Energy and Water Fluxes at the Soil Atmosphere Interface of Water Repellent Soils

vorgelegt von
Dipl.-Ing. Technischer Umweltschutz
Horst Georg Schonsky
geb. in Kiel

von der Fakultät VI – Planen Bauen Umwelt
Institut für Ökologie, FG Standortkunde und Bodenschutz
der Technischen Universität Berlin
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Promotionsausschuss:
Vorsitzender: Prof. Dr. Martin Kaupenjohann
Gutachter: Prof. Dr. Gerd Wessolek
Gutachter: Prof. Dr. (apl) Jörg Bachmann

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Preface

At the beginning of the work on my doctorate I had little knowledge on energy transport, apart from a few fundamental lectures on basic physics and energy- and impulse-transport. I come from a background of environmental engineering, where I devoted rather much of my time on the study of water in drinking water treatment, industrial waste water processing, soil water transport, hydrogeology and aquatic chemistry. I am glad that I had the possibility to learn more on energy, its transport and transformation during my doctorate.

During my early searches on soil water repellency I found many papers related to plant wilting on golf courses caused by inhibited wetting behaviour. ‘Am I really doing golf course research here?’ was one of my first thoughts. It did not take me too long to realise that soil water repellency in fact touches a lot more than golf courses, of which many things awoke my curiosity.

I am thankful that I had the time to learn more on surface and physical chemistry, on microbiology, on proteins and hydrophobins and their folding, on hydrology, meteorology, boundary layer meteorology, deserts, wild fires, catchment scale modelling and many others things, of which very few actually found a direct way into my work, but many of them influenced my understanding of and the approach to the topics I was tackling.

I wish to use the opportunity here to thank a whole lot of people. First of all Gerd Wessolek for his support and his honest interest in giving all his PhD students the best possible chance to finish their work. Thanks to Helena Schmischek for keeping our department running and dealing with the monsters of TU bureaucracy. I would like to thank Michi Facklam and Reinhold Schwartengräber for their vast amounts of practical knowledge and for their support in my experiments. Thank goes to Steffen Trinks and Joachim Buchholz for spending endless hours in the damp, cold, cramped lysimeter vault, to get the whole equipment up and running. Thanks to Stefan Abel, Moritz Werkenthin, Arvid Markert and Marie Hölscher for being wonderful chums on the way. Thanks to Alex Toland for great discussions, many different viewpoints and for keeping my English up. All the folks from the department of Bodenkunde for just being a wonderful sociotope. A big fat thanks to Marieke Hoffmann for being an ingenious masters student and being painfully critical towards measurements, concepts and results. Marcus Bork for being an ugly freshman and many things more. A big thank to Björn Kluge for being a great coauthor, a pleasure to work with and just a grand colleague. A special thank I want to dedicate to Andre Peters, for being an ingenious scientist, for
challenging views, for one of the fastest brains I have ever seen in action and for being in its entirety a superb person.

Thank you to my wife, Antje Schonsky, for being there, for keeping in contact in a real sense, for choosing to travel our route together. And last but not least to my little son, Paul Enok Schonsky, who was born during my work on the stuff you hold in your hands right now. Thanks to him for being a wonderful person, a sunshine and for even in his fuming moments being approachable and great.

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**Related Theses**

In this project on the soil atmosphere energy balance of water repellent soils several other theses have been written. I mention these here to call the readers attention to these works as they might be of interest for further studies.

The dynamics of the fluid solid contact angle under drying conditions were investigated by Steyer (2013). The most interesting finding was that the contact angle was dependent on drying time.

The relationship of water content and thermal conductivities of water repellent and wettable soil was investigated in another work (Schröder, 2013). The measurements were undertaken in drying experiments, where the soil was initially saturated. During saturation the water repellent soil became wettable, no differences between wettable and water repellent had been observed.

In capillary rise experiments with artificially water repellent sand and water and ethanol as wetting fluids it was found that ethanol can not be assumed to be a perfectly wetting fluid (contact angle greater than 0°) (Lacour, 2013). This implies that assumptions on the wetting capabilities of ethanol made in many capillary rise experiments might be wrong.

