signal noise of every data point i ($s_{\mathrm{res},i}$) (Peters et al., 2013) from 25, 28 and 29 June, since these dates are used for further analysis in Chapter 4.

$$s_{res,i} = \sqrt{\frac{1}{r}\sum_{j=1}^{r}[x_j - \widehat{x_j}]^2} \ , \tag{3.2}$$

Here, r is the number of data points within the time window of the applied smoothing function, x_j are the measured data and $\widehat{x_j}$ are the fitted values within the respective time window. This measure is based on the assumption that the fitted values describe the real data sufficiently good (Peters et al., 2014). The mean of $s_{\mathrm{res},i}$ over time and depth was calculated in order to have one value per lysimeter and day to compare with the relative bias between predicted ($\tilde{x}$) and observed (x) daily evapotranspiration (Eq. 2.16).

To investigate the influence of the magnitude of evapotranspiration and thus soil water depletion over one day, measured evapotranspiration was correlated with the relative bias (Eq. 2.16). Here, all days with undisturbed soil water content measurement where considered.

Additionally, the correlation between the sand content of each lysimeter with b gives an indication whether the operation of the *msml* is influenced by the texture. The sand content was chosen since it is negatively correlated with the silt and clay content of the respective soils and thus represents the texture well.

3.2.5 Stable isotope measurements

Preferential water uptake depth of all species present in each plot was additionally estimated by analyzing the natural ^{18}O isotopic composition of soil and xylem water. Therefore on 18 and 19 July 2012 three soil samples were taken on each plot with a soil auger of 1 cm diameter (Eijkelkamp, The Netherlands) in nine different soil depths (0-3, 3-6, 6-10, 10-20, 20-30, 30-40, 40-50, 50-55, and 55-60 cm). Soil samples in each depth were pooled, resulting in nine soil samples per plot.

For each species present on each plot, root crowns of three to five individuals were collected and pooled by species. All samples were immediately placed into 12 ml glass vials (Labco Limited, UK), sealed with a cap and parafilm and kept frozen until cryogenic water extraction.

Xylem water in the root crowns and soil water was extracted using cryogenic water extraction (Barnard et al. 2006). Isotopic composition of oxygen in the xylem and soil water was measured with a TC/EA high-temperature conversion/elemental analyzer coupled with a DeltaplusXP isotope ratio mass spectrometer via a ConFlo III interface (Thermo-Finnigan, Bremen, Germany; further information can be found in Werner et al. 1999). Oxygen isotopic composition of the samples was measured as $\delta^{18}O = (R_{Sample}/R_{Standard}) - 1$, where R is the ratio of ^{18}O to ^{16}O of the sample and the standard. Values are expressed in ‰. The measurements were V-SMOW (Vienna Standard Mean Ocean Water) and the precision of the measurements was 0.1 ‰.

The respective proportional contribution of the soil water to the xylem signature of $\delta^{18}O$ was estimated with the multi-source mixing model SISUS (Stable Isotope Sourcing using Sampling, http://statacumen.com/sisus/). Further information on the SISUS model can be found in Erhardt (2009). SISUS was applied on each lysimeter separately using the measured $\delta^{18}O$ of the soil water as source proportion and the several plants as target mixtures for all soil depths mentioned above.

To compare the estimated root water uptake profiles from the *msml* method and the SISUS model, we integrated the uptake proportion in accordance with the soil moisture measurement depths (10 cm, 20 cm, 30 cm, and 60 cm). Additionally, the community uptake was calculated from individual species weighted means based on specific leaf area, as the transpirations strongly correlate with the leaf area index. For several plants some of the measured xylem $\delta^{18}O$ values were not in the range of the source ratios. Schwendenmann et al. (2014) suggest that this will indicate a water uptake below the lowest soil source measurement. However, we found that this was mainly the case for plants with a shallow root system and thus excluded these lysimeters from the comparison with the *msml* method. Furthermore we also excluded lysimeters were not every grown species was sampled, as this would lead to a bias in the community transpiration and root water uptake. Finally we could use lysimeter #4 (4 species mixtures) and #7 (16 species mixtures) to validate the *msml*.

3.2.6 Evaluation criteria and statistical analysis

Analogue to Chapter 2 we used the correlation coefficient (R) (Eq. 2.14), the coefficient of determination R^2, the relative variability (RV) (Eq. 2.15) and the bias (b) (Eq. 2.16) as evaluation criteria to test the quality of the estimation of evapotranspiration.

Further, the moment of inertia (moi) was calculated as a measure of the scatter of the correlation between observed (E_{obs}) and predicted evapotranspiration (E_{msml}) for each lysimeter (Eq. 3.3), where values close to zero indicate that the scatter cloud arranges around the 1:1 line.

$$moi = 0.5 \cdot \frac{1}{n} \sum_{k=1}^{n} (ET_{obs,k} - ET_{msml,k})^2 \tag{3.3}$$

Statistical analysis on the relation between evapotranspiration, sand content and the measure for the signal noise s_{res} with the relative bias was conducted by using the LinearModel.fit function and the anova function of the Statistics toolbox in Matlab R2012.b

3.3 Results

We compared evapotranspiration rates of 12 lysimeters from a measurement campaign from 15th June to 21st July 2012 with predicted values. Soil water contents below 60 cm were not included in this study since they did not change regarding evapotranspiration.

3.3.1 Prediction of evapotranspiration

The *msml* method predicted the community evapotranspiration with a high correlation between measured (E_{obs}) and predicted (E_{msml}) values. The linear model explains about 79 % of the variation in the measured evapotranspiration. Fig. 3.3 shows that the *msml* results match well the 1:1 line between E_{obs} and E_{msml}, with a slight overestimation over the entire range of evapotranspiration.

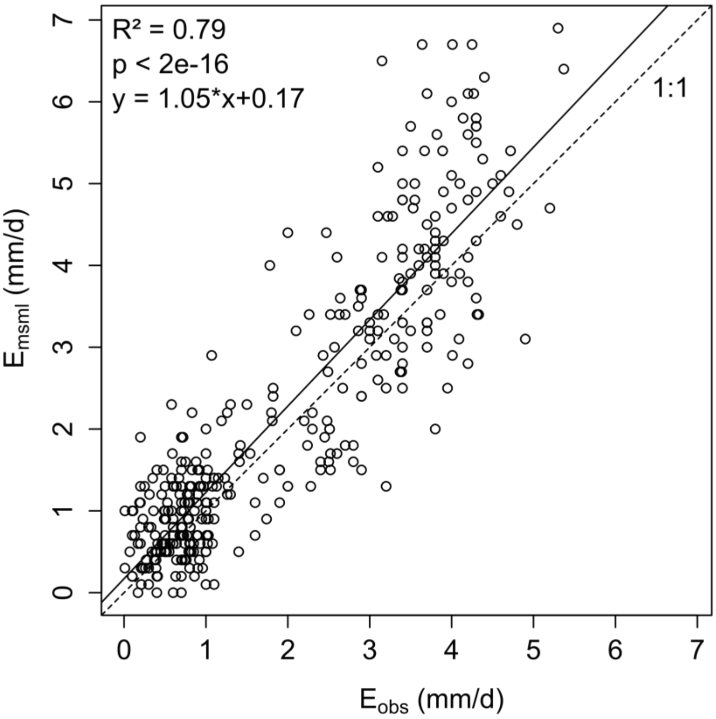


Figure 3.3 Comparison of observed (E_{obs}) and predicted (E_{msml}) values of daily evapotranspiration from a lysimeter experiment conducted in the CRNS Ecotron, Montpellier on 12 weighable lysimeters. The solid line is the regression line and the dashed line represents the 1:1 line.

A disentangling and comparison of the evaluation criteria according to the particular lysimeters indicates that the mean relative bias is comparatively small (20 %) whereby lysimeter #5 and #11 have a higher error of about 50 % (Tab. 3.1). The model performance criteria are summarized in Table 3.1. The correlation was relatively high for each lysimeter ($R > 0.8$), except lysimeter #12. The reproduction of the observed variance show considerable differences among the lysimeters with a range from 0.83 to 1.48. This is also apparent in Fig 3.4, where the regression between E_{obs} and E_{msml} show over- and underestimations depending on the particular lysimeter. Regardless, the predicted values of each lysimeter match well the 1:1 line between E_{obs} and E_{msml}.

Table 3.1 Comparison of the model performance of the *msml* regarding reproducing the observed evapotranspiration of each lysimeter. SR (species richness) denotes the number sown of species in the respective lsimeter, $\bar{E}$ is the mean daily evapotranspiration (mm day^{-1}) over the respective time period and the numbers in brackets indicate the standard deviation. The model performance is expressed, similar as in Chapter 2, as correlation coefficient R, relative variability RV and relative bias (b). Note that the lengths of the compared time series of the lysimeters differ due to different failures of the weight or the TDR sensors.

Lysimeter	SR	$\bar{E}$	R	RV	b (%)	moi
1	16	6.3 (±1.4)	0.89	1.21	27.7	0.44
2	4	4.2 (±0.9)	0.95	1.41	17.9	0.17
3	16	5.9 (±1.5)	0.94	0.83	-16.9	0.15
4	4	5.4 (±2.1)	0.89	1.06	9.2	0.28
5	4	6.2 (±1.0)	0.94	1.48	49.5	0.56
6	16	5.5 (±1.7)	0.91	0.93	-0.8	0.16
7	16	6.6 (±0.7)	0.95	1.27	28.7	0.35
8	4	5.0 (±1.5)	0.92	0.89	6.8	0.13
9	16	5.6 (±1.3)	0.92	1.07	17.3	0.19
10	4	6.4 (±1.3)	0.94	1.21	4.4	0.15
11	16	6.5 (±0.8)	0.93	1.22	46.6	0.44
12	4	4.1 (±1.4)	0.76	0.91	-15.9	0.15
mean			0.91	1.12	|20.1|	0.34

Furthermore, Fig. 3.4 shows that the lysimeters differ in their magnitude of evapotranspiration according to the grown species mixture. This variation in evapotranspiration is related to the leaf area of the respective plant community, an issue what is further discussed in Chapter 4.

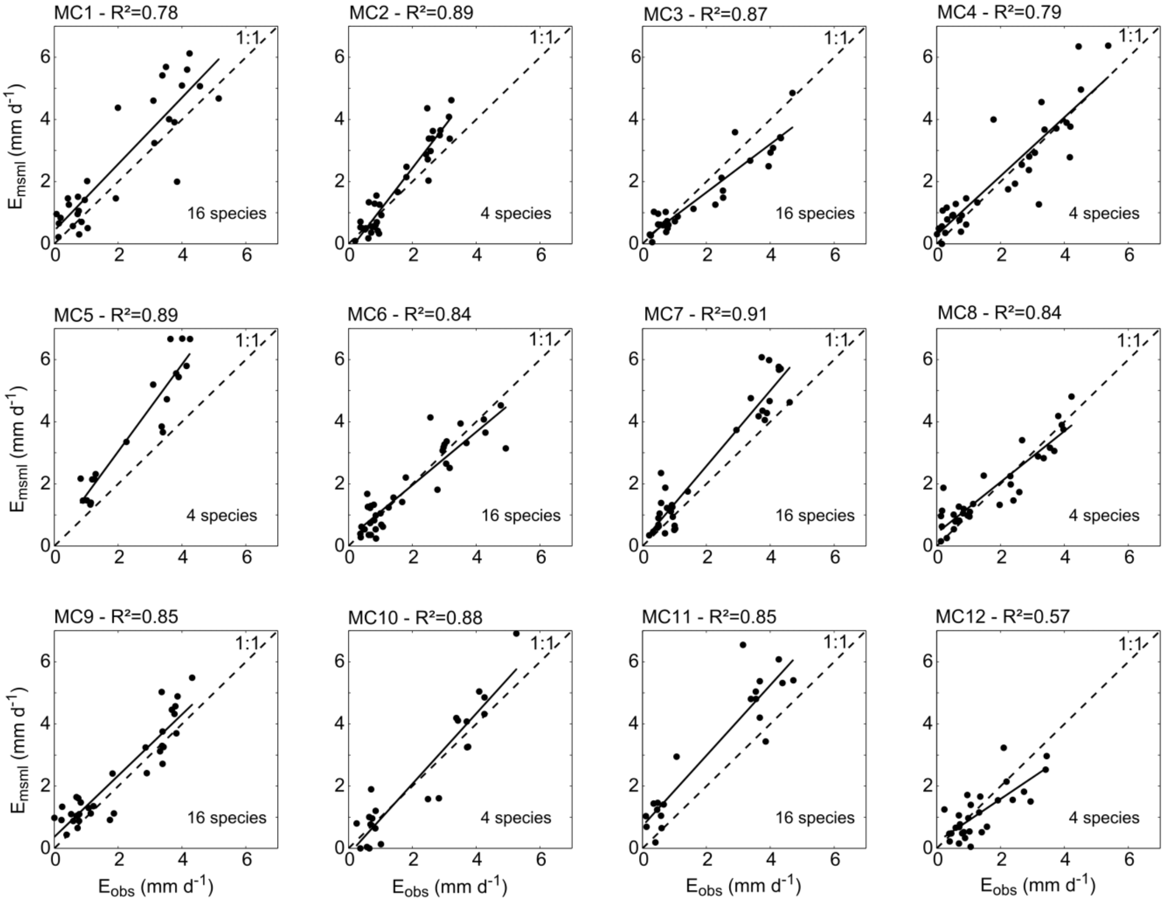


Figure 3.4 Comparison of observed (E_{obs}) and predicted (E_{msml}) values of daily evapotranspiration for each lysimeter. The lysimeters contain two different diverse plant communities (4 and 16-species mixtures). The coefficient of determination (R^2) are shown in the title of the figures, respectively. The solid lines are the regression lines and the dashed lines represent the 1:1 line.

3.3.2 Effects on the quality of predicted evapotranspiration

The relations between E_{obs} and E_{msml} shown in Fig 3.4 suggest that the prediction of root water extraction and thus evapotranspiration could be influenced by biotic and abiotic factors. The experimental setup of the 12 lysimeters, containing different ecosystems and soil texture distributions, has great capacity to investigate these factors.

Effect of the magnitude of evapotranspiration

It was found that the magnitude of evapotranspiration has a significant effect ($p < 0.001$) on the quality of the predicted values. Fig. 3.5 (a) shows that the relative bias between E_{obs} and E_{msml} decreases with increasing evapotranspiration. The estimates scattered when evapotranspiration was small, i.e. smaller than 2 mm/d. Furthermore, the depletion of soil moisture is significantly and positively related to the magnitude of evapotranspiration ($p < 0.001$). Thus, the strength of water depletion also influences the quality of predicting evapotranspiration.

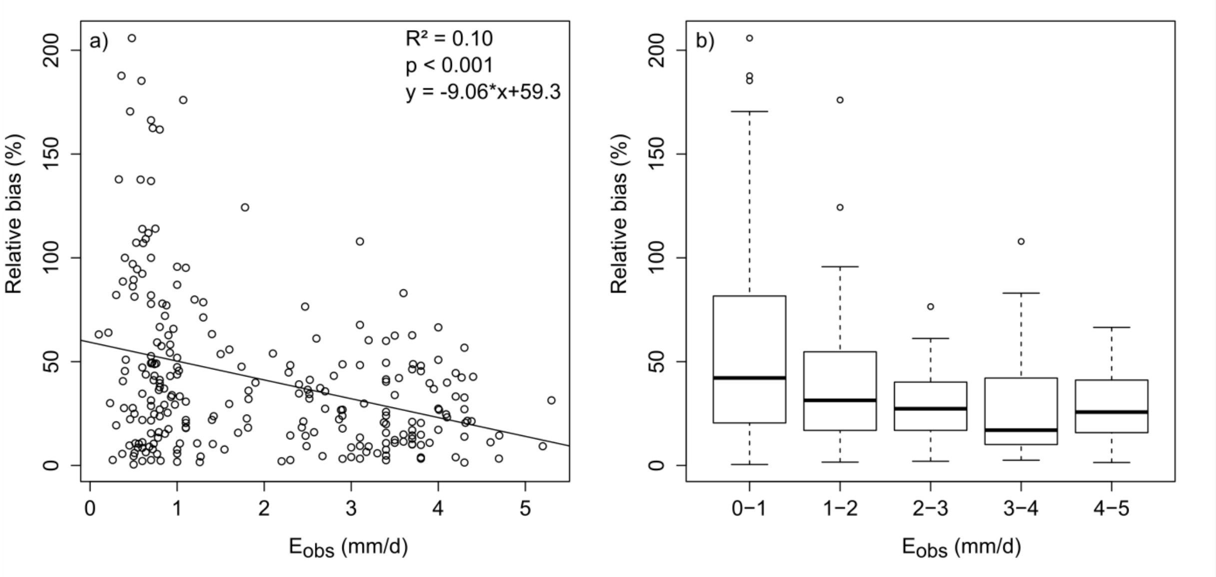


Figure 3.5 Significant effect of the magnitude of observed evapotranspiration E_{obs} (mm/d) on the relative bias between calculated (E_{msml}) and observed evapotranspiration (E_{obs}) from weight changes of the respective lysimeter (a). Additional boxplots indicate the course of the median of the relative bias (b). E_{obs} was calculated from the difference of measured weight changes between 5:00 am – 6:30 pm (day) and 6:30 pm – 5:00 am (night). The black line in a) is the regression line.

Influence of soil texture

The soil monoliths represent the natural variation of soil texture from sandy loam to silty clay of the experimental field site, whereas only the sand content was used as proxy for the mean texture of the respective soil column. Although the bias is slightly higher for lower sand contents, the mean sand content of each lysimeter has no significant effect on the error of the predicted evapotranspiration ($R^2 = 0.059$, $p = 0.44$; Fig. 3.6).

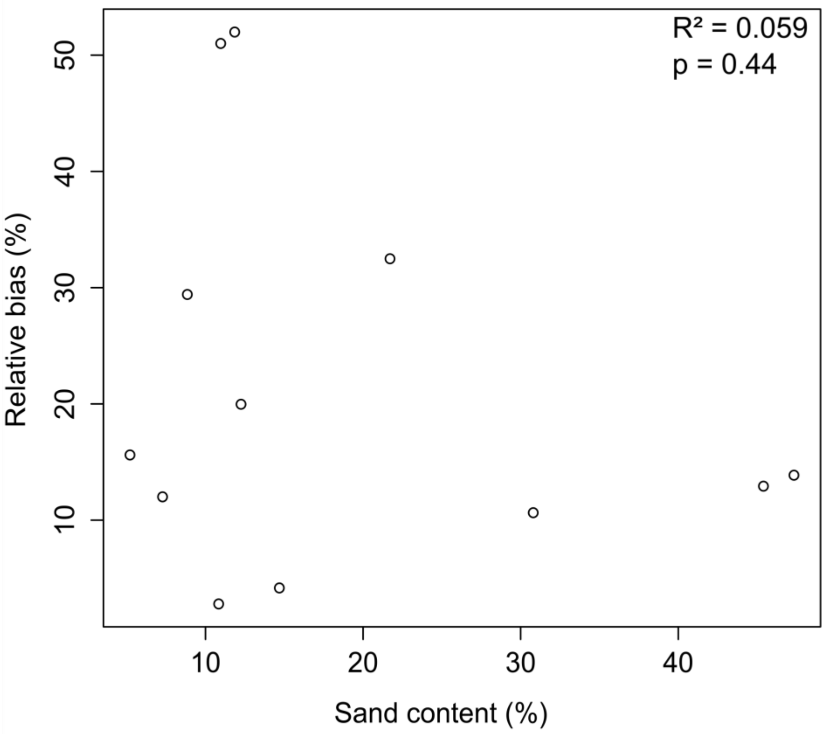


Figure 3.6 Effect of sand content (%) on the mean relative bias between calculated (E_{msml}) and observed evapotranspiration (E_{obs}). The sand content is a proxy for the mean texture of the respective soil column.

Influence of signal noise and smoothing filter

In Fig. 3.7, the mean noise of the measurements (s_{res}) for each of the three considered days is shown. For all three days, the filter window width was 241 minutes for the soil layers 10 cm and 20 cm, and 721 minutes for 30 cm and 60 cm depths.

In all three cases we found no significant effect of the signal noise (s_{res}) on the relative bias between E_{obs} and E_{msml}. The statistical measures R^2 and the statistical significance value (p) are summarized in Table 3.2. Additionally, Fig. 3.2 shows how the fitted data describes the course of the soil moisture compared to the noisy data. Especially, in Fig. 3.2c it is evident that disturbances of the data, which occurred over a longer time than the window width, could not be removed by the filter. However, with a manual selection of the considered days the applied filter has no impact on the quality of the msml method.

Table 3.2 Coefficient of determination (R^2) and statistical significance (p) between the noise of the measurements (s_{res}) and the relative bias for the data estimated on 25, 28 and 29 June 2012.

Date	R^2	p
25 June	0.144	0.22
28 June	0.004	0.85
29 June	0.003	0.86

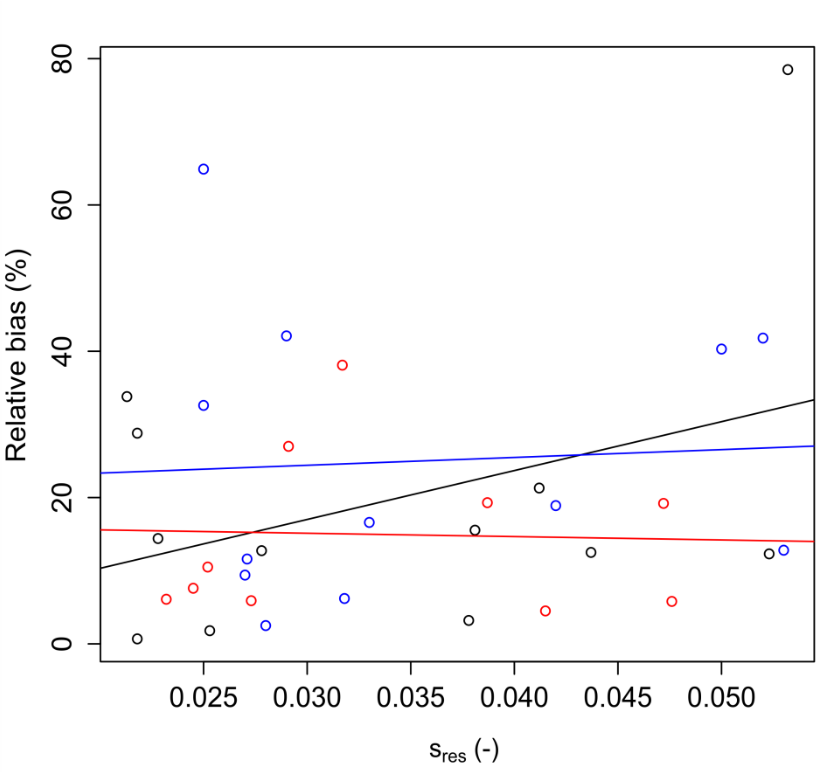


Figure 3.7 Relation between the noise of the measurements (s_{res}) on the mean relative error between calculated (E_{msml}) and observed evapotranspiration (E_{obs}) for 25 June (black dots), 28 June (blue dots) and 29 June (red dots). The lines represent the respective fitted linear models, but do not indicate any significant effect.

Comparison of root water uptake estimates with stable isotope measurements

As an additional evaluation of the *msml* method, the estimated community root water uptake profile was compared with those derived from the isotope measurements (SISUS model). We used two lysimeters (#4, #7), where nearly all species present in the dome were sampled (100 % and 98 %, respectively) with a proportion of total biomass of 85 % and 89 %, respectively. For lysimeter #4 (Fig. 3.8a), both estimated uptake profiles show the same course with nearly the same percentage of uptake in all considered depths. Figure 3.8b indicates an underestimation of the proportional root water uptake in 0 - 15 cm estimated with the *msml* compared to the SISUS model. However, this is vice versa in the sampled layers below. Overall, the root water uptake patterns match very well. Note that the community water uptake profiles derived from stable isotopes are not applicable to evaluate the *msml*, since they are based on a Bayesian model to estimate source contributions (Erhardt, 2009). However, they can be used to double-check the proposed method.

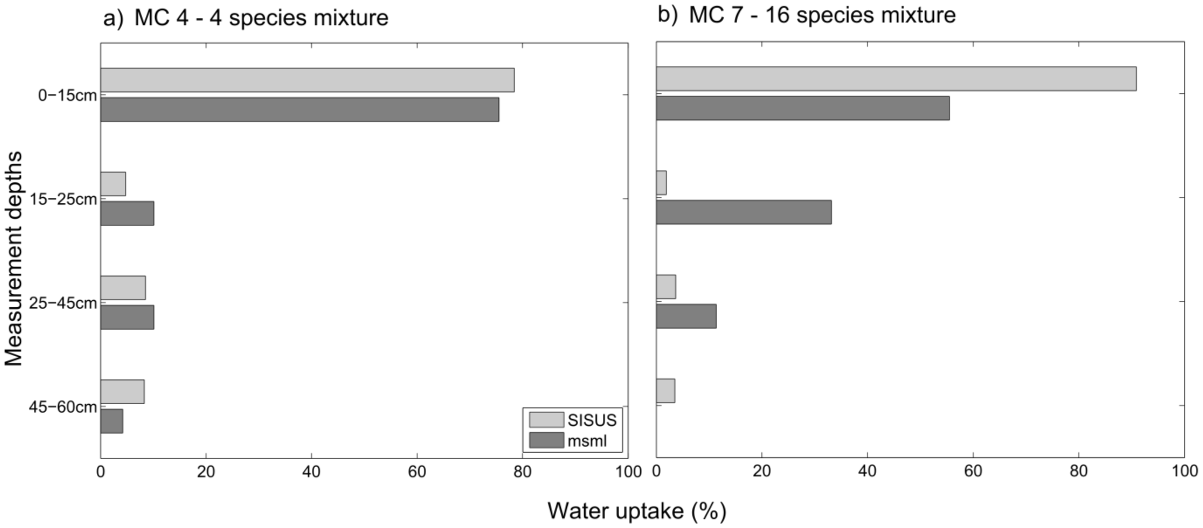


Figure 3.8 Comparison of the *msml* with root water uptake profiles estimated with the multi-source mixing model SISUS from stable isotope measurements for (a) lysimeter (MC) 4 (isotope measurements on 100 % of realized plant species) and (b) lysimeter (MC) 7 (isotope measurements on 98 % of realized plant species).

3.4 Discussion

We evaluated the application of the introduced Multi Step Multi Layer Regression method (*msml*) to estimate actual evapotranspiration and root water uptake patterns on 12 weighing lysimeters. Up to now, no standard method is available to derive evapotranspiration and root water uptake patterns from soil water content measurements (Molz, 1981; Feddes et al., 2001; Hopmans and Bristow, 2002). Guderle and Hildebrandt (2015) showed based on a numerical study that the *msml* applied here has great potential for predicting the actual evapotranspiration and root water uptake during periods without rainfall. A validation with experimental data was still missing and weighable lysimeters are well suited to calibrate and evaluate water balance methods and water transport models (Durner et al., 2008; Schelle et al., 2012) since they deliver a precise and realistic measure of evapotranspiration by registration of weight changes (Meissner et al., 2007; Allen et al., 2010; Peters et al., 2014). Moreover, the knowledge of evapotranspiration and additionally the registration of drainage flux allows for closing the water balance of the entire lysimeter, which is representative for the considered ecosystem from where it originates and the transpiring surface of the respective lysimeter.

By comparing the evapotranspiration estimated from the *msml* method with the measured evapotranspiration, it is directly evident that the *msml* is able to predict the actual evapotranspiration of the lysimeters from soil water content measurements. Furthermore, the upscaling to a transpiring surface of two m^2 does not influence the results negatively. The overall error is about 20 %, which is in the same range as obtained in the numerical study (Chapter 2) and for common soil water balance methods (Allen et al., 2010). Nevertheless, this overestimation could be caused by the unavoidable neglect of soil water fluxes at times at which night-time evapotranspiration occurred. During those times, vertical fluxes could not be determined, which leads to overestimation of evapotranspiration (as already suggested in Chapter 2). The conditions during the evaluation period were comparatively wet (frequent irrigation), which suggests the presence of vertical flow components.

However, it became obvious that the *msml* method is more robust against measurement errors in soil moisture time series than the soil water balance methods since the latter one is applied to only two time points per day, namely at the start and the end of the transpiration period. The considering of vertical soil water fluxes is an additional advantage of the *msml* compared to soil water balance methods.

Similar to the numerical study in Chapter 2, we found that the magnitude of evapotranspiration has a significant effect on the quality of the predicted evapotranspiration, which increase with increasing evapotranspiration. In turn, higher evapotranspiration rates induce a higher depletion of the soil moisture. This is expressed as steeper decreasing course of the daytime soil moisture time series, which can be better described by the fitted linear function of the *msml* method. A similar proneness to error was observed by Zhu et al. (2011) for estimation of evapotranspiration from groundwater fluctuations. Even though there is a slight overestimation of evapotranspiration and thus of the water uptake profiles, differences in water uptake profiles between ecosystems with different evapotranspiration behaviours are not negatively influenced, since this overestimation occurs over the entire range of evapotranspiration. Consequently this does not negate the application on ecological investigations. Despite the slight overestimation of evapotranspiration and taking into account that errors are also attached to the lysimeter weight measurements (5-15 %, Allen et al., 2010), the predicted values of evapotranspiration close the water balance of the lysimeters, and give a first confirmation of the *msml* method on experimental data. The next step is an analysis of the vertical profiles.

Root water extraction profiles play a central role in ecology and eco-hydrology (Davis and Mooney, 1986; Le Roux, 1995; Jackson et al., 1996; Ogle et al., 2004; Leimer et al., 2014; Schwendenmann et al., 2014) as already stated in Chapter 2. The knowledge of these profiles allows understanding of resource partitioning and ecosystem structure (Arnold et al., 2010). The predicted evapotranspiration is the integrated sink term over the entire soil profile according to Eq. 2.3 (Chapter 2) and thus our results suggest that the predicted water extraction profile represents the true profile caused by the ecosystem on top of the lysimeter. This assumption was already proven by the numerical study in Chapter 2.

However, the numerical study neglects the natural horizontal heterogeneity in soil water contents, which propagates to uncertainties of water uptake profiles in real world situations (Guderle and Hildebrandt, 2015). In general, lysimeter studies do not provide any water uptake profile data for validation, but the comparison of stable isotope compositions in the plants and the soil water enables an additional determination of the water uptake profiles (Ehleringer and Dawson, 1992; Ogle et al., 2004; Schwendenmann et al., 2014). Based on the Bayesian multi-source mixing model SISUS, stable isotope measurements are used to derive a relative uptake profile in percentage of the total uptake. These cannot be used to evaluate them since the results of the multi-source mixing models are no unique solution (Asbjornsen et al., 2007; Phillips and Gregg, 2003; Schwendenmann et al., 2014). A further error source for the mixing model is the fact that it estimates the proportional contribution to the plant isotope signature for single plants. Thus, the community uptake has to be calculated from individual species weighted means based on specific leaf area to capture the proportion of community transpiration of the respective plant. Though, transpiration depends not only on the leaf area but also on the opening of stomata, which could not be considered with the described method. Nevertheless, the stable isotope ratios can be used to double-check such methods like the *msml.* The estimation of water uptake patterns from isotope measurements was not possible for all lysimeters since not all realized plant species could be sampled during the labelling campaign. One reason for the slight overestimations of the *msml* predicted water uptake compared to the stable isotopes could be because the *msml* method cannot distinguish between evaporation and transpiration (Chapter 2; Guderle and Hildebrandt, 2015) whereas the stable isotope measurements can only capture transpiration. Nevertheless, the root uptake patterns estimated from isotope measurements and the *msml* method compare well for the considered lysimeters, which corroborate the potential of the *msml* method.

The conducted lysimeter experiment holds further possibilities for disentangling different environmental and non-environmental influences on the application of the msml method.

First, even though the twelve lysimeters were hosted under controlled environmental conditions like irrigation, irradiance and humidity, they were taken from plots equally distributed across the Jena Experiment and thus contain soils with different soil texture (sandy loam to silty clay). However, it was found that the quality of the *msml* predictions was not influenced by soil texture. This robustness is an additional advantage of the *msml* method for real world application, where soil properties are often difficult to obtain. In particular inverse numerical root water uptake models require soil parameters for solving the Richards equation. Those parameters have also been shown to be a major source of error and limitation of these procedures (Musters and Bouten, 1999; Musters et al, 2000; Vrugt et al., 2001; Hupet et al., 2002).

Second, we can also re-examine the influence of sensor uncertainty, already discussed in Chapter 2. Since we are unable to identify calibration errors, we only discuss precision errors. Precision errors are realized as a noise in the data, which we eliminated by applying a smoothing filter. Since the noise (s_{res}) (Peters et al., 2013) does not correlate with the prediction error (bias), we conclude that the smoothed time series describes the real data sufficiently well and thus the measurement uncertainty does not influence the prediction of water uptake and evapotranspiration. Please note, we used a slightly revised smoothing filter compared to Chapter 2, which was necessary since the soil moisture measurements have a higher temporal resolution with a considerable measurement noise as well as abnormalities/disturbances in their course.

The practical implementation of the *msml* showed that a carefully check regarding abnormalities/disturbances in the course of the applied soil moisture time series is a mandatory requirement. Such irregular disturbances in the data are hard to eliminate and can lead to severe errors in predicting evapotranspiration and water uptake profiles. A possible alternative to using the smoothing filter with a fixed window width (used here) is to apply in the future a dynamic filter routine with an adaptive window width depending on signal strength (Peters et al., 2013).

Important pre-requisites for applying the *msml* are a high temporal resolution of soil moisture measurements to capture the diurnal cycle and a high spatial resolution of soil moisture sensors over the entire soil column. The latter one is important to record the non-linear nature of the root water uptake (Kumar et al., 2013; Guderle and Hildebrandt, 2015). The placement of sensors in the entire rooting zone is recommended to sample the particular water extraction (Wilson et al., 2001). An installation as deep as possible in the soil is still better to get information on the contribution of capillary rise and redistribution on soil water fluxes. In any case, as already discussed in Chapter 2, a high spatial and temporal resolution of the soil sensors is suggested since this allows a more reliable determination of evapotranspiration (Schwärzel et al., 2009; Clausnitzer et al., 2011; Garré et al., 2013) and accounting for precision errors.