Hoffmann (2014) undertook an extensive data analysis for long term high temporal resolution lysimeter measurements. Unfortunately the lysimeter measurements did not yield impressive results. This is further discussed in the main part of my thesis.
Abstract

Soil water repellency (SWR), the inhibited wetting of soils, is a characteristic shown by soils of all types and in all climatic regions around the world; SWR seems to be rather the norm than the exception. The hydraulic effects of SWR have been studied reasonably well and are still studied up to date. The effects of SWR on the soil atmosphere energy balance on the other hand have not been the subject of thorough investigations so far. Via evapotranspiration the soil atmosphere energy balance is directly linked to the soil water balance. Therefore it is of utmost importance to measure the water balance in order to gauge the energy balance.

The aim of my doctorate was to attain quantitative information on the effects of SWR on the soil atmosphere energy balance.

To achieve this we, my colleagues and me, employed different methods. First we conducted a numerical study of the soil water balance and especially evapotranspiration in a conceptual frame to get an idea on the quantitative effects to be expected from SWR. Secondly we measured longwave radiation (infrared) in a field study from an extremely water repellent and an artificially wettable soil to obtain differences in temperature and thermal radiation from these soils. Thirdly we attempted to measure the soil atmosphere energy balance differences of water repellent and artificially wettable soil employing weighable lysimeters.

In the numerical study we estimated a reduction in evapotranspiration from 30–300 mm per year or 9%–76% less evapotranspiration from water repellent soil. During our field study we found differences in emitted thermal radiation between water repellent and wettable soil. When the radiation difference is transferred from units of energy per square meter to an amount of water vaporized per square meter the difference translates to 0.13 mm per day, which is a very small value. If the reduction of evapotranspiration postulated in our first study is true this implies that the main part of energy not going into evapotranspiration leaves the soil via sensible heat flux. Our lysimeter study to measure the soil atmosphere energy balance did not yield strong results on the effects of SWR for the energy balance. Nonetheless we managed to develop a new filter algorithm for smoothing lysimeter data, which is better suited than commonly used algorithms to discern between measurement noise and desired signals.

We developed a better tool for analysing lysimeter data, which can aid in future lysimeter studies, not only regarding SWR. Overall we managed to derive information on the effects of SWR on the soil atmosphere energy balance on a conceptual level and to measure differences in thermal radiation caused by SWR. It can be concluded that future studies of the effects of
SWR on the soil atmosphere energy balance should best be approached interdisciplinary, with expertise from the fields of soil physics, plant physiology and micro meteorology.
Kurzfassung

Viele Böden weltweit zeigen Benetzungshemmung gegenüber Wasser (engl.: Soil Water Repellency, SWR) unabhängig von Bodentyp oder Klimazone; Benetzungshemmung von Böden scheint eher die Norm, als die Ausnahme zu sein. Die hydraulischen Auswirkungen der Benetzungshemmung wurden und werden recht ausgiebig erforscht. Andererseits sind die Auswirkungen der Benetzungshemmung auf die Energiebilanz zwischen Boden und Atmosphäre bisher nicht tiefgehend analysiert worden. Durch Evapotranspiration besteht eine direkte Verbindung der Bodenenergiebilanz und der Bodenwasserbilanz, daher ist die Erfassung der Wasserbilanz unumgänglich für die Ermittlung der Energiebilanz.


In der numerischen Studie haben wir eine Verringerung der Evapotranspiration von 30–300 mm pro Jahr, das entspricht 9%–76% Verringerung, durch Benetzungshemmung geschätzt. In der Feldstudie haben wir Unterschiede in der emittierten thermischen Strahlung gefunden. Wird der unterschied in Ausstrahlung von Energie pro Quadratmeter in ein Volumen verdampftes Wasser pro Quadratmeter umgerechnet ergibt sich ein unterschied von 0.13 mm pro Tag. Dies ist ein relativ kleiner Unterschied. Wenn die in unserer ersten Studie postulierte Abnahme der Evapotranspiration zutreffend ist, dann bedeutet das, dass der Hauptteil der nicht in die Verdunstung gehenden Energie über fühlbare Wärme abtransportiert wird. Unsere Lysimeterstudie zur Messung der Energiebilanz hat keine klaren Ergebnisse erbracht. Nichtsdestotrotz ist es uns gelungen einen neuen Filteralgorithmus zum Glätten von Lysimeterdaten zu entwickeln, der besser als allgemein gebräuchliche Algorithmen geeignet ist, um zwischen Messrauschen und gewollten Signalen zu unterschieden.
Eidesstattliche Versicherung

Ich versichere an Eides statt, dass ich die Arbeit selbstständig und eigenständig angefertigt sowie keine anderen als die angegebenen Hilfsmittel benutzt habe. Wörtlich oder sinngemäß aus anderen Quellen übernommene Textstellen, Bilder, Tabellen u. a. sind unter Angabe der Herkunft kenntlich gemacht.
Weiterhin versichere ich, dass diese Arbeit noch keiner anderen Prüfungsbehörde vorgelegt wurde.

Berlin den 11.10.2014

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Horst Schonsky
# Table of Contents

Preface ...................................................................................................................................... III  
Abstract ..................................................................................................................................... V  
Kurzfassung ............................................................................................................................. VII  
1 General Introduction ........................................................................................................ .. 1  
  1.1 Mikroscale Causes ...................................................................................................... 3  
  1.2 Water Movement ........................................................................................................ 5  
  1.3 Soil Atmosphere Energy Balance .............................................................................. 5  
  1.4 Meteorological Surface Energy Balance Measurements ........................................... 7  
2 Methods ..................................................................................................................... ......... 8  
  2.1 Numerical Modelling ................................................................................................. 8  
  2.2 IRT Field Measurements .......................................................................................... 11  
  2.3 Lysimeters ................................................................................................................ 13  
3 Overall Conclusion .......................................................................................................... . 15  
  3.1 Water Balance .......................................................................................................... 15  
  3.2 Soil atmosphere energy balance ............................................................................... 15  
  3.3 Possible Effects on Climate ...................................................................................... 16  
  3.4 Future Studies ........................................................................................................... 17  
References ................................................................................................................................ 19  
Appendices ............................................................................................................................... 18
List of Figures

Figure 1 Droplet of water on water repellent sand. Droplet diameter approx. 5mm (from Atwell et al., 1999) .................................................................................................................... 1

Figure 2 A possible feedback loop between SWR and climate. The yellow oval indicates the area studied in this thesis ........................................................................................................... 3

Figure 3 Schematic illustration of possible spatial orientations of organic matter (OM), consisting of the carbon backbones chains (solid gray) and the functional groups (solid black circles) toward the mineral surface depending on the relations between the number of OM molecules the mineral surfaces and the SOM/mineral ratio (adopted from Ellerbrock et al., 1998) .......................................................................................................................................... 4

Figure 4 Daytime energy balance elements without precipitation. Wettable soil (top). Water repellent soil with wettable flow fingers (bottom). Black arrows indicate energy flow for the wettable case; red arrows indicate possible changes due to SWR ............................................ 6

Figure 5 Comparison of van Genuchten Mualem model (top) and the new model suggested by Peters (2013) (bottom). On the left the water retention characteristics are shown and on the right the hydraulic conductivity. The parameter values for the van Genuchten Mualem model are: $\theta_s = 0.4 \text{ m}^3 \text{ m}^{-3}$, $\theta_r = 0.04 \text{ m}^3 \text{ m}^{-3}$, $\alpha = 0.05 \text{ m}^{-1}$, $n = 1.6$, $l = 0.5$ and $K_s = 100 \text{ cm d}^{-1}$. For the new model the same parameters were used, additional parameters were: $h_a = \alpha^{-1}$, $h_0 = 6.3 \times 10^6 \text{ cm}$, $w = 1 - (\theta_r \theta_s^{-1})$, $a = -1.5$ and $\omega = 10^{-4}$ .................................................................. 10