In summary, in spite of the slight overestimation of evapotranspiration and thus of the water uptake profiles, the *msml* method can be used for comparison of root water uptake profiles of different ecosystems. The root water uptake profiles of ecosystems with various evapotranspiration rates are not affected by the deviations since they occur over the entire range of evapotranspiration.

3.5 Conclusions

The overall aim of this study was to find out a simple and straight forward method for estimating root water uptake patterns to investigate the influence of different ecosystems on the soil water status. To evaluate the procedure of the *msml* method, we applied it on 12 weighable lysimeter taken from the Jena Experiment. This allowed for testing the effects of various evapotranspiration rates and soil textures on the quality of prediction by the *msml*. Moreover, we could validate the predicted root uptake profiles in tow lysimeters using stable isotope measurements.

The *msml* was shown to predict evapotranspiration with a small deviation from the real values. Even though there is a slight overestimation of evapotranspiration and thus of the water uptake profiles, differences in water uptake profiles between ecosystems with different evapotranspiration behaviours are not negatively influenced. Hence, this does not negate the application on ecological questions since the overestimation occurs over the entire range of evapotranspiration. The main advantage of this method is the low requirement of information of soil texture, soil hydraulic properties, and plant and root distribution parameter compared to numerical models.

Furthermore, the following conclusions were found in this analysis: (1) The uncertainty of the *msml* method decreases with increasing evapotranspiration respectively soil water depletion. (2) Soil texture had no influence on the prediction quality of root water uptake. (3) The proposed filter routine describes the real data sufficiently well and thus the measurement uncertainty has no influence on the prediction of water uptake and evapotranspiration.

The proposed method should be tested in the future additionally with a smarter filter routine (Peters et al., 2013).

Chapter 4

Plasticity in root water uptake facilitates efficient water use of higher diverse plant communities

4 Plasticity in root water uptake facilitates efficient water use of higher diverse plant communities

Abstract

Efficient extraction of soil water is important for productivity and survival of plants and plant communities. However, the individual interaction of plants regarding soil and water resources, especially the effect of biodiversity on transpiration and root water uptake profiles, has been rarely examined. The overarching aim of our study was to answer the question, whether diverse plant communities exploit soil water more efficiently than less diverse ones. So far, research on this question has been conducted without the measurement setup allowing for the estimation of root water uptake profiles. To address this knowledge gap, we used short term fluctuations of soil moisture data in a lysimeter setup hosting 12 experimental grasslands of contrasting species richness (4 and 16 sown species) to derive root water uptake profiles. Additional measurements of leaf water potential, stomatal conductance and root traits were used to shed light on the effects of functional groups on root water uptake strategies of different plant communities. We found that evapotranspiration increased with increasing leaf area. Furthermore, our results indicate, that higher diverse communities in this experiment comprise more plants with a root structure that allows to adjust their root water uptake strategy, such that the water uptake per root area was increased and the water uptake is more equally distributed over depth. Particularly the plant functional group of tall herbs in higher species mixtures contributed to a dynamic niche partitioning (plasticity) in root water uptake. The setup of this experiment allowed for evaluating the influence of biotic factors (e.g. species richness) on evapotranspiration as well as root water uptake patterns and receiving deeper process understanding concerning root water uptake strategies.

4.1 Introduction

Efficient use of available soil water is a key factor for plant growth and survival. For example, water stress is alleviated if root systems are able to adjust to site-specific conditions, like a shallow water table (Feddes et al., 2001). This holds also true for plant communities where the ecosystem transpiration can be considered as the sum of the root water uptake of all individuals (Zea-Cabrera et al., 2006). Up to now, only few studies investigated the impact of plant species interactions on root water uptake and particularly, the effect of species richness on transpiration as well as evapo-transpiration, while root water uptake patterns have been very little explored. For instance, Kreutziger (2006) and Van Peer et al. (2004) found enhanced ecosystem transpiration with increasing plant species richness. But this could either be explained due to higher leaf and thus transpiring area (Li et al., 2005), which in those cases coincided with higher biodiversity (Van Peer et al., 2004; Roscher et al., 2005) or by more efficient water extraction or both. However, niche-partitioning and complementarity were suggested as the basis for coexistence in highly diverse communities (Hooper, 1998; Loreau and Hector, 2001; Schenk, 2006) indicated by the positive relationship between biodiversity and ecosystem functioning (Cardinale et al. 2011, 2012; Hooper et al. 2012). For example, plant communities containing species with different root distribution might increase the spatial acquisition of soil resources compared to communities containing species with similar root distributions (Berendse 1982; Mommer et al., 2010; De Kroon et al., 2012; Mueller et al., 2013). In this context, root traits such as root length density (RLD), root depth, root foraging behavior and root system architecture potentially play a key role for ecosystem functioning (Schenk, 2006), being even more important than the taxonomic richness, as they allow taking advantage of different spatial niches in diverse plant communities (Cody 1986; Silvertown, 2004; Stubbs and Wilson, 2004; Schenk, 2006). Such niche differentiation in plant communities may result in specific root uptake profiles, soil water fluxes and storage, which are probably the key to understanding efficient water use in diverse plant communities (Zea-Cabrera et al., 2006, Schwendenmann et al., 2014). However, one main question is from where within the soil profile roots obtain water (Ogle et al., 2004). To answer this question, information on root water uptake and soil water fluxes are necessary, but their survey is still a major challenge in plant ecology and ecohydrology (Jackson et al., 2000).

To date, it is not possible to measure soil water flow directly (Vereecken et al., 2008) and this prevents obtaining root water uptake profiles. Our knowledge about changes of ecosystem root water uptake profiles with increased plant diversity is rudimentary, because soil water fluxes can only be estimated, either (i) through inverse modelling or (ii) as integrated water budgets derived from large soil monoliths in lysimeters.

Commonly, water uptake profiles are modeled as a function of rooting parameters (Gale and Grigal, 1987; Jackson et al., 1996; Schenk, 2008; Kuhlmann et al., 2012). The parameterization of root water uptake profile functions, especially root length density, are cumbersome to measure in the field and their relevance for root water uptake distribution is strongly uncertain (Hamblin and Tennant, 1987; Ong et al., 1999, Lai and Katul, 2000; Li et al., 2002; Doussan et al., 2006; Garrigues et al., 2006; Schneider et al., 2009; Bechmann et al., 2014). The most critical point in water flow models is the fact that they assume that root activity and thus root water uptake is directly related to measured RLD. There are, however, several indications that this is not necessarily the case in reality (Hamblin and Tennant, 1987; Perrochet, 1987; Prasad, 1988; Jarvis, 1989; Kleidon and Heimann, 1998). Root water uptake is related to the activity of roots (Nimah and Hanks, 1973; Kulmatiski et al., 2010; Kulmatiski and Beard, 2013), soil salinity and the transpiring demand from leaves as well as the hydraulic conductance of roots (Jackson et al., 2000; Steudle, 2000; Quijano et al., 2012). Thus a direct relation between RLD and root water uptake may be valid only for certain conditions and plant species identity (Hamblin and Tennant, 1987) and temporal and spatial plasticity in belowground resource use could be a major characteristics in niche partitioning and competition, respectively (Callaway et al., 2003; Ashton et al., 2010; Kulmatiski and Beard, 2013).

The overarching aim of our study was to answer the question, whether diverse plant communities exploit soil water more efficiently than less diverse ones. We hypothesized that diverse plant communities transpire more water and show increased complementarity in water uptake. Specifically, we investigated (1) whether in diverse plant communities root water uptake is achieved by exploiting greater depths (spatial complementarity), (2) if there is a vertical belowground niche separation due to different rooting distributions between the two diversity levels and (3) how root traits of the composing species influence community root water uptake patterns.

To date, the studies investigating the relations between species richness and water use have been conducted without estimating root water uptake profiles and soil water fluxes. To address this knowledge gap, we applied a data-driven method interpreting short term fluctuations of measured soil moisture, especially comparing changes in dynamics between day and night (Li et al., 2002; Guderle and Hildebrandt, 2015). This method allows a first order distinction between root water uptake and soil water flux and thus the estimation of root water uptake patterns over depth and time. We compare estimated root water uptake patterns with measured leaf water potentials, stomatal conductance and root traits in order to investigate how root water uptake strategies differ between plant communities varying in species and functional group diversity. This allows for deeper process understanding concerning root water uptake strategies. For this, we used a measurement campaign on twelve excavated lysimeters with soil-vegetation monoliths from the Jena Biodiversity Experiment (Roscher et al., 2004), which cover two diversity levels (4 and 16-species mixtures). The experiments were conducted in a controlled environment for ecosystem research (CNRS Ecotron, Montpellier). The Ecotron offered the unique opportunity of testing the influence of biotic factors on evapotranspiration as well as root water uptake patterns, since it allows simultaneous measurements of evapotranspiration and water fluxes from ecosystems varying in plant species richness under the same controlled conditions.

4.2 Material and Methods

4.2.1 Plant communities

The Jena Experiment is a long-term grassland biodiversity experiment located on the floodplain of the Saale River in Jena, Germany (50° 55´ N, 11° 35´ E, 130 m above sea level) (Roscher et al., 2004). Mean annual precipitation is 587 mm and mean annual temperature is 9.3 °C (Kluge and Müller-Westermeier, 2000). The experiment was established in 2002 and the site was previously used as arable land. Plant communities originating from two sown diversity levels (four and 16 species) of the Jena Experiment were used to analyse the influence of species diversity on evapotranspiration and root water uptake. Therefore, we used a measurement campaign on twelve lysimeters (2 m^2, diameter of 1.6 m, 2 m depth with a weight of 7-8 tonnes), which were excavated in December 2011. The lysimeters were buried to the top edge near the experimental field, before being transported to the Ecotron facility in March 2012. This allowed recovering after excavation disturbances (Milcu et al., 2014). The twelve plots were selected according to the following criteria: (1) all four plant functional groups (grasses, legumes, small and tall herbs) were present, (2) realised species numbers were close to sown species richness and (3) plots were equally distributed across the experimental blocks of the field site to account for different soil textures. The selected plots met the aforementioned criteria with the exception of one plot were no grasses had been sown. A detailed description of the experimental setup in the Ecotron is given in Chapter 3, Section 3.2.1 “Lysimeter setup in the CNRS Ecotron facility”.

4.2.2 Multi Step Multi Layer Regression (msml)

The Multi Step Multi Layer Regression (*msml*) was used to estimate evapotranspiration and sink term profiles from diurnal fluctuation of soil water content measurements (Li et al., 2002; Guderle and Hildebrandt, 2015). It applies a regression over multiple time steps on soil moisture time series of each measurement depth. Here we used measurements in 10 cm, 20 cm, 30 cm and 60 cm. The transpirational time is defined by the activity of plant stomata or rather by their opening and closure, which is driven by the supply of solar energy (Loheide, 2008; Maruyama and Kuwagata, 2008; Sánchez et al., 2013). We defined the transpirational time between 05:30 am until 06:30 pm. A detailed description of the method can be found in Chapter 2 and in Guderle and Hildebrandt (2015), the method evaluation as well as a description of the used soil water content measurements is given in Chapter 3.

4.2.3 Selected times

The *msml* method was validated by comparing the estimated evapotranspiration with measured evapotranspiration from weight changes. Although the weight changes and thus the actual evapotranspiration were continuously registered in the Ecotron facility, the lysimeter weights were unavoidable disturbed through experimental work, which is a constraint for possible evaluation times. Furthermore, the *msml* method could only be applied for dry conditions as irrigation caused rapid changes of soil water contents and thus blurs the signal of root water uptake. After a first selection of dry days with undisturbed soil water content measurements, we chose soil moisture measurements to estimate root water uptake for 25, 28, 29 of June 2012 and for 17 and 18 of July 2012.

The latter period was selected because measurements of stable isotopes, leaf water potential, stomatal conductance and root traits (root length density, root diameter, root biomass etc.) were done at these days (17 July to 19 July 2012).

4.2.4 Leaf water potential and stomatal conductance

Leaf water potential was measured with a pressure chamber (Pressure Chamber Instruments Model 600, PMS Instrument Company, Albany, Oregon, USA) at predawn (04:00 am – 06:00 am) and midday (01:30 pm – 04:00 pm) for the most abundant species on each plot. Two to three species were chosen in the 4-species mixtures, and five to eight species in the 16-species mixtures. All measurements were done within three days (17 to 19 July 2012). Measurements were carried out on young, but fully expanded leaves of four individual shoots per species per plot. Stomatal conductance (gs, mmol m^{-2} s^{-1}) was measured with a portable leaf porometer (SC-1 Leaf porometer, Decagon Devices, Pullman, USA) on three leaves growing at different shoots for each available species per dome. Measurements were done in the auto mode for 30 seconds. Table B.1 in appendix lists the species included in measurement of leaf water potential and/or stomatal conductance for each plot.

4.2.5 Leaf area index (LAI), leaf area index per species (LAI_s), average root diameter (d_{root}) and root area index (RAI)

Leaf area index (LAI)

Leaf area index (*LAI*) was measured with a portable LAI-2000 plant canopy analyzer (LI-COR, Lincoln, USA). The average *LAI* was measured under diffused light conditions (evening) with five measurements near ground level and at different positions on each lysimeter. A reference measurement was done above the canopy. More detailed information on the *LAI* measurements can be found in Milcu et al. (2014).

Leaf area index per species (LAI_s)

We estimated the specific leaf area index per species (LAI_s, cm^2 cm^{-2}) (Eq. 4.1) from leaf dry weight *ldw* (g cm^{-2}) and the specific leaf area *SLA* (mm^2 mg^{-1}) of the respective species (Table B1). The unit of *SLA* had to be converted in cm^2 g^{-1} for further calculations.

$$LAI_s = ldw \cdot SLA \tag{4.1}$$

For estimation of *SLA*, we collected three to five fully expanded leaves growing on different shoots for each available species per plot. Leafs (pooled per plot and species) were put in moist tissue paper, sealed in plastic bags and stored at 4 °C overnight. Then, leafs were plotted dry with tissue paper and leaf area of the bulk samples was measured with the LI-3100A area meter (LICOR, Lincoln, USA). Samples were dried for 48 h at 70 °C and weighted. *SLA* was calculated as the ratio of leaf area to dry weight in mm^2 mg^{-1}. For the dry weight estimation, the vegetation was clipped at ground level in a rectangle of 0.8 x 1.0 m per plot, dried at 65 °C for three days and sorted for species. A subsample of biomass of each species per dome was separated into the plant compartments (leafs, shoot and flowers), which was used to calculate *ldw*.

Root length density (RLD), average root diameter (d_{root}) and root area index (RAI)

Three soil cores (diameter 3.5 cm) in 0-60 cm depth were sampled per macrocosm. Each core was divided into six layers (0-5, 5-10, 10-20, 20-30 and 40-60 cm). The respective layers were pooled per macrocosm, washed with tap water, and sieved (mesh size 200 µm) to obtain the root samples. Roots were weighed and a subsample of the fresh roots (approx. 2 g) was stored in 70 % ethanol before it was dyed (with neutral red solution), scanned (Scanner Optical STD4800 Regent Instruments Inc.), and analysed with WinRHIZO (Reg 2009c, Regents Instruments Inc.) to get root traits (root length density, average root diameter, root surface).

The *RAI* was calculated from measured root surface A_r (cm^2 cm^{-3}) and thickness of the respective soil layers z_i (cm) (Eq. 4.2):

$$RAI_i = A_r \cdot z_i, \tag{4.2}$$

The total RAI per plot is the sum over all soil layers *i*.

4.2.6 Statistical analysis

Statistical analyses were conducted with the statistical software R 3.0.2 (R Development Core Team, http.//www.R-project.org). We checked the data for heteroscedasticity, and they were log-transformed if required. We used linear mixed-effects models using the package nlme (Pinheiro et al., 2014) in R, considering species richness as fixed factor and the lysimeter as random effect. Additional fixed effects and their interaction were added stepwise to a constant null model containing only the fixed factor and random effects. Significant improvement of the model after adding the fixed effects was tested with the maximum likelihood method and likelihood ratio tests. Effects of species richness on evapotranspiration over time was analysed separately for June (25, 28 and 29 June 2012, later stated as June) and July (17 and 18 July 2012, later stated as July), considering species and time as additional fixed factors. Effects of species richness on root water uptake profiles were also analysed separately for June and July, similar to evapotranspiration but with depth as additional fixed effect. Further, we tested for differences in root water uptake in every measurement depth separately, applying the model as described for evapotranspiration.

Statistical analyses of leaf water potential and stomatal conductance were done using the package multcomp (Hothorn et al. 2008) in R. Values of leaf water potential and stomatal conductance of the individual shoots were averaged per species per plot. Effects of species richness and functional group identity were tested considering plot and species as random effects and species richness (SR) and functional group identity (FG) as fixed effects. Differences among functional groups were identified with Tukey's HSD tests using ghlt function in the multcomp package.

Effects of species richness on root length density, belowground biomass (BGBM), RAI and RAI:LAI ratio were done using a one way ANOVA. We used a simple linear regression to analysis the relation of leaf area index and evapotranspiration.

4.3 Results

4.3.1 Species richness effects on evapotranspiration

The measured evapotranspiration of all 16-species mixtures was higher on all investigated days than the measured evapotranspiration of the 4-species mixtures (Fig. 4.1). On average, the measured evapotranspiration was in June 18 % and in July 27 % higher than in the 4-species mixtures. However, the effect was significant only for June ($p = 0.043$, Tab. 4.1). In July, there is a clear time effect, which is indicated by the strong increase of evapotranspiration on 17 July.