Figure 6 Measurement area of the infrared thermography field study. Shortly after set up at the 2013-07-05 (left) and at the beginning of the camera recordings at the 2013-08-15 (right). Date format YYYY-MM-DD .................................................................................................. 12

Figure 7 Infrared thermography camera mounted on tripod (left) and recorded plot (right) ........................................................................................................... 13

Figure 8 View of the lysimeters ........................................................................................................... 14

Figure 9 Possible consequences of SWR on climate mechanisms ............................................................................................................................ 17
1 General Introduction

Soil water repellency (SWR) is the property of soils to exhibit prolonged wetting behaviour (Doerr and Ritsema, 2006). Water repellant soils display solid-liquid contact angles greater than 90° (see Figure 1) (Bachmann et al., 2003).

Figure 1 Droplet of water on water repellent sand. Droplet diameter approx. 5mm (from Atwell et al., 1999).

A lot of research on SWR has been conducted as several review articles highlight. The history of research on SWR was summarized by DeBano (2000), a general overview on SWR, its causes, occurrence and characteristics was given by Doerr et al. (2000), amelioration strategies were highlighted by Hallet (2008) and Müller and Deurer (2011) and a summary of knowledge from a surface chemistry viewpoint was given by Diehl (2013). The awardees of the Don and Betty Kirkham Soil Physics Award identified SWR as part of the main problems to be tackled in future soil physics investigations (Jury et al., 2011).

SWR can increase surface runoff and thereby erosion, preferential flow and the exposure of groundwater to contamination (Doerr and Ristema, 2000; Leighton-Boyce et al., 2007); it may also lead to less available water for plants, thereby increase dry patches, wilting and agricultural production losses (Kostka, 2000; Roper, 2005). It is also argued that SWR may have positive effects by reducing evapotranspiration from soils in arid regions (Hallet, 2008). SWR can occur in soils of all types, i.e. sand, loam, silt or clay (Doerr et al., 2006) and in all climates (Jaramillo et al., 2000). Permanently vegetated sites are far more likely to exhibit SWR than are tilled sites (Doerr et al., 2006).

Jaramillo et al. (2000) tested for a correlation of SWR and climate, they found no such correlation. Hallet (2008) stated that global warming might lead to an increase in SWR.
Goebel et al. (2011) reasoned that lowered soil water content and heightened soil temperatures may lead to increased SWR.

It has been shown that SWR is caused by organic substances coating soil particles (Ellerbrock et al., 2005; Horne and McIntosh, 2000) although the exact mechanisms are not yet full understood (Diehl, 2013). Rillig et al. (2010) found that fungi cause SWR by excreting hyrophobins, ubiquitous proteins found in filamentous fungi. Hydrophobins can reverse water repellency and wettability on surfaces (Bayry et al., 2012; Wösten and de Vocht, 2000).

In soil science literature the terms soil water repellency, water repellency and hydrophobicity are often used interchangeably. In other disciplines a clear distinction between hydrophobicity and water repellency is made; where hydrophobicity refers to substances with non-polar, i.e. hydrophobic, groups and water repellency refers to surfaces that have a microstructure that hinders wetting (Callies and Quéré, 2005). This differentiation is not made in soil science. In more recent soil science literature I observed a trend to solely use the term soil water repellency. It makes the language clearer and no advantage arose from the interchangeable terms.

Water repellency and hydrophobicity are studied in many disciplines, among which are material sciences, medical sciences, biology and surface chemistry (Bayry et al., 2012; Callies and Quéré, 2005). Many of these fields are of minor importance to applications in soil science; this is a strong reason to use the term soil water repellency and not only water repellency, in order to clarify the soil scientific context.

The main goal of my thesis was to investigate the effects SWR has on the soil atmosphere energy balance, which could influence microclimate. It is possible that a change in microclimate would then affect global climate, which might have an effect on global climate; this would imply a feedback mechanism on climate. In my thesis I focused on the soil science aspects of the problem, i.e. SWR and its effects on the soil atmosphere energy balance (see Figure 2).
In the following paragraphs I will give a more detailed overview of the causes and consequences of SWR.