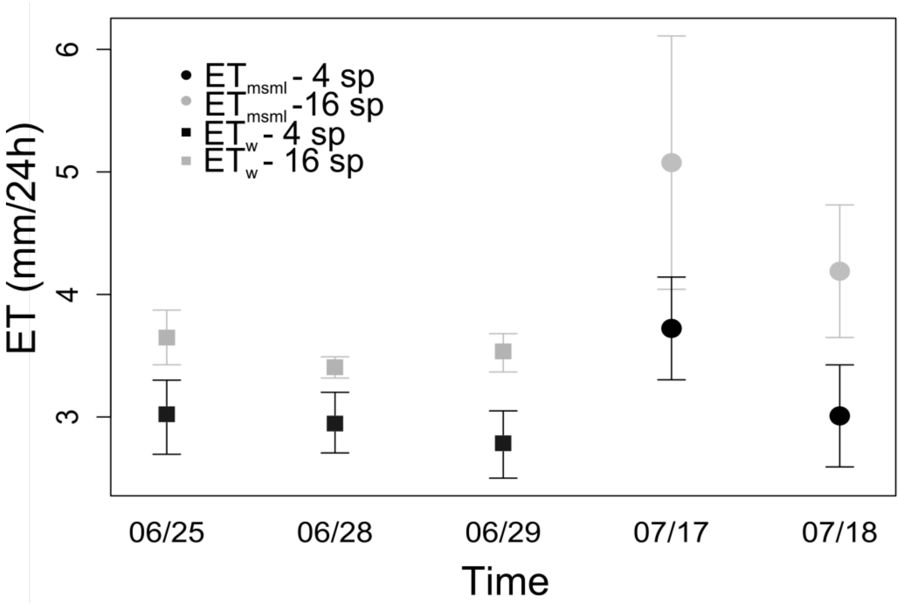


Figure 4.1 Comparison between mean evapotranspiration of 4-species mixtures (black dots) and 16-species mixtures (grey dots) on 25, 28 and 29 of June, and 17 and 18 of July 2012. The error bars indicate the standard error. Evapotranspiration was estimated from weight changes (ET_{w} - squares) and with the *msml* method (ET_{msml} - circles).

Table 4.1 Summary of linear mixed-effects model analysis for the evapotranspiration from 25-28-29 June and 17-18 July 2012.

	June			July		
Source of variation	df	L-ratio	*p*	df	L-ratio	*p*
SR	4	4.09	**0.0431** ↑	4	2.36	0.1244
Time	6	4.50	0.1054	5	5.20	**0.0226**
SR*Time	8	3.54	0.1707	6	0.08	0.7831

Models were fitted by stepwise inclusion of fixed effects. Listed are the results for degrees of freedom (df), the likelihood ratio tests (L-ratio) and the statistical significance of the fixed effects (p value). Arrows indicate increase (↑) or decrease (↓) of evapotranspiration with species richness. SR = species richness

Leaf area index and evapotranspiration were significant positively related ($R^2 = 0.73$, $p < 0.001$), whereby the communities with 16-species mixtures on average have higher LAI than 4-species mixtures (Fig. 4.2, respectively).

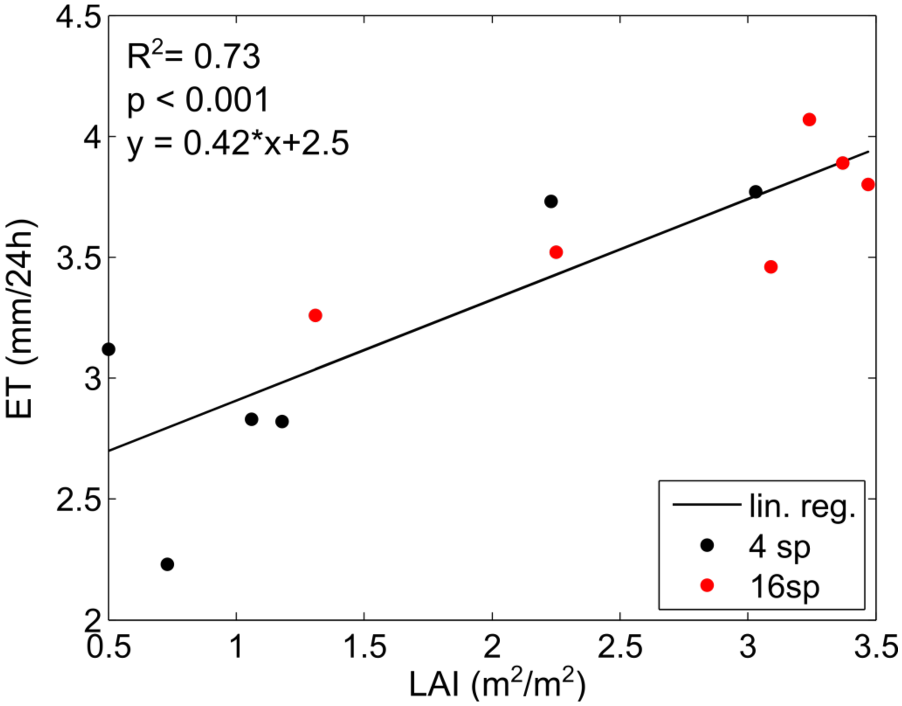


Figure 4.2 Correlation between leaf area index and evapotranspiration. Black dots indicate communities with 4-species mixtures and red dots indicate communities with 16-species mixtures.

4.3.2 Species richness effects on root water uptake patterns

Species richness (SR) had no significant effect on root water uptake in individual soil layers in June, but root water uptake decreased significantly with depth ($p < 0.001$) and depends on the time ($p = 0.027$) (Tab. 4.2). In contrast, SR significantly increased root water uptake in individual layers in July ($p = 0.004$) and again root water uptake decreased significantly with depth ($p < 0.001$). The interactions between SR, depth and time had no influence on the root water uptake at both considered times. Nevertheless, the uptake profiles between 4 and 16-species mixtures were considerably different, especially in 20 cm and 30 cm depth (June) and additionally in 60 cm in July (Fig. 4.3). Here, it becomes evident that the 16-species mixtures had higher uptake rates in these depths than the 4-species mixtures. Separate analyses per depth showed, that 16-species mixtures had a significantly higher root water uptake in 30 cm depth ($p = 0.028$), and also tended to have a higher root water uptake in 20 cm depth ($p = 0.061$) compared to 4-species mixtures in June (Tab. 4.3). In July, when the vapor pressure deficit increased (Fig. B.1), we found an enhanced water uptake in 30 cm ($p = 0.013$) and in 60 cm depth ($p = 0.015$) in the 16-species compared to the 4-species mixtures (Tab. 4.4). There were no differences of root water uptake in the topsoil.

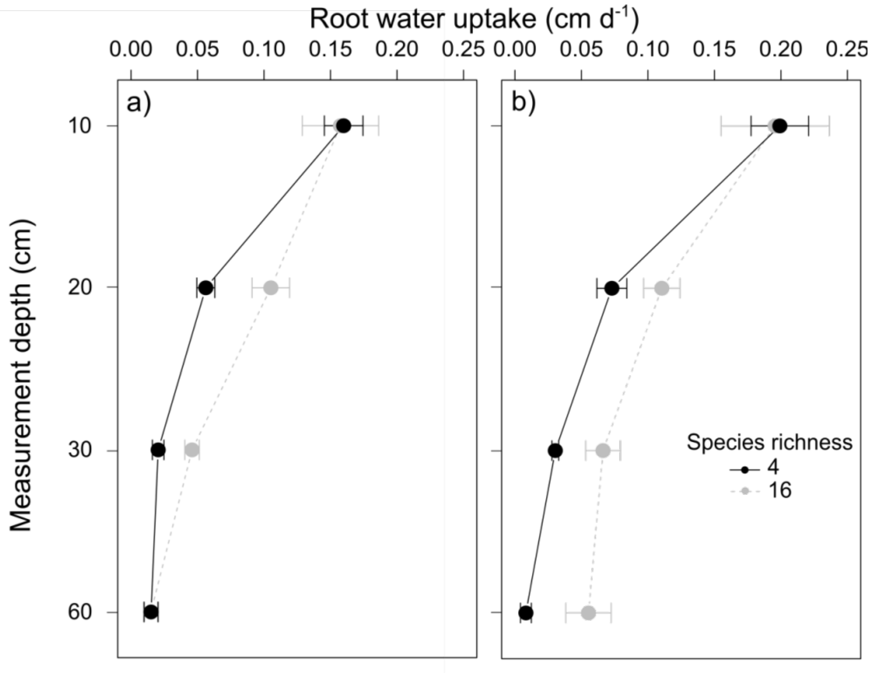


Figure 4.3 Comparison of mean root water uptake profiles for every measurement depth between 4-species mixtures (black dots) and 16-species mixtures (grey dots) for 25, 28 and 29 of June (a) and for 17 and 18 of July (b). The error bars indicate the standard error.

Table 4.2 Summary of linear mixed-effects model analysis for root water uptake profiles from 25-28-29 June and 17-18 July 2012.

	June			July		
Source of variation	df	L-ratio	p	df	L-ratio	p
SR	12	0.60	0.439	12	8.22	**0.004↑**
Depth	15	51.82	**<0.001**	15	48.76	**<0.001**
Time	17	7.22	**0.027**	16	0.75	0.386
Depth x Species	20	6.15	0.104	19	1.18	0.757
Depth x Time	26	3.66	0.721	22	3.75	0.289
Species x Time	28	3.12	0.210	23	1.92	0.166
Depth x Species x Time	34	1.91	0.928	26	0.98	0.806

Models were fitted by stepwise inclusion of fixed effects. Listed are the results for degrees of freedom (df), the likelihood ratio tests (L-ratio) and the statistical significance of the fixed effects (p value). Arrows indicate increase (↑) or decrease (↓) of root water uptake with species richness. SR = species richness

Table 4.3 Summary of linear mixed-effects model analyses for root water uptake in 10 cm, 20 cm, 30 cm and 60 cm for 25-28-29 June 2012.

	10 cm			20 cm			30 cm			60 cm		
Source of variation	df	L-ratio	p	df	L-ratio	p	df	L-ratio	p	df	L-ratio	p
SR	5	1.87	0.172	5	3.52	**0.061**	5	4.81	**0.028** ↑	5	0.00	0.993
Time	7	0.10	0.950	7	0.16	0.923	7	8.03	**0.018**	7	2.71	0.258
SR xTime	9	0.09	0.955	9	0.92	0.629	9	1.32	0.516	9	1.06	0.589

Models were fitted by stepwise inclusion of fixed effects. Listed are the results for degrees of freedom (df), the likelihood ratio tests (L-ratio) and the statistical significance of the fixed effects (p value). Arrows indicate increase (↑) or decrease (↓) of root water uptake with species richness. SR = species richness

Table 4.4 Summary of linear mixed-effects model analyses for root water uptake in 10 cm, 20 cm, 30 cm and 60 cm for 17-18 July 2012.

	10 cm			20 cm			30 cm			60 cm		
Source of variation	df	L-ratio	p	df	L-ratio	p	df	L-ratio	p	df	L-ratio	p
SR	5	0.00	0.953	5	2.58	0.108	5	6.18	**0.013** ↑	5	5.94	**0.015**↑
Time	6	9.99	**0.002**	6	0.01	0.908	6	0.15	0.697	6	0.61	0.434
SR x Time	7	2.30	0.129	7	0.39	0.533	7	0.36	0.546	7	1.04	0.309

Models were fitted by stepwise inclusion of fixed effects. Listed are the results for degrees of freedom (df), the likelihood ratio tests (L-ratio) and the statistical significance of the fixed effects (p value). Arrows indicate increase (↑) or decrease (↓) of root water uptake with species richness. SR = species richness

4.3.3 Dependence of root water uptake on root length density

Depth distribution of root water uptake was clearly related to root length density (RLD) in the 4-species mixtures on 17 and 18 July (Fig. 4.5a, c), since both, root water uptake and RLD, follows the same curve shape over the entire soil profile. On the contrary, the root water uptake profiles of the 16-species mixtures showed weak relationships to RLD (Fig. 4.5b, d). Here, root water uptake is substantially smaller than RLD in 10 cm depth while it is considerably higher than RLD in deeper layers. Interestingly, this is reinforced on 17 July when evapotranspiration had the highest value within the considered days. Furthermore, root water uptake in the 16-species mixtures showed a greater variance, as evident from the wide grey band in Fig. 4.5b and 4.5d, which indicates the maximum and minimum values. Interestingly, we found no significant difference in root length density between both diversity levels (Fig. 4.4a, Tab. B.2) and only a slight trend for greater belowground biomass in the 16-species mixtures (Fig. 4.4b, Tab. B.2).

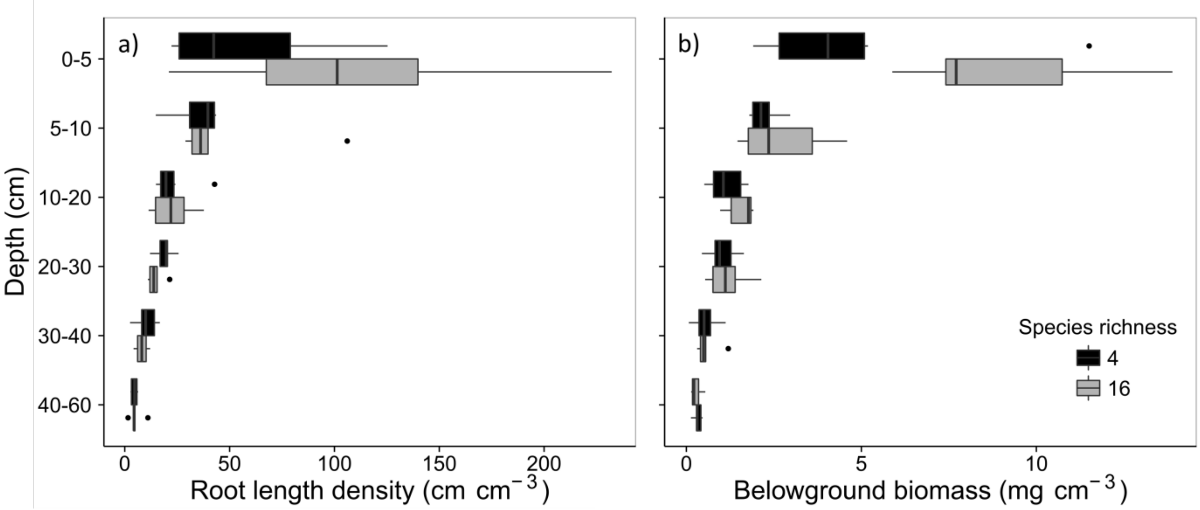


Figure 4.4 Comparison of the root length density profiles of 4 and 16-species mixtures (a) and the belowground biomass profiles of 4 and 16-species mixtures (b).

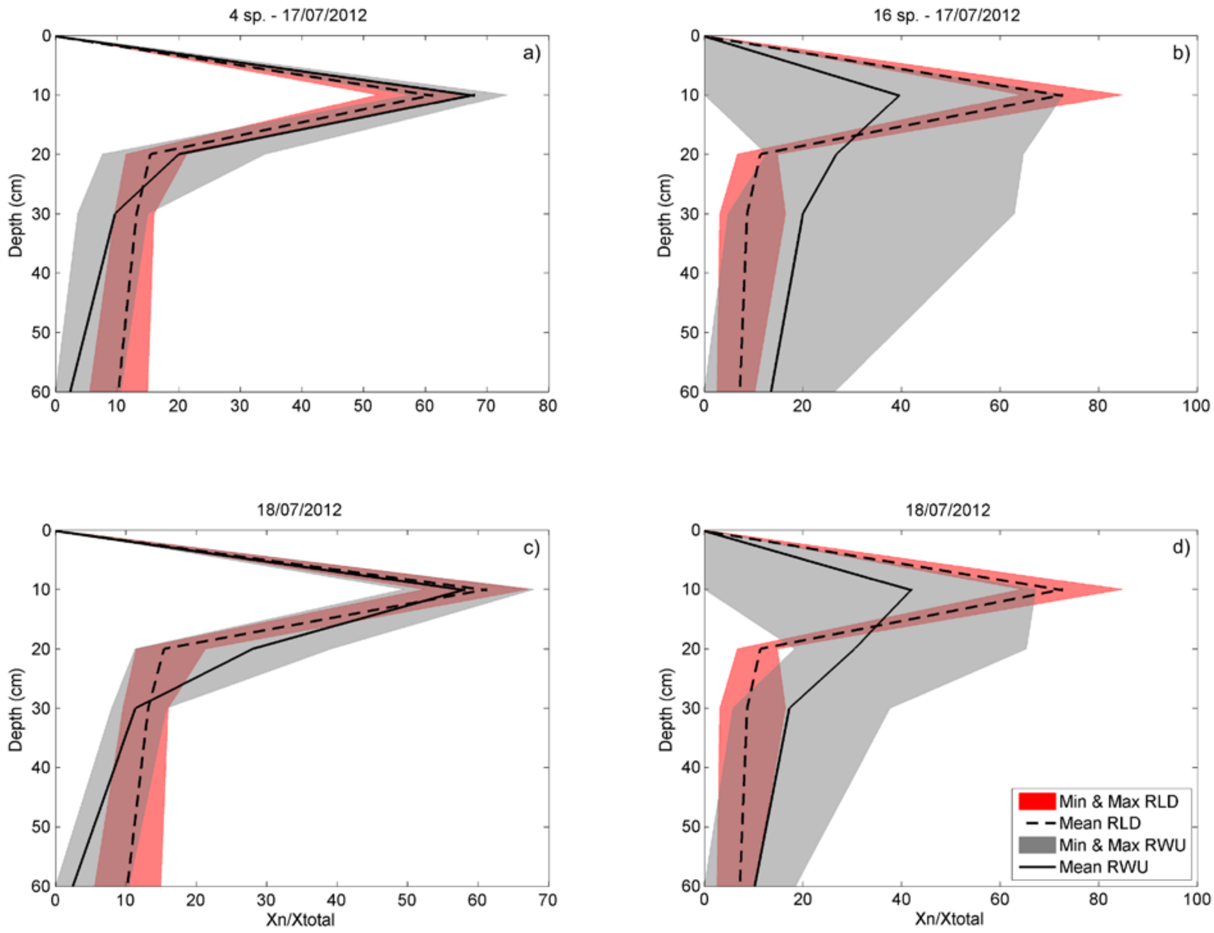


Figure 4.5 Mean root length density (dashed black line) and root water uptake profile (solid black line) for 17 of July and for 4-species mixtures (a) and for 16-species mixtures (b) as well as for 18 of July (c - 4-species mixtures; d - 16-species mixtures). The shaded areas indicate the maximum and minimum measured values of 6 lysimeters, respectively for root length density (red) and root water uptake (grey).

4.3.4 Effect of species richness on root area and RAI:LAI ratio

The root area index (RAI) as a measure of root surface per area soil was not significantly different between diversity levels (Fig. 4.6a, Tab. B.3). The ratio between RAI and LAI provides information on the ratio between transpiring area and water acquiring areas. LAI is used because it is directly related with evapotranspiration (Fig. 4.2). Unlike the RAI, the RAI:LAI ratio was slightly higher in 4-species mixtures than in 16-species mixtures ($p = 0.053$, Tab. B.3) suggesting that the potentially transpirational surface areas are higher in 16-species mixtures while the relative surface for water uptake is reduced as the RAI is nearly equal in both diversity levels. Hence uptake velocity (flux per unit root area) is likely increased in 16-species mixtures.

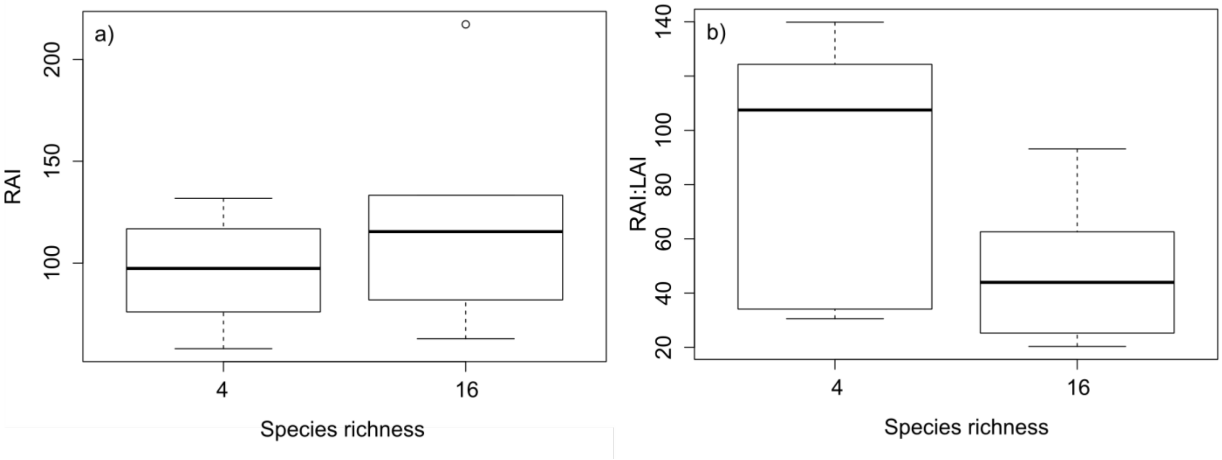


Figure 4.6 Comparison of the root area per soil area (root area index - RAI) for 4 and 16 species mixtures (a) and the RAI:LAI ratio for 4 and 16-species mixtures (b).

4.3.5 Leaf water potential and stomatal conductance of functional groups

Species richness (SR) and functional group (FG) identity had no significant effect on measured predawn leaf water potential (PLWP), whereas we found a significant interaction between SR x FG identity ($p = 0.011$, Tab. 4.5). This interaction was obviously due to the difference of PLWP of grasses, which showed more negative values and a higher variance in the 4 species mixtures compared to 16-species mixtures (Fig. 4.7a). Although the differences in the PLWP of grasses between the two species richness levels were not significant (Tab. 4.5) they point to a higher water stress of grasses in less diverse communities. Further, plant diversity did not affect midday leaf water potential (MLWP) but MLWP differed between functional groups ($p < 0.001$). Grasses had a more negative MLWP than the other three functional groups in both diversity levels (Fig. 4.7b). Moreover, the MLWP of tall herbs differed between diversity levels ($p = 0.003$, Tab. 4.5). The MLWP of tall herbs in 4-species mixtures was less negative than that of tall herbs in 16-species mixtures, which was in the same range with small herbs and legumes (Fig. 4.7).

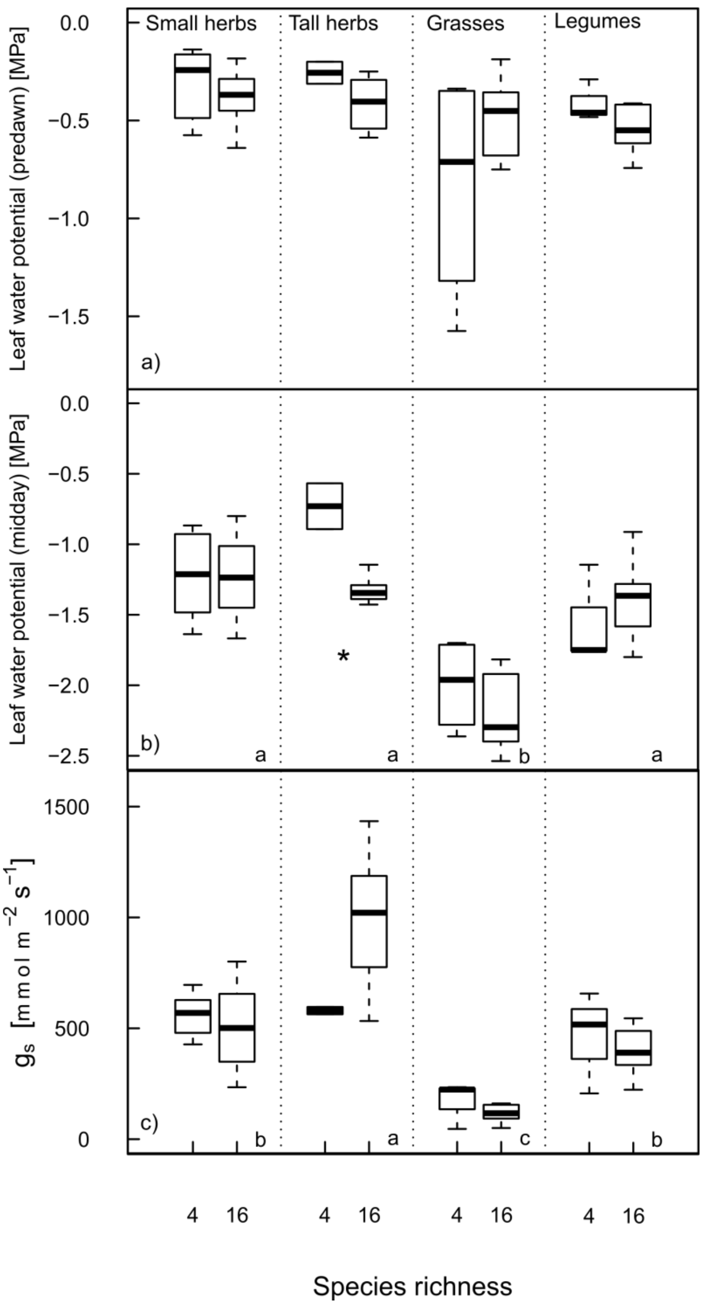


Figure 4.7 Boxplots measured leaf water potential (predawn (a) and midday (b)) and measured stomatal conductance (c) of functional groups (small herbs, tall herbs, grasses and legumes) for 4 and 16-species mixtures (17-19 July 2012). Differences among functional groups are marked with lower case according the Tukey's HSD test. * indicate significant differences of functional groups between 4 and 16-species.

Table 4.5 Summary of linear mixed-effects model analysis for leaf water potential and stomatal conductance for 17-19 July 2012.

	LWP predawn		LWP midday		g_s	
	X^2 ratio	p	X^2 ratio	p	X^2 ratio	p
SR (log-linear)	0,34	0,559	0,18	0,676	3,54	0,06
FG.ID	7,24	0,065	32,61	**< 0.001**	21,83	**< 0.001**
SR x FG.ID	11,06	**0,011**	5,91	0,116	18,01	**< 0.001**
Small herbs						
SR	1,06	0,302	0,3	0,584	0,03	0,873
Tall herbs						
SR	3,43	0,064	8,72	**0,003↑**	11,79	**< 0.001↑**
Grasses						
SR	2,79	0,095	0,54	0,462	0,1	0,750
Legumes						
SR	0,73	0,392	0,48	0,487	0,27	0,605

The fixed effects and their interaction were added stepwise to a constant null model containing only the random effects. Significant improvement of the model after adding the fixed effects was tested with maximum likelihood method and likelihood ratio tests (χ2 ratio). p values are the statistical significance of the effects. Arrows indicate increase (↑) or decrease (↓) of leaf water potential (LWP) or stomatal conductance (gs) with species richness, SR is the species richness and FG.ID is the functional group identity.

Stomatal conductance (g_s) differed between functional groups ($p < 0.001$) and plant diversity on stomatal conductance differed between functional groups (SR x FG identity, $p < 0.001$, Tab. 4.5). Tall herbs had higher and grasses much lower stomatal conductance than the other two functional groups. Tall herbs in higher diverse mixtures had higher g_s values with a higher variance than in 4-species mixtures. Stomatal conductance of small herbs, grasses and legumes did not differ between diversity levels.

4.3.6 Rooting types of functional groups

The comparison of different rooting types within the functional groups (based on literature data, Roscher et al., 2004) indicates that there is a clear distinction between tall herbs and grasses. Nearly 80 % of all tall herbs have a large primary root system with additional secondary fibrous roots, whereas the root system of all present grass plants consist of an extensive secondary root system with only short-living primary roots (Fig. 4.8). Similarly, about 61 % of all small herbs and 55 % of all legumes have also an extensive secondary root system. Plants with beet- or stake-like taproots were only in a few cases represented.

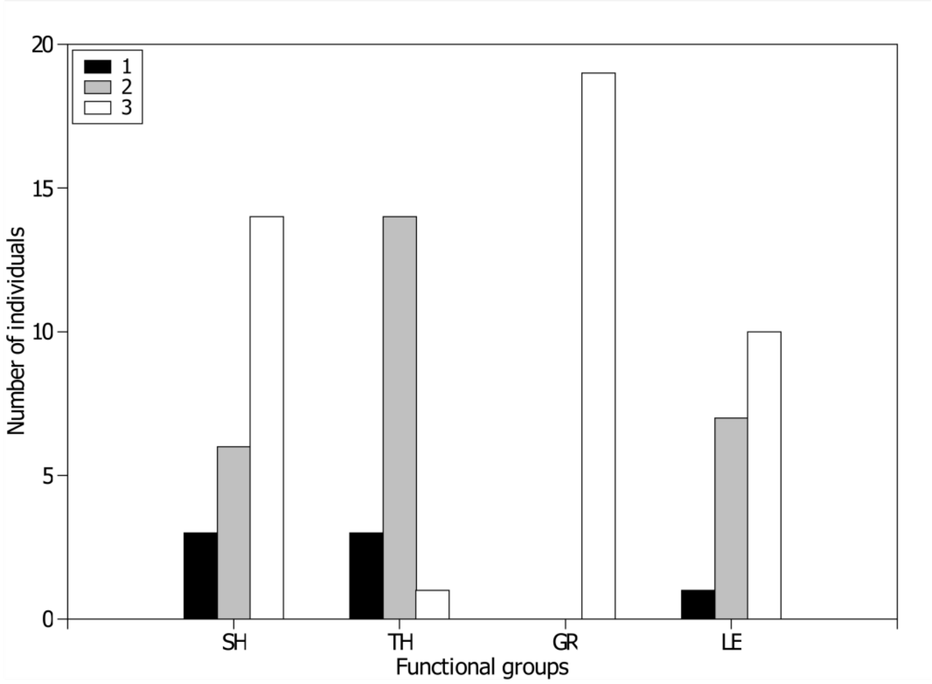


Figure 4.8 Overview of the distribution of different rooting types of the functional groups present in the species pool of the lysimeter experiment in the Ecotron based on literature (see Roscher et al., 2004; Gubsch et al., 2011). Rooting type is distinguished into three categories: 1 = long-living primary root system (beet- or stake-like taproots), 2 = secondary fibrous roots in addition to the primary root system, 3 = short-living primary root system, extensive secondary root system.

4.3.7 Distribution of functional groups by leaf area index

The proportion of each functional group on total leaf area index is given in Fig. B.2. In 4-species mixtures, half of the studied communities were dominated by small herbs. The other three lysimeters had a different composition and were mainly composed of tall herbs, grasses or legumes. In 16-species mixtures, tall herbs were the most abundant functional group as confirmed by the comparison of leaf area index between diversity levels (Fig. B.3).

4.4 Discussion

In this study we investigate whether higher evapotranspiration rates in more diverse plant communities can be explained by a more efficient depletion of the soil water reservoir. Especially, we examined (1) whether this is driven by exploitation of greater depths or (2) by a vertical below ground niche differentiation of the respective rooting systems and thus a more efficient water uptake within the respective depth, and (3) how root traits of the composing species influence community root water uptake patterns.

We found that the root water uptake of 16-species mixtures was shifted to deeper soil layers compared to 4-species mixtures. Further, we could show that this shift of root water uptake is associated with a decrease in leaf water potential, which is a pre-requisite for exploring deeper layers. This is reinforced when the evapotranspiration demand per unit root length is increased. However, a particular plant root structure is required, which allows a more efficient exploitation of the soil water reservoir. We will discuss these points in detail in the following sections.

Effects of species richness on evapotranspiration rates

For all investigated times (25, 28 and 29 June, 17 and 18 July 2012) we found an enhanced (although not significant trend) of actual evapotranspiration for the 16-species mixtures compared to the 4-species mixtures, similar to studies of Kreutziger (2006) and Van Peer et al. (2004). An increase in transpiration with greater leaf area has been reported for several plant communities (Eavis and Taylor, 1979; Irritz and Lindroth, 1996; Rosset et al., 1997; Li et al., 2005; Li et al., 2006; Zhongmin et al., 2009) and our study confirms this finding for evapotranspiration over two biodiversity levels. In our study higher leaf area coincided with higher biodiversity (Spehn et al., 2000b; Van Peer et al., 2004; Roscher et al., 2005; Marquard et al., 2009). In contrast, other studies also reported that a higher leaf area and thus a greater plant cover of more diverse plant communities reduced soil evaporation but show an increased transpiration, whereas plant communities with reduced species richness show an enhanced soil evaporation and lower transpiration (Spehn et al., 2000a; Leimer et al, 2013). This opposite effects of soil evaporation and transpiration in communities with different diversity levels may explain that we found only a small difference in evapotranspiration between the two considered species mixtures. However, the high correlation between LAI and evapotranspiration indicates that transpiration is the substantial portion of evapotranspiration.

Higher exploitation of deeper soil layers in 16-species mixtures

At higher species diversity (16-species mixtures) we found a significantly higher root water uptake in 30 cm and 60 cm in July. This shift of root water uptake to deeper layers can be explained with the increased evapotranspiration demand during this time. These results are in line with those of Verheyen et al. (2008), who observed a higher exploitation of soil water by more diverse grassland systems.

Following a common assumption, vertical root water uptake profiles are related to the distribution of root length density over the soil profile (e.g. Perrochet, 1987; Prasad, 1988; Jarvis, 1989, Feddes et al., 2001). Here we found no difference in the distribution of root length density (RLD) over the soil profile between 4 and 16-species mixtures. This is opposed to the assumption that a vertical differentiation in the root system between different species mixtures and functional groups should be visible (Berendse 1982; Brassard et al., 2011). In our study, there was only a small difference in RLD and slight significant difference in belowground biomass in the upper 5 cm and thus there is no evidence for a spatial root niche differentiation in the plant-soil monoliths in the Ecotron, which is in line with the findings of Ravenek et al. (2014) for the entire Jena Experiment.

Nevertheless, for 16 species mixtures we could show, that the root water uptake was reduced compared to RLD in the upper layers, but intersects the RLD from 20 cm to 60 cm. This shift of root water uptake from soil layers with higher RLD to less densely rooted soil layers was also observed by others (e.g. Lai and Katul, 2000; Li et al., 2002; Dousson et al., 2006; Garrigures et al., 2006) and agrees with models of root water uptake (Schneider et al.,2009; Bechmann et al., 2014). For instance, Dousson et al. (2006) showed that the proportion of water uptake by a specific root portion changes dynamically with time and the position of a root portion in the entire root system. Hence, the root water uptake is linked to plant hydraulic properties and also to soil properties and can therefore not be related to RLD entirely.