In the second chapter a more extensive description of methods employed for the publications is given, than was possible in the publications themselves. The third chapter right away deals with the overall conclusion and points for promising new research are discussed.

Appendices one and three contain published articles and Appendix 2 contains an article in preparation. Appendix 1 is a numerical study on the effects of SWR on evapotranspiration and the soil atmosphere energy balance in a conceptual frame, Appendix 2 describes the effect of SWR on soil surface temperature and topsoil water dynamics and Appendix 3 describes a new filter routine to evaluate lysimeter measurements, needed for precise determination of precipitation and evapotranspiration; and thus latent energy transport at the soil atmosphere interface.

1.1 Mikroscale Causes

In the following paragraph I am giving a short synopsis on the micro-scale causes of SWR. These are not directly related to my work, but I want to point out that the understanding of microscopic reasons of SWR is essential for understanding macroscopic effects.

Soil water repellency is caused by aliphatic organic molecules and waxes (Capriel, 1997; Franco et al., 2000). Aliphatic molecules have got polar groups that are wettable, as they form hydrogen bonds with water molecules, and non-polar groups that exhibit water repellent behaviour (Ellerbrock et al., 2005). Soil organic matter (SOM) can either coat soil minerals or
exist as a bulk phase inside the soil. It is generally accepted that SWR is caused by SOM. Ellerbrock et al. (2005) suggested a model how SOM influences SWR (Figure 3).

**Surface Properties**

<table>
<thead>
<tr>
<th>Water Repellent</th>
<th>Wettable</th>
<th>Water Repellent</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Diagram" /></td>
<td><img src="image2.png" alt="Diagram" /></td>
<td><img src="image3.png" alt="Diagram" /></td>
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Figure 3 Schematic illustration of possible spatial orientations of organic matter (OM), consisting of the carbon backbones chains (solid gray) and the functional groups (solid black circles) toward the mineral surface depending on the relations between the number of OM molecules the mineral surfaces and the SOM/mineral ratio (adopted from Ellerbrock et al., 1998).

The sources of compounds causing SWR are wildfires, decomposing organic matter, plant root exudates, surface waxes from plants and hydrophobins, i.e. hydrophobic proteins, from fungi (Doerr et al., 2000). Soil texture influences how prone soils are to exhibit SWR (Doerr et al., 2000). The actual state of SWR is influenced by soil temperature, water content, pH, ionic strength and microbial activity (Diehl, 2013; Doerr et al., 2000).

The time dependent degree of water repellency is partially attributed to rearrangement of non-polar and polar groups of SOM during drying and wetting (Diehl, 2013; Ellerbrock, 2005). The theory is that SOM, during desiccation, rearranges so that the hydrophobic carbon backbone of organic molecules and hydrophobic groups are oriented towards the capillaries of the soil. During wetting polar groups are rearranging to face into the soil capillaries (Diehl, 2013).

Hydrophobins can not only render wettable surfaces water repellent, but also make water repellent surfaces wettable (Bayry, 2012). This is made possible by their amphiphilic character, with polar and non-polar groups. All surfactants have got this amphiphilic characteristic in common and it is therefore well possible that any surfactant might not only alleviate but also increase water repellency. Gruber et al. (2007) tested if surface active
substances extracted from water repellent soil lessen water repellency if applied to soil, but
did not find an effect.
In a seminal experiment Horne and McIntosh (2000) showed that water repellent soil can
become wettable when an extraction with non-polar solvent is made and that water repellency
reappears when a second extraction is made with polar solvent; they actually repeated these
extraction cycles four times with slightly decreasing levels of SWR for each extraction step. It
is well imaginable that these different extraction steps remove layers of polar and nonpolar
molecules from the soil particle surfaces which would be well in accordance with the
previously mentioned model suggested by Ellerbrock et al. (2005) (Figure 3).