Dynamic niche partitioning in 16 species mixtures

In contrast to other diversity experiments, for instance the Cedar Creek experiment (Mueller et al., 2013), RLD measurements did not indicate spatial niche differentiation of roots within the two considered species mixtures. Similar results were found for standing root biomass within all species mixtures of the Jena Experiment (Ravenek et al., 2014). These results are in line with Mommer et al. (2010) and similar findings were also reported in the review of De Kroon et al. (2012). One explanation for this could be the nutrient rich soil of the Jena Experiment (Bessler et al., 2009). As the Jena Experiment was a former agricultural field, N availability is comparably high and was not reduced after establishing the experiment (Oelmann et al., 2011). Bessler et al. (2009) suggested that the high availability of nutrients, especially N, lead to an increased root growth during the first years of the experiment so that the exploitation of soil resources is maximized. When competition for belowground resources, especially nutrients, is low (Hodge et al., 1999) and competition for light increases, plants invest more in aboveground biomass production to be competitive, especially in higher diverse species mixtures. Therefore, biodiversity experiments general show increase in above-ground biomass production with increased species richness (e.g. Naem et al., 1994; Tilman et al., 2001; Hector et al., 1999; Spehn at al., 2005; Cardinale et al., 2007, Bessler et al., 2009; Marquard et al., 2009; Mommer et al., 2010).

A consequence of higher biomass production is an increased leaf area, which leads to increased transpiration (Eavis and Taylor, 1979; Van Peer et al., 2004), which in turn has to be met by higher root water uptake. Referring to the RLD in this study, the limiting factor for water uptake might be, comparatively to the higher transpiration, the reduced active root surface in 16-species mixtures rather than the absolute availability of soil water (Rajcan and Swanton, 2001). To verify this point, we introduced the ratio between root area index (RAI) and leaf area index (LAI) because the amount of root water uptake as well as transpiration depends strongly on the active uptake surface of roots and the surface of leafs. Although we found no higher root area in 16-species mixtures, the RAI:LAI ratio was much smaller in 16-species mixtures than in 4-species mixtures.

Thus, the water uptake per root area in 16-species mixtures was increased, which should theoretically induce more negative xylem potentials. This allows for a more complete use of the root system (Bechmann et al., 2014). The decreasing RAI:LAI ratio should also affect leaf water potential. In general, the leaf water potential describes the potential gradients between leafs and soil, which drives the water uptake and shows a daily pattern with a minimum in the afternoon where transpiration is maximized (Sala et al., 1981). During 17, 18 and 19 July 2012 we measured predawn and midday leaf water potential for all functional groups in mixtures of both diversity levels. The midday leaf water potential of tall herbs in 4-species mixtures showed a smaller decrease compared to 16-species mixtures, where it was in the same range as those of small herbs and legumes. This can be explained by two processes. First, the smaller decrease in the lower species mixture may be interpreted as less lower stress. Alternatively, the very negative matric potentials in tall herbs in the diverse mixture may indicate an adaptation of the plant to take up more water per root area and at the same time from deeper soil layers. The latter one can be denoted as a dynamical niche partitioning. Stomatal conductance (*gs*) may help to clarify whether it is the first or the latter process, as it is a measure for the transpiration flux trough open stomata. If *gs* is still high, as it is the case for the tall herbs in 16-species mixtures, it indicates that the plants are still able to transpire. In case of the tall herbs in 16-species mixtures, we suggest that the plants obtain a greater proportion of soil water from deeper layers. This might explain the wide range in the root water uptake patterns in the 16-species mixtures, because these plants adjust their uptake depth according to their demand within the community.

This is different for grasses, which had in the diversity levels, and compared to the other functional groups, strongly reduced leaf water potentials. The measured g_s of grasses indicate that they transpire little, irrespective of their very negative leaf water potential.

Briefly, our results indicate a dynamic niche partitioning by tall herbs, which transpire most and decrease leaf water potentials in a way that water uptake can be extended deeper into the soil.

Plant root structure and shift of ecosystem composition enables redistribution of root water uptake

With a rooting system, that mainly consist of extensive secondary roots (only short-living primary roots) (Roscher et al., 2004; Kulmatiski and Beard, 2013), grasses use exhaustively soil water from the upper soil layer (Kulmatiski and Beard, 2013; Leimer et al., 2014). Grasses also root in deeper soil layers, but the structure of secondary roots is not able to establish the required pressure heads to take up water and thus grasses face earlier water stress than plants with a more heterogeneous root system

(Leimer at al., 2013; Bechmann et al., 2014). In comparison, tall herbs mainly have a primary root system (taproots for water transport) combined with secondary fibrous roots (fine roots for water uptake), which allow water uptake from deeper soil layers (Hamblin and Tennant, 1987; Bechmann et al., 2014) and thus are more competitive and contribute to a more sustainable water use in plant communities of higher diversity (Leimer et al., 2013).

In our study, small herbs and additionally grasses built the main part of the plant communities in 4-species mixtures (Fig. B.3 and B.4). In contrast, tall herbs and to smaller proportion legumes were the functional groups with the highest proportion of leaf area in 16-species mixtures. Beside growth stature, these functional groups differ in rooting type. As stated above, tall herbs mainly have a distinct heterogeneous root system whereas grasses and small herbs have a homogeneous secondary root system. These conclusions suggest that the community transpiration in 16-species mixtures is dominated by the tall herb contribution, whereby they show a complementarity in belowground exploitation regarding the resource soil water. This plasticity in root water uptake is possible due to their root system and is indicated by the shifted root water uptake in deeper layers.

In summary, in more diverse communities in this experiment consisted of more plants of functional groups that are able to adjust their root water uptake strategy, based on the root system structure, in a way that the water use of the entire community is optimized (De Boeck et al., 2006; Naeem and Li, 1997) and the water uptake is more equally distributed over the depth profile. Additionally, plants with more heterogeneous root systems are in advantage because they can explore the soil water more effectively. In addition, they suffer less from drop of xylem potential when enhancing flow. Furthermore, the comparison between June and July showed that species in more diverse plant communities can escape a possible competition for water resources by exploiting deeper water resources, especially if the evapotranspiration demand is increased. Particularly tall herbs in 16-species mixtures contributed to a dynamic niche partitioning regarding root water uptake.

Unfortunately, this lysimeter experiment allowed only the investigation of two species richness levels and only for a few days during vegetation period. We therefore suggest further studies with more diverse environmental situations, and under a larger range of soil moisture conditions, to get deeper process understanding concerning the change of root water uptake strategies within the particular communities. Additional detailed stable isotope analysis could further improve these studies.

4.5 Conclusions

The aim of this study was to investigate the effect of plant diversity on community evapotranspiration and especially on the distribution of root water uptake. We used a data-driven method to estimate root water uptake profiles based on short term fluctuations of soil moisture data, measured in a lysimeter experiment considering contrasting species richness. To date, estimation of root water uptake has not been attempted for research on the relation between species richness and water use, which is the novel on this thesis.

Although we found no spatial niche differentiation, neither of root length density nor of root biomass, the root water uptake profiles show that 16-species mixtures take up more water from deeper layers than plants in 4-species mixtures. This indicates a niche partioning regarding soil water use in communities of higher species richness, which is, contrary to common assumptions, not characterized by root length density distribution but from plasticity in belowground resource use. Additional leaf water potential measurements reveal that this shift of root water uptake is associated with a decrease in leaf water potential, which is a pre-requisite for exploring deeper layers. The second pre-requisite is a particular plant root structure with a well-developed transport root system, which is typical for tall herbs and allows a more efficient exploitation of the soil water reservoir.

However, to draw general statements on the effect of plant biodiversity on root water uptake, we suggest further studies, especially on more ecosystems with more different diverse plant communities. Additionally, investigations of different environmental situations, i.e. from dry to wet conditions, are needed to get deeper process understanding concerning the change of root water uptake strategies within the particular communities. Since the investigation on root structure was only done with data from literature, we further suggest the combination of extensive stable water isotope measurements with a detailed examination of the root structure of the respective sampled plant individuals.

More broadly, this study shows that the investigation of root water uptake profiles in combination with plant physiology is crucial for understanding the processes of water use and water uptake strategies in ecosystems.

Chapter 5

Synthesis

5 Synthesis

The main focus of this thesis was to identify a simple but sufficient accurate method for estimating water uptake from soil water content measurements and their application to answer the eco-hydrological question, whether co-existing plant species affect community root water uptake. The resulting process understanding is relevant i.e. for developing sustainable management strategies to maintain ecosystem functions. This becomes particularly important in the light of multitude pressures evoked through increasing globalization and economic interests of human society, associated with changes of ecosystems and a tremendous loss of plant species diversity. For those reasons, minimal-invasive and easy to use methods for estimating root water uptake on plant and ecosystem level are needed. However, in a hydrological framework, a variety of different approaches are suggested ranging from simple water balance methods to complex model applications. Each method has its own assets and drawbacks, which renders an appropriate selection difficult, especially for non-hydrologists. Certainly, this might be a reason why studies investigating the relations between species richness and water use have been conducted without estimating root water uptake profiles. In this context, this dissertation deals with measuring and understanding ecosystem root water uptake in plant communities of varying species diversity. This chapter summarizes the results of the present thesis by answering and concluding the research questions posed in Chapter 1.

5.1 Summary of the results

Since the first aim was to find a simple method for estimating root water uptake profiles, Chapter 2 deals with the evaluation of four different complex water balance methods, which do not require any a priori information on root distribution parameters. We set this prerequisite for the method selection because these parameters are cumbersome to measure in the field and also the relevance for root water uptake distribution is uncertain (Hamblin and Tennant, 1987; Lai and Katul, 2000; Li et al., 2002; Doussan et al., 2006; Garrigues et al., 2006; Schneider et al., 2009). The simplicity is required by the fact that the method are suggested also for application by non-hydrologists respectively researcher, who are not familiar in the field of modelling. The evaluation of each method was performed stepwise on a synthetic experiment, while after each step the worst method was rejected. The first two steps comprised the testing of accuracy for estimating evapotranspiration and water uptake profiles considering different measurement frequencies. In the last step, we investigated the influence of sensor uncertainties on the outcomes of the two remaining methods. To summarize, the conclusion of Chapter 2 of the thesis are:

1. *Which data-driven method can be adopted to obtain accurate estimates of evapotranspiration and root water uptake from standard volumetric soil water content measurements?*

The most suitable approach to estimate evapotranspiration and root water uptake was found to be the Multi Step Multi Layer Regression (*msml*). This simple method derives root water uptake from diurnal fluctuation of soil water content measurements (Li et al., 2002; Guderle and Hildebrandt, 2015). It applies a regression over multiple time steps on soil moisture time series of each measurement depth. This method allows a first order distinction between root water uptake and soil water flux and thus the estimation of root water uptake patterns over depth and time. The *msml* method does not require soil hydraulic parameters, which is a benefit in light of the application on real world data compared to the more complex Inverse Model. Commonly soil hydraulic parameters have to be calibrated before application in soil water flow models. In turn, this introduces additional uncertainties in the parameter due to the non-uniqueness of calibrated parameter sets (Hupet et al., 2002) and thus in simulated soil water fluxes and root water uptake (Dardanelli et al., 2004; McIntyre et al., 1995; Hopmans and Bristow, 2002; Zuo et al., 2002). For application of the *msmsl*, only volumetric soil water and rainfall measurements have to be available, however, in temporal and spatial high resolution. This leads to the second issue addressed in this part of the thesis.

2. *Which impact has the measurement frequency on the prediction of evapotranspiration and root water uptake?*

In general, our results show that the required measurement frequency of soil water content depends on the different methods. Following up on the chosen method, the Multi Step Multi Layer Regression showed better applicability for measurements with a temporal resolution of 3h or less. This method analyses the diurnal cycle of soil water content, which is only captured by a high measurement frequency. Furthermore, higher measurement frequencies better reflects the temporal variance of evapotranspiration, which may be considerable over the course of a day (Jackson et al., 1973).

Beside the impact of parametrization and the measurement frequency, uncertainties arise also from the sensor itself, especially from measurement noise (precision) and calibration (accuracy). Therefore, the following question was asked:

3. *How are the estimates of evapotranspiration and root water uptake influenced by sensor uncertainties?*

This issue is a critical point in light of the application on real world data. The fact that accurate estimation of soil water content at field scale is intricate (Hupet, 2003) can have significant impacts on data-driven approaches and soil hydrological models (Spank et al., 2013). The performance of the Inverse Model is strongly influenced by the sensor uncertainties, putting it's appropriateness for estimating real world water uptake into question. In contrast, the simpler Multi Step Multi Layer Regression is comparable robust towards measurement errors. Although, it was somewhat affected by sensor precision, the calibration errors barely influenced the estimates of evapotranspiration and root water uptake (see Tab. 2.4). These results were expected, since random scatter of measured data, which are introduced by measurement noise, blurry the required course of the diurnal cycle of soil moisture. In contrast, imprecise sensor calibration does not affect the course of the soil moisture desiccation, but the absolute value of measurements. Sensor precision uncertainty cannot be avoided, since this is a technical property of sensors, and thus additional noise reducing filters are suggested for further application (Li et al., 2002; Peters et al., 2014).

The feature that water flow, evapotranspiration and water uptake profiles are known in numerical experiments makes them an ideal tool for method respectively model assessments. As these components are notoriously unknown under field conditions, such evaluations are necessary before final application of methods. To close the gap between numerical and field experiments, Chapter 3 follows the line of the analysis of Chapter 2, but on real field data from a lysimeter experiment. Lysimeters are well suited for this excercise since they deliver a precise and independent measurement of evapotranspiration by registration of weight changes (Meissner et al., 2008; von Unhold and Fank, 2008; Allen et al., 2010; Peters et al., 2013). An accuracy assessment considering magnitudes of evapotranspiration, soil texture variability, sensor uncertainty, and implicitly upscaling was carried out for the Multi Step Multi Layer Regression. For this, we employed measurements of soil moisture from 12 weighable lysimeters. To summarize, the conclusions of the second part of the thesis are:

4. *How does the magnitude of evapotranspiration influence the prediction of evapotranspiration and root water uptake?*

This study indicates that the Multi Step Multi Layer Regression is able to predict the actual evapotranspiration of the lysimeters from soil water content measurements. Although the evapotranspiration and thus the of distribution of water uptake is slightly overestimated, the overall error of about 20 % is in the same range as obtained in the numerical study (Chapter 2) and for common soil water balance methods (Allen et al., 2010). However, the results indicate that the method shows a sensitivity regarding the magnitude of evapotranspiration. From the comparison of predicted and measured evapotranspiration of the single lysimeters, we see that the uncertainty of the method decreases with increasing evapotranspiration. Higher evapotranspiration rates lead to a steeper decreasing course of the daytime soil moisture time series, which can be better described by the fitted linear function of the *msml* method.

5. *Is the method restricted by soil texture variability?*

Soil texture had no influence on the prediction quality of root water uptake. Indeed, this constitutes a major advantage compared to numerical soil water flow models like the Inverse Model examined in Chapter 2 and already discussed in Question 1.

Beside the aforementioned discussed sources of error, sensor uncertainties are an additional source of error scientist encounter while measuring soil water content insitu. Therefore, the following issue was investigated:

6. *How to deal with real sensor uncertainties?*

We showed in Chapter 2 that sensor imprecision somewhat affected predictions of root water uptake by the Multi Step Multi Layer Regression. However, it is difficult to disentangle sensor imprecision of real field measurements and we therefore suggested using a filter routine for smoothing the time series of soil water content measurements. The results indicate that the filter routine, proposed in Chapter 3, describes the real data sufficiently well such that the measurement uncertainty has no influence on the prediction of water uptake and evapotranspiration.

Overall, the results of Chapter 3 corroborate the findings from Chapter 2 that the Multi Step Multi Layer Regression is a sufficiently accurate method for estimating root water uptake from soil water content measurements and can be regarded as complementary means to more complex methods.

Compared to the previous Chapters, in Chapter 4 we focused on the application of the Multi Step Multi Layer Regression to improve our understanding on the effect of co-existing plant species on the community root water uptake. Especially, we investigated whether diverse plant communities exploit soil water more efficiently than less diverse ones. So far, research on this question has been conducted without the measurement setup allowing for the estimation of root water uptake profiles. The application of the Multi Step Multi Layer Regression on lysimeters with soil-vegetation monoliths of a long-term grassland biodiversity experiment (Jena Biodiversity Experiment) combined with measurements of leaf water potentials, stomatal conductance and root traits, constitutes the novelty of this research. To summarize, the conclusion of Chapter 4 of the thesis are:

7. *Is root water uptake in diverse plant communities achieved by exploiting greater depths (spatial complementarity)?*
8. *Is there a vertical belowground niche separation due to different rooting distributions between two diversity levels?*

The estimated root water uptake profiles show that 16-species mixtures take up more water from deeper layers than plants in 4-species mixtures. However, we found no spatial niche differentiation, neither of root length density nor of root biomass. Interestingly, this is contrary to the common assumptions that root water uptake is characterized by root length density distribution (e.g. Perrochet, 1987; Prasad, 1988; Jarvis, 1989, Feddes et al., 2001). Additional leaf water potential measurements reveal that this shift of root water uptake is associated with a decrease in leaf water potential, which is a pre-requisite for exploring deeper layers. Briefly, in combination with measurements of stomatal conductance (g_s), our results indicate plasticity in belowground resource use and dynamic niche partitioning by tall herbs, which transpire most and decrease leaf water potentials in a way that water uptake can be extended deeper into the soil.

However, Casper and Jackson (1997) elucidated that root characteristics like biomass, fine root density and total surface area determine the degree of soil exploitation and thus are important for belowground competition respectively complementarity. Hence, we additionally examined the following question:

9. *How do root traits of the involved species influence community root water uptake patterns?*

Our results suggest that plant root structure may be a pre-requisite for exploring deeper layers. The root structure of tall herbs consists mainly of primary root system combined with secondary fibrous roots, which allow water uptake from deeper soil layers (Hamblin and Tennant, 1987; Bechmann et al., 2014). The adjustment or rather the enhancement of root water uptake by leaf water potential becomes effective with such a root system.

In comparison, grasses and small herbs have a homogeneous secondary root system, which is not able to establish the required pressure heads to take up water. Thus, grasses use predominantly soil water from the upper soil layer (Kulmatiski and Beard, 2013; Leimer et al., 2014).

5.2 Perspectives of future research

In the course of this thesis a comparative study on a numerical experiment was carried out to come up with a suitable method for estimating evapotranspiration and root water uptake from standard soil water content measurements. Furthermore, the most suitable method (Multi Step Multi Layer Regression) was evaluated on a lysimeter experiment. These parts of the thesis were motivated by a practical question in ecohydrological applications.

From the model evaluation, we could draw the following conclusion, which are suggested to be considered while planning the instrumentation of further experiments. First, a pre-requisite for applying the Multi Step Multi Layer Regression method is a high temporal resolution of soil moisture measurements to capture the diurnal cycle. Additionally, we recommend a high spatial resolution of soil moisture sensors over the entire soil column. This is important to record the non-linear nature of the root water uptake (Kumar et al., 2013; Guderle and Hildebrandt, 2015). An installation as deep as possible in the soil is suggested to sample the contribution of capillary rise and the redistribution on soil water fluxes.

The results of this work put forward that soil water content measurements contain a great deal of information for estimating evapotranspiration and root water uptake. Indeed, the respective sensor precision uncertainties have to be considered and can be eliminated by applying a smoothing filter. Since the applied filter routine used a fixed window width, we suggest using a dynamic smoothing filter with an adaptive window width like proposed in Peters et al. (2013). Moreover, a carefully check regarding abnormalities/disturbances in the course of the applied soil moisture time series is strongly recommended.

As part of the comparative study of Chapter 2, we found that the Inverse Model was strongly affected by calibration uncertainties of soil moisture sensors, whereas sensor precision had a much smaller effect. Based on this result, we rejected this model for further use. However, we suggest testing this method on lysimeter experiments where all sensors in the profile are well calibrated.

The second part of this thesis comprised the investigation of the ecological issue whether diverse plant communities exploit soil water more efficiently than less diverse ones. The conducted lysimeter experiment allowed only the investigation of two richness levels and only for a few days during vegetation period. The finding of this study provides first hints on the processes associated with root water uptake in plant communities in non-water limited environments. However, more research is needed to disentangle the single impacts on root water uptake strategies for a thorough understanding of ecosystem functioning. In particular, our sample was small and our findings should be confirmed on a larger dataset with higher plant diversity gradients. Moreover, investigations of different environmental situations, i.e. from dry to wet conditions, are essential.

In this work, we draw conclusions on how root structure influence water uptake. Since, the investigation on root structure was only done with data from literature; we further suggest the combination with extensive stable water isotope measurements with a detailed examination of the root structure of the respective sampled plant individuals.

For future research, such facilities like the CNRS Ecotron are valuable, because they allow simultaneous high resolution measurements of evapotranspiration and water fluxes from of different ecosystems under the same controlled conditions.

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Appendices

Appendix A

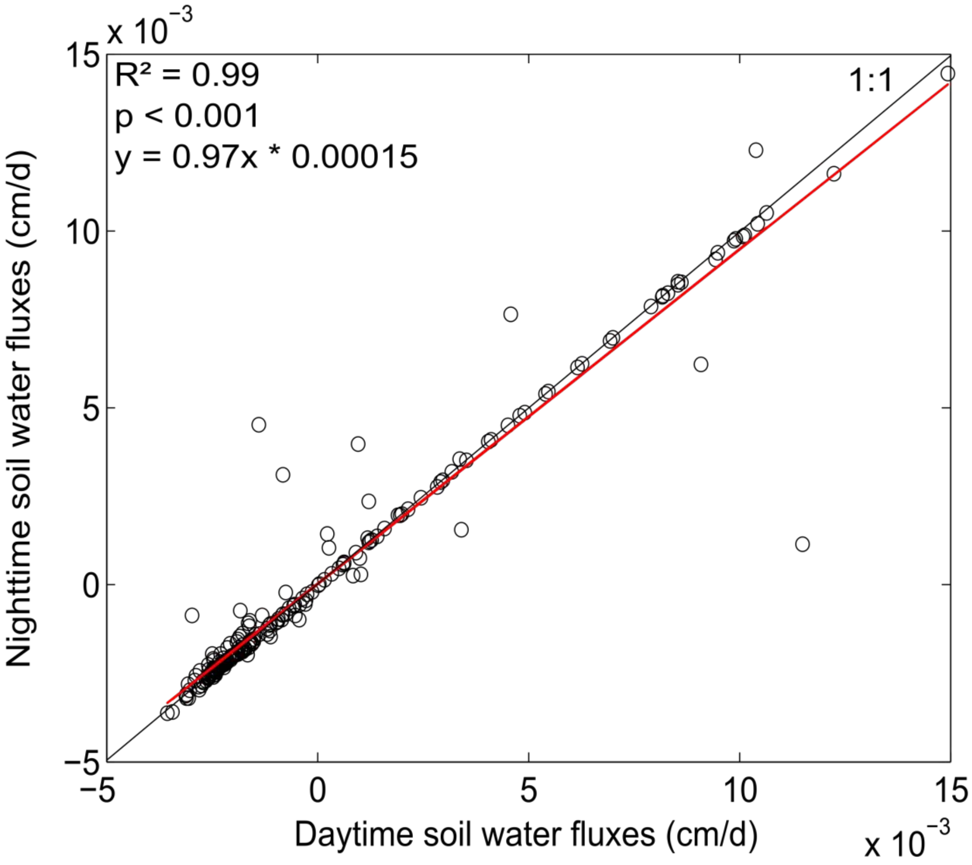


Figure A.1 Correlation between simulated mean fluxes of the respective day and the mean fluxes in the nights before and after one particular day. The solid red line is the regression line and the solid black line represents the 1:1 line. The analysis was conducted with the LinearModel.fit function of the Statistics toolbox in Matlab R2012.b.

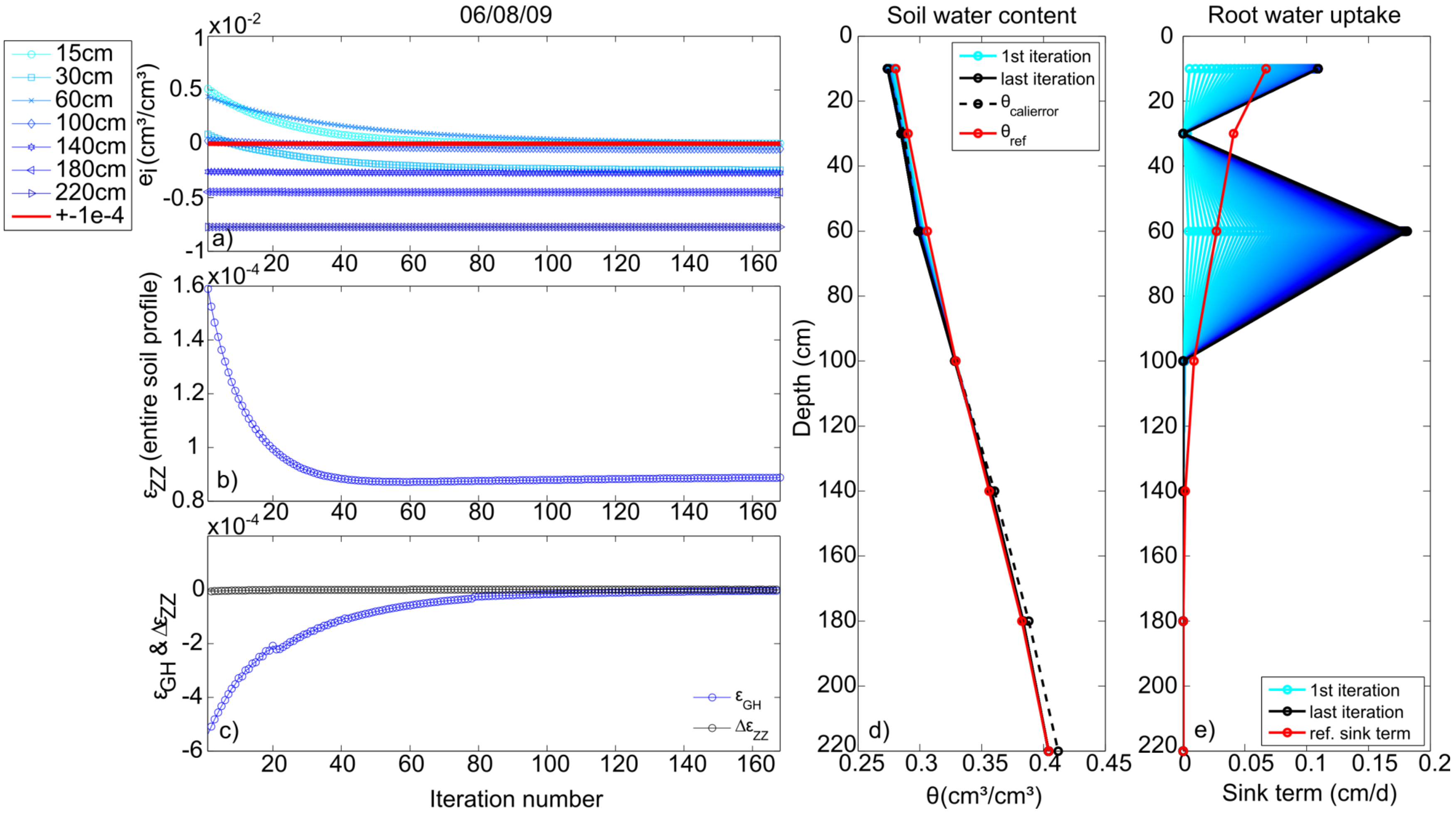


Figure A.2 Evaluation of the inversion process with disturbed soil water content data (calibration uncertainty) of the im method (daily resolution). Subplot a) shows the difference of simulated and observed soil water content e_i (from Eq. 12) for each conducted iteration step in each depth. Suplot b) shows the evolution of the decision criteria ε_{ZZ} at each iteration step and c) depicts the convergence criteria $\Delta\ \varepsilon_{ZZ}$ and ε_{GH} for each iteration step until the reach their value for termination. Subplot d) shows the reference soil water content profile (θ_{ref}), the perturbed soil moisture profile ($\theta_{calierror}$) and the respective iterations. Subplot e) shows the reference sink term and the evaluation of the estimated sink term over depth for each conducted iteration.

Appendix B

Table B.1 Overview of the species which were sampled for leaf water potential and for specific leaf area index (SLAI). Plot is the denomination of the position on the Jena Experiment field site, SR means species richness, FG indicates the functional group (SH – small herbs, TH – tall herbs, GR – grasses and LE – legumes), date is the sampling date for leaf water potential and x indicate if the species was sampled for leaf water potential (LWP) and specific leaf area (SLAI).

Lysimeter	Plot	SR	Species	FG	Date	LWP	SLAI
1	B2A22	16	Achillea millefolium	TH	17.07.2012	x	x
1	B2A22	16	Campanula patula	TH			
1	B2A22	16	Centaurea jacea	TH			
1	B2A22	16	Cynosurus cristatus	GR			
1	B2A22	16	Festuca pratensis	GR	17.07.2012	x	x
1	B2A22	16	Lathyrus pratensis	LE	17.07.2012	x	x
1	B2A22	16	Lotus corniculatus	LE			
1	B2A22	16	Onobrychis viciifolia	LE			x
1	B2A22	16	Phleum pratense	GR			
1	B2A22	16	Poa trivialis	GR			x
1	B2A22	16	Rumex acetosa	TH	17.07.2012	x	x
1	B2A22	16	Sanguisorba officinalis	TH			
1	B2A22	16	Trifolium hybridum	LE			
1	B2A22	16	Trifolium repens	LE			x
1	B2A22	16	Trisetum flavescens	GR	17.07.2012	x	x
1	B2A22	16	Vicia cracca	LE			x
2	B4A04	4	Anthriscus sylvestris	TH			

Lysimeter	Plot	SR	Species	FG	Date	LWP	SLAI
2	B4A04	4	Arrhenatherum elatius	GR	17.07.2012	x	x
2	B4A04	4	Plantago lanceolata	SH	17.07.2012	x	x
2	B4A04	4	Trifolium campestre	LE			
3	B1A01	16	Ajuga reptans	SH	17.07.2012	x	
3	B1A01	16	Anthoxanthum odoratum	GR			x
3	B1A01	16	Anthriscus sylvestris	TH			
3	B1A01	16	Avenula pubescens	GR	17.07.2012	x	x
3	B1A01	16	Bromus hordeaceus	GR			
3	B1A01	16	Carum carvi	TH			
3	B1A01	16	Geranium pratense	TH	17.07.2012	x	x
3	B1A01	16	Lathyrus pratensis	LE	17.07.2012	x	x
3	B1A01	16	Lotus corniculatus	LE			
3	B1A01	16	Plantago lanceolata	SH	17.07.2012	x	x
3	B1A01	16	Poa pratensis	GR			x
3	B1A01	16	Ranunculus repens	SH			
3	B1A01	16	Taraxacum officinale	SH	17.07.2012	x	x
3	B1A01	16	Tragopogon pratensis	TH			
3	B1A01	16	Trifolium campestre	LE			
3	B1A01	16	Vicia cracca	LE			x
4	B1A04	4	Campanula patula	TH			
4	B1A04	4	Festuca pratensis	GR	17.07.2012	x	x

Lysimeter	Plot	SR	Species	FG	Date	LWP	SLAI
4	B1A04	4	Onobrychis viciifolia	LE			
4	B1A04	4	Plantago lanceolata	SH	17.07.2012	x	x
5	B3A23	4	Bromus hordeaceus	GR			
5	B3A23	4	Leucanthemum vulgare	TH			
5	B3A23	4	Ranunculus repens	SH	18.07.2012	x	x
5	B3A23	4	Trifolium fragiferum	LE	18.07.2012	x	x
6	B2A18	16	Ajuga reptans	SH	18.07.2012	x	x
6	B2A18	16	Alopecurus pratensis	GR	18.07.2012	x	x
6	B2A18	16	Anthriscus sylvestris	TH			
6	B2A18	16	Bromus hordeaceus	GR			
6	B2A18	16	Campanula patula	TH			x
6	B2A18	16	Cardamine pratensis	TH			
6	B2A18	16	Cynosurus cristatus	GR			
6	B2A18	16	Geranium pratense	TH	18.07.2012	x	x
6	B2A18	16	Medicago lupulina	LE			
6	B2A18	16	Plantago media	SH	18.07.2012	x	x
6	B2A18	16	Poa pratensis	GR	18.07.2012	x	x
6	B2A18	16	Primula veris	SH			
6	B2A18	16	Ranunculus repens	SH			x
6	B2A18	16	Trifolium campestre	LE			
6	B2A18	16	Trifolium dubium	LE			

Lysimeter	Plot	SR	Species	FG	Date	LWP	SLAI
6	B2A18	16	Trifolium repens	LE			
7	B4A18	16	Alopecurus pratensis	GR			x
7	B4A18	16	Bromus hordeaceus	GR			
7	B4A18	16	Carum carvi	TH			
7	B4A18	16	Crepis biennis	TH			x
7	B4A18	16	Cynosurus cristatus	GR			
7	B4A18	16	Heracleum sphondylium	TH			x
7	B4A18	16	Lathyrus pratensis	LE	18.07.2012	x	x
7	B4A18	16	Leontodon autumnalis	SH			
7	B4A18	16	Luzula campestris	GR			
7	B4A18	16	Onobrychis viciifolia	LE	18.07.2012	x	x
7	B4A18	16	Pimpinella major	TH	18.07.2012	x	x
7	B4A18	16	Plantago media	SH	18.07.2012	x	x
7	B4A18	16	Taraxacum officinale	SH	18.07.2012	x	x
7	B4A18	16	Trifolium campestre	LE			
7	B4A18	16	Trifolium hybridum	LE			
7	B4A18	16	Veronica chamaedrys	SH	18.07.2012	x	x
8	B2A01	4	Anthoxanthum odoratum	GR	18.07.2012	x	x
8	B2A01	4	Knautia arvensis	TH	18.07.2012	x	x
8	B2A01	4	Prunella vulgaris	SH	18.07.2012	x	x
8	B2A01	4	Trifolium pratense	LE			