1.2 Water Movement
One of the main influences of SWR is how it affects water dynamics in soils. Most current
models assume that a dry soil which is wetted from above will exhibit a uniform wetting
front. It has been shown that this is rather often not the case. Even in homogeneous soils
preferential flow does occur (Hillel, 1998). Nonetheless it has been observed that water
repellent soils are especially prone to exhibit preferential flow (Ritsema and Dekker, 2000;
Täumer et al., 2005). Preferential flow paths in water repellent soils are not static and change
over the course of a year (Wessolek et al., 2009). Preferential flow causes water to only flow
through the topsoil via preferential flow paths, thereby reaching deeper soil layers faster and
bypassing large parts of the topsoil. As the topsoil is the biologically most active soil region,
this can heighten the risk of contaminants reaching the groundwater (Ritsema and Dekker,
2000).
On the laboratory scale, for bare soil Or et al. (2013) have shown, that SWR can inhibit
evapotranspiration as less water is available in the topsoil. Most plants only root in the upper
soil layers, which are also drier under water repellent than under wettable conditions. Wilting
patterns caused by SWR are a well known phenomenon (Kostka, 2000). To my knowledge no
studies have been undertaken that quantitative measure the effects of SWR on
evapotranspiration on the field scale.
Another effect of SWR is the increase of surface runoff (Biemelt et al., 2011). This is caused
by the inhibited wetting behaviour of the soil.

1.3 Soil Atmosphere Energy Balance
The energy balance is given by:
\[ 0 = R_s \downarrow - R_s \uparrow + R_L \downarrow - R_L \uparrow - H \uparrow - LE \uparrow - G \downarrow \]  
(1),
where $R$ denotes radiation, the subscripts S and L stand for short and long wave and $\downarrow$ for downward fluxes and $\uparrow$ for upward fluxes. $H$ is the sensible heat flux, $LE$ the latent heat flux and $G$ the ground heat flux. All balance elements are given in $[\text{W m}^{-2}]$. The daytime energy balance of a wettable soil is shown in Figure 4 (top). The energy balance is set up at the soil-atmosphere boundary layer. Therefore the balance system has no volume and no storage term needs to be accounted for. Incoming energy originates from the sun in the form of short wave radiation and backscattering from the sky ($R_S\downarrow$), and to a minor degree from anthropogenic light sources, and from long wave radiation ($R_L\downarrow$) from the atmosphere and the sun. The incoming $R_S$ can be reflected from the surface due to albedo causing $R_S\uparrow$ leaving the balance domain. The soil emits long wave radiation ($R_L\uparrow$) at the soil atmosphere boundary layer. Energy will also be transported to or away from the soil surface by convection, i.e. sensible heat ($H\uparrow$). Latent heat ($LE\uparrow$) is energy leaving the soil surface due to vaporization of water and subsequent water vapour transport. The last term of the energy balance is made up of the ground heat flux ($G\downarrow$).

This energy balance does not contain heat brought into the system by precipitation (rain, dew, snow). Only atmospheric energy sources are considered, i.e. contributions of geothermal heat flux and heat produced by soil biota are assumed to be negligible.

I now assume a partially WR soil with preferential flow paths and derive some conclusions on changes I do expect to happen to the energy balance. The incoming radiation ($R_S\downarrow$ and $R_L\downarrow$) does not change if feedback mechanisms of WR on the atmosphere are minor. WR will cause
the soil in the vicinity of the surface to become drier, which has a number of further implications: (i) the soil surface will become brighter and the albedo will increase, causing $R_s \uparrow$ to increase, (ii) the heat capacity of the soil decreases, as the water is replaced by air, leading to an increase of surface temperature at day time, which will cause more thermal radiation, i.e. $R_L \uparrow$ increases, (iii) the thermal conductivity of the soil decreases, this would decrease the ground heat flux ($G_\downarrow$) and at the same time the surface temperature should rise, thereby increasing the driving gradient, this would increase the ground heat flux ($G_\downarrow$), therefore it is unclear how the ground heat flux ($G_\downarrow$) is influenced, (iv) the increased soil temperature will also lead to an increased soil atmosphere temperature gradient, which will cause an increase in sensible heat flux ($H_\uparrow$) and (v) the decrease of soil moisture will result in less water availability for evaporation and therefore in decreased energy transport away from the soil by latent heat ($LE_\uparrow$). These hypothesized implications are schematically summarized in Figure 4, bottom.

During nighttimes the lowered heat capacity of the soil will lead to faster cooling of the soil and thereby less radiant energy emission ($R_L \uparrow$) and very often negative sensible heat flux ($H_\uparrow$; directed from the atmosphere to the soil). Daytime changes in energy balance are by far more important than night time changes, as daytime fluxes are orders of magnitude higher (Foken, 2006).

If enough water is available, the main energy flow away from the soil surface is contributed by the latent heat flux ($LE_\uparrow$) (Foken, 2006; Hillel, 1998). Therefore I expect the major contribution to changes in the energy balance to origin from the reduction of evapotranspiration ($LE_\uparrow$).

### 1.4 Meteorological Surface Energy Balance Measurements

The earth surface atmosphere energy balance is a core topic of boundary layer meteorology and naturally meteorologists have a lot of knowledge about this topic (Foken, 2006), contributions from soil physics can be complementary contributions from a related field of science. The best meteorological method, with the least balance residuals, to date is the eddy covariance method (Foken, 2008). For the eddy covariance method atmospheric turbulences are analysed by the use of rather cost intensive eddy measurement towers. Boundary layer fluid mechanics is employed to derive the results. Because of the hard to predict, chaotic behaviour of turbulent systems the eddy covariance method is at the moment limited to measurements in homogeneous environments, i.e. areas with wide stretches of similarly
structured ground. Up till now it can not be reliably employed to measure for example in heterogeneous environments, e.g. urban areas.

2 Methods

2.1 Numerical Modelling

Water movement in porous media is governed by gradients in chemical potential. Under most circumstances only the gravitational and the matric (or pressure) potential need to be considered to describe water transport satisfactory. Instead of the matric potential very often suction is used, which is the negative of the matric potential. Suction is convenient, as it is positive when matric potential is equal or lower than atmospheric pressure, which is always the case in unsaturated soils.

A central mechanistic approach to describe combined heat and moisture transport in the soil has been developed by Philip and de Vries (1957). This theory has found its way into modern modelling software. Further important contributions to the description of the soil atmosphere energy balance have been published by Chung and Horton (1987) and Horton (1989).

In my work my co-authors and I used a conceptual model to simulate the soil water balance under dynamic SWR conditions. For the simulation we employed the Hydrus 1D software and spreadsheet calculations. The results of this work have been published, see Appendix 1. In the following I am giving a more detailed description of the models employed in our study, than the limited space in publications permits.

The soil water retention as a function of suction, \( \theta(h) \) [m\(^3\) m\(^{-3}\)], is often described using the van Genuchten Equation:

\[
\theta(h) = \frac{\theta_s - \theta_r}{\left[1 + (\alpha \cdot h)^n\right]^m} + \theta_r
\]

(2),

where \( h \) is suction [cm], \( \theta_r \) is the residual water content, \( \theta_s \) is the saturated water content, both in units of [m m\(^{-3}\)] and \( \alpha \) [cm\(^{-1}\)], \( n \) [-] and \( m \) [-] are fitting parameters, \( m = 1 - n^{-1} \) is often used.

To keep numbers small, suction is often expressed as pF, where pF = log (h [cm]).

A problem of the van Genuchten equation is that \( \theta_r \) is rather an empirical fitting parameter than mechanistically describing a physical process. It has been shown that soils keep on losing water even in the very dry range (Rossi and Nimmo, 1994), i.e. the idea of residual water content is not suited to describe soil water retention in the very dry range. Therefore Peters
(2013) suggested a new model, in which soil water retention is described by the sum of capillary bound water, $\theta^{\text{cap}}(h) \text{[m}^3 \text{m}^{-3}]$, and adsorbed water, $\theta^{\text{ad}}(h) \text{[m}^3 \text{m}^{-3}]$:

$$\theta_{\text{tot}}(h) = \theta^{\text{cap}}(h) + \theta^{\text{ad}}(h) \quad (3).$$

The formulation of the capillary bound water is similar to the van Genuchten Equation:

$$\theta^{\text{cap}}(h) = \theta_s w \left( \frac{1}{1 + (\alpha \cdot h)^w} \right)^w \quad (4),$$

where $w$ is a weighing factor describing the fraction of capillary bound water, with $0 \leq w \leq 1$.