Lysimeter	Plot	SR	Species	FG	Date	LWP	SLAI
9	B3A22	16	Ajuga reptans	SH	19.07.2012	x	x
9	B3A22	16	Anthoxanthum odoratum	GR			
9	B3A22	16	Bellis perennis	SH	19.07.2012	x	x
9	B3A22	16	Bromus erectus	GR			
9	B3A22	16	Crepis biennis	TH	19.07.2012	x	x
9	B3A22	16	Festuca rubra	GR			x
9	B3A22	16	Galium mollugo	TH	19.07.2012	x	x
9	B3A22	16	Geranium pratense	TH	19.07.2012	x	x
9	B3A22	16	Onobrychis viciifolia	LE			
9	B3A22	16	Phleum pratense	GR			
9	B3A22	16	Ranunculus repens	SH			x
9	B3A22	16	Rumex acetosa	TH			x
9	B3A22	16	Trifolium dubium	LE			
9	B3A22	16	Trifolium fragiferum	LE			
9	B3A22	16	Veronica chamaedrys	SH	19.07.2012	x	x
9	B3A22	16	Vicia cracca	LE	19.07.2012	x	x
10	B2A16	4	Knautia arvensis	TH	19.07.2012	x	x
10	B2A16	4	Leontodon autumnalis	SH			
10	B2A16	4	Plantago media	SH	19.07.2012	x	x
10	B2A16	4	Vicia cracca	LE	19.07.2012	x	x
11	B3A24	16	Ajuga reptans	SH	19.07.2012	x	x

Lysimeter	Plot	SR	Species	FG	Date	LWP	SLAI
11	B3A24	16	Anthoxanthum odoratum	GR			
11	B3A24	16	Arrhenatherum elatius	GR	19.07.2012	x	x
11	B3A24	16	Avenula pubescens	GR	19.07.2012	x	x
11	B3A24	16	Bromus hordeaceus	GR			
11	B3A24	16	Festuca pratensis	GR	19.07.2012	x	
11	B3A24	16	Glechoma hederacea	SH	19.07.2012	x	x
11	B3A24	16	Lotus corniculatus	LE			x
11	B3A24	16	Medicago x varia	LE	19.07.2012	x	
11	B3A24	16	Poa trivialis	GR			
11	B3A24	16	Prunella vulgaris	SH			
11	B3A24	16	Ranunculus repens	SH			x
11	B3A24	16	Taraxacum officinale	SH	19.07.2012	x	x
11	B3A24	16	Trifolium pratense	LE			
11	B3A24	16	Trifolium repens	LE			
11	B3A24	16	Vicia cracca	LE	19.07.2012	x	x
12	B4A11	4	Heracleum sphondylium	TH			x
12	B4A11	4	Medicago x varia	LE	19.07.2012	x	x
12	B4A11	4	Tragopogon pratensis	TH			
12	B4A11	4	Trisetum flavescens	GR	19.07.2012	x	x

Statistical analysis of root length density and belowground biomass

Table B.2 reports the results of statistical analysis of the difference between root length density and belowground biomass of 4 and 16 species mixtures. Table B.3 shows the results for statistical analysis for the root area index and the RAI:LAI ration.

Table B.2 Summary of analysis of variance (ANOVA) for root length density (RLD) and belowground biomass (BGBM).

	RLD			BGBM		
Depth	df	F-value	Pr(>F)	df	F-value	Pr(>F)
0-5 cm	1	2.39	0.153	1	4.87	**0.0518↑**
5-10 cm	1	0.80	0.391	1	0.84	0.38
10-20 cm	1	0.00	0.949	1	2.59	0.139
20-30 cm	1	3.24	0.102	1	0.25	0.626
30-40 cm	1	0.80	0.39	1	0.02	0.894
40-60 cm	1	0.14	0.712	1	0.34	0.572

Listed are the results for degrees of freedom (df), the F-value and the level of significance (Pr(>F)). Arrows indicate increase (↑) or decrease (↓) of RLD or BGBM with species richness.

Table B.3 Summary of analysis of variance (ANOVA) for root area index (RAI) and RAI:LAI ratio.

	RAI			RAI:LAI		
Source of variation	df	F-value	Pr(>F)	df	F-value	Pr(>F)
SR	1	1.02	0.336	1	3.678	**0.0841↑**

Listed are the results for degrees of freedom (df), the F-value and the level of significance (Pr(>F)). Arrows indicate increase (↑) or decrease (↓) of RLD or BGBM with species richness.

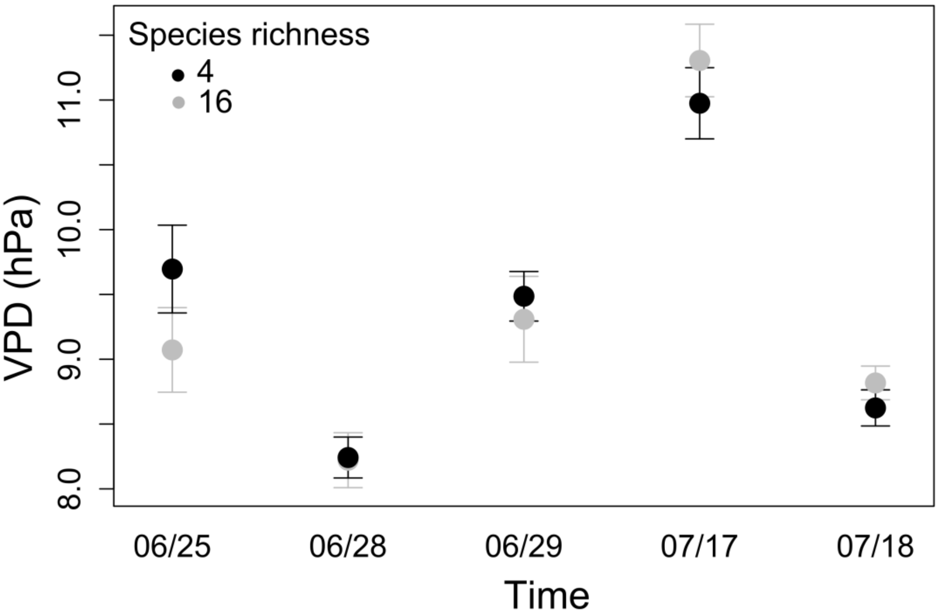


Figure B.1 Comparison between mean vapor pressure deficit of 4 species mixtures (black dots) and 16-species mixtures (grey dots) on 25, 28 and 29 of June and 17 and 18 of July 2012. The error bars indicate the standard error.

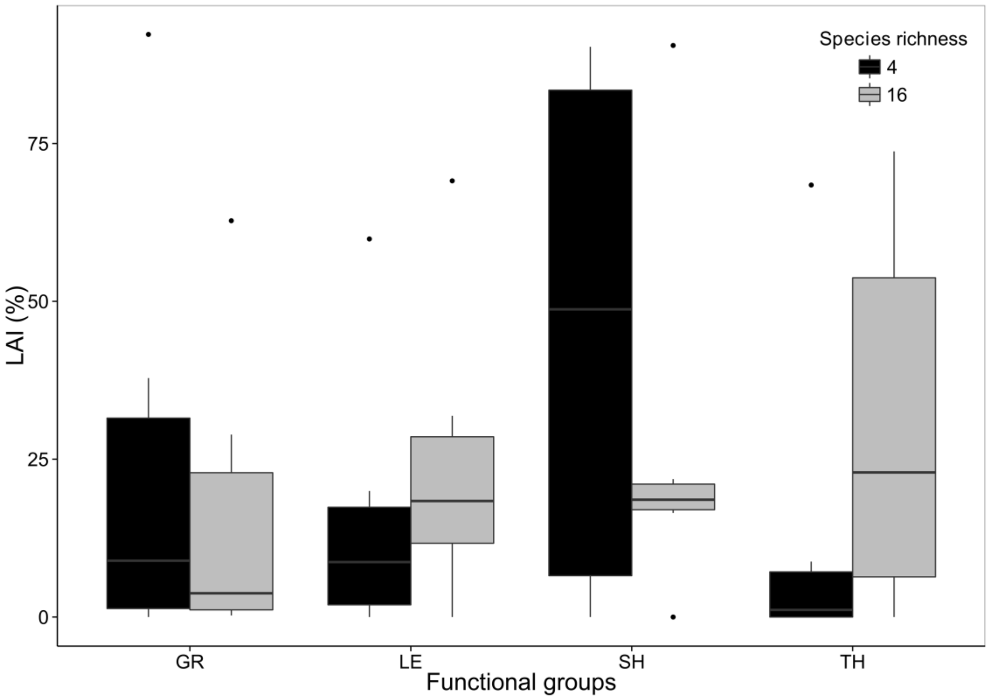
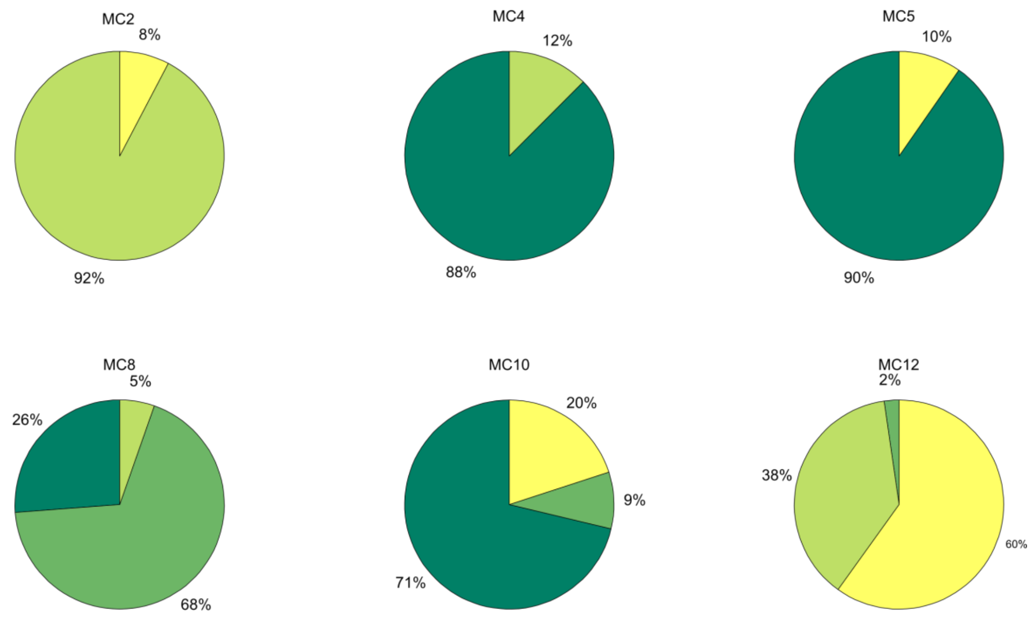


Figure B.2 Proportion of leaf area per area soil of functional groups (GR - grasses, LE – legumes, SH – small herbs and TH – tall herbs) for 4 (grey) and 16-species mixtures (black).

a) Leaf area of all functional groups in 4 species mixtures:



b) Leaf area of all functional groups in 16 species mixtures:

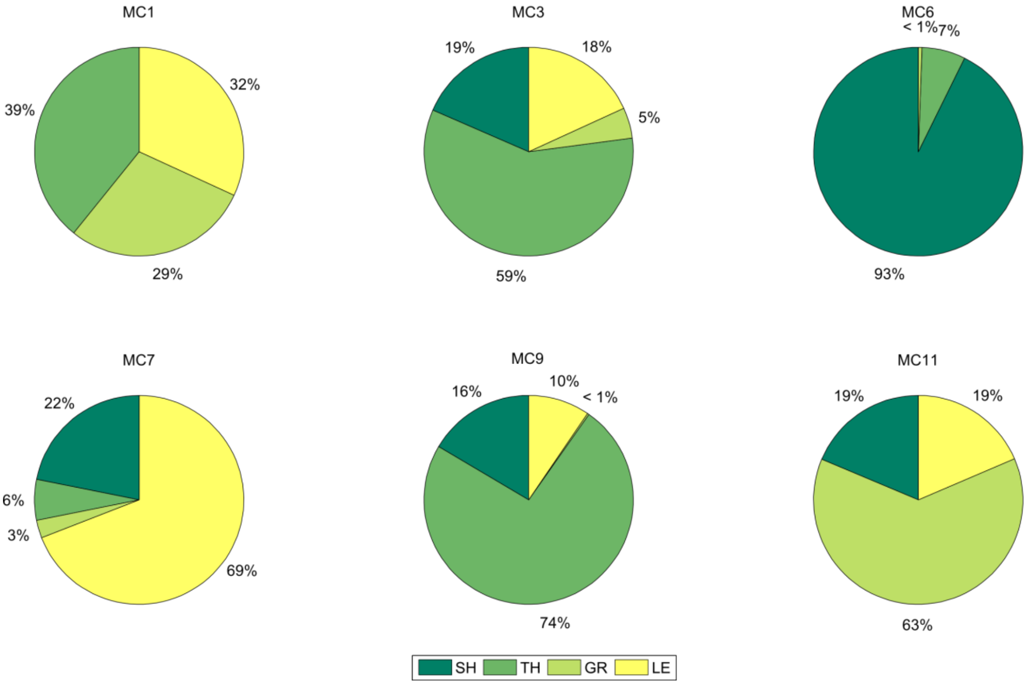


Figure B.3 Proportion of leaf area per area soil of all realized functional groups on the respective lysimeter (MC) with 4-species mixtures (a) and 16-species mixtures (b). The different colored pie slices indicate the functional groups small herbs (SH - dark green), tall herbs (TH - green), grasses (GR – light green) and legumes (LE - yellow).

Selbstständigkeitserklärung

Ich erkläre, dass ich die vorliegende Arbeit selbstständig und unter Verwendung der angegebenen Hilfsmittel, persönlichen Mitteilungen und Quellen angefertigt habe.

Ort, Datum	Unterschrift des Verfassers

Author contribution

Chapter 2 (Manuscript 1): Guderle, M. and Hildebrandt, A.: Using measured soil water contents to estimate evapotranspiration and root water uptake profiles – a comparative study, Hydrol. Earth Syst. Sci., 19, 409-425, doi:10.5194/hess-19-409-2015, 2015.

- M. Guderle is the first author and responsible for writing this paper. He carried out the numerical experiment, processed the inverse model and programmed the termination criteria, analyzed and discussed the data.
- A. Hildebrandt was responsible for the overall design of the study, reviewed and edited drafts of the manuscript.

Chapter 2: Evaluation of the Multi Step Multi Layer Water Balance on a lysimeter study

- M. Guderle is responsible for writing this chapter. He established the method, estimated the water uptake, analyzed and discussed the data.
- D. Bachmann and N. Buchmann provided stable isotope data and the related methods.

Chapter 3 (Manuscript 2): Guderle, M., Bachmann, D., Milcu, A., Gockele, A., Bechmann, M., Fischer, C., Roscher, C., Roy, J., Landais, D., Ravel, O., Devidal S., Gessler A., Buchmann, N., and Hildebrandt, A.: Plasticity in root water uptake facilitates efficient water use in more diverse plant communities, In preparation.

- M. Guderle is the first author and responsible for writing this paper. He established the method, estimated the water uptake, analyzed and discussed the data.
- C. Roscher, D. Bachmann, A. Gockele, A. Gessler, and N. Buchmann provided vegetation-related methods and data.
- A. Milcu, J. Roy, D. Landais, O. Ravel, and S. Devidal provided Ecotron related methods and data.

- A. Hildebrandt was responsible for the overall design of the study, reviewed and edited drafts of the manuscript.
- All authors contributed to revision of this manuscript.

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PUBLICATIONS

2015 **Guderle, M.** and Hildebrandt, A.: Using measured soil water contents to estimate evapotranspiration and root water uptake profiles – a comparative study, Hydrol. Earth Syst. Sci., 19, 409-425, doi:10.5194/hess-19-409-2015, 2015.

2014 **Guderle, M.** and Hildebrandt, A.: Using measured soil water contents to extract information on summer evapotranspiration and root water uptake patterns, 1. PhD conference on Earth System Science, Jena, 12-14 März, 2014.

2014 Milcu, A., Roscher, C., Gessler, A., Bachmann, D., Gockele, A., **Guderle, M.**, Landais, D., Piel, C., Escpape, C., Devidal, S., Ravel, O., Buchmann, N., Gleixner, G., Hildebrandt, A., Roy, J.: Functional diversity of leaf nitrogen concentrations drives grassland carbon fluxes, Ecology Letters, 2014.

2013 **Guderle, M.**, Roy, J., Milcu, A., Landais, D. and Hildebrandt, A.: Using soil water content for calculation of ecosystem root water uptake patterns. 15. Gumpensteiner Lysimetertagung, Gumpenstein, 16-17 April, 2013.

2013 **Guderle, M.** and Hildebrandt, A.: Using measured soil water contents to extract information on summer evapotranspiration and root water uptake patterns. General Assembly European Geoscience Union 2013, Wien, 8-12 April, 2013.

2012 **Guderle, M.** and Hildebrandt, A.: Inverse modeling of root water extraction by means of a sink term. EuroSoil 2012, Bari (Italy) 2-6 Juni, 2012.

2011 Walser, S.; Schütze, N.; **Guderle, M.;** Liske, S.; Schmidhalter, U.: Evaluation of the transferability of a SVAT model - results from field and greenhouse applications. Irrigation and Drainage 60 (1), 59-70, 2011.