The adsorptive bound water is described by:

$$\theta^{\text{ad}} = \begin{cases} \theta_s (1-w) X_m \left( \frac{1 - \ln \left( \frac{1 + h/\h_a}{\ln (1 + h_0/\h_a)} \right)}{\ln \left( 1 + h_0/\h_a \right)} \right), & \text{for } h > \h_a \\ \theta_s (1-w), & \text{for } h \leq \h_a \end{cases} \quad (5)$$

with

$$X_m = \left( 1 - \frac{\ln(2)}{\ln \left( 1 + h_0/\h_a \right)} \right)^{-1}, \quad (6),$$

where $X_m$ is a fictitious parameter slightly greater than one [-], $\h_a$ [cm] is the air entry point for adsorptive water and is set to a value of $\alpha^{-1}$ and $h_0$ [cm] is the suction at which the soil is defined to be completely dry, i.e. oven dried for 24 h at 105°C.

The new soil water retention function declines linearly on the semi-log scale in the dry range (Figure 5, bottom, left; next page). Therefore it is much better suited to describe soil water dynamics in the extremely dry range.

Soil water conductivity was described by van Genuchten, coupling his soil water retention function and a capillary model suggested by Mualem:

$$K(h) = K_s \left( \frac{\theta(h) - \theta_s}{\theta_s - \theta_r} \right)^\tau \left( 1 - \left( \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \right)^{1/w} \right)^w \quad (7),$$

where $K_s$ is the saturated hydraulic conductivity [cm d$^{-1}$] and $\tau$ is the pore-connectivity parameter [-].

Peters (2013) pointed out that adsorbed water films and water vapour contribute to water transport in the dry range. I am going to describe the film flow model and the differences of the coupled capillary and film flow model and the classical van Genuchten Mualem model.
here. I am omitting the vapour transport model, as the important modelling implications can be shown by just discussing film flow. Further information on the model and its still continuing advance can be found in the original article by Peters (2013), a comment to the article by Iden and Durner (2014) and a reply to the comment by Peters (2014).

Figure 5 Comparison of van Genuchten Mualem model (top) and the new model suggested by Peters (2013) (bottom). On the left the water retention characteristics are shown and on the right the hydraulic conductivity. The parameter values for the van Genuchten Mualem model are: \( \theta_s = 0.4 \, \text{m}^3 \, \text{m}^{-3}, \theta_r = 0.04 \, \text{m}^3 \, \text{m}^{-3}, \alpha = 0.05 \, \text{m}^{-1}, n = 1.6, l = 0.5 \) and \( K_s = 100 \, \text{cm} \, \text{d}^{-1} \). For the new model the same parameters were used, additional parameters were: \( h_a = \alpha^1, h_0 = 6.3 \cdot 10^6 \, \text{cm}, w = 1-(\theta_r/\theta_s)^{-1} = 0.1, a = -1.5 \) and \( \omega = 10^4 \).

Analogous to the soil water retention function, the hydraulic conductivity function is an addition of two functions:

\[
K_{\text{tot}}(h) = K_{\text{cap}}(h) + K_{\text{film}}(h)
\]

The capillary hydraulic conductivity is simply a fraction of the hydraulic conductivity from the van Genuchten Mualem model:

\[
K_{\text{cap}}(h) = (1-\omega)K(h)
\]
where $\omega$ is a weighing factor.

Film flow is described by:

$$K_{\text{film}}(h) = \omega K_s \left( \frac{h_0}{h_o} \right)^{ \alpha \left( 1 - \frac{\theta_s}{\theta_c ([0 - w])} \right) }$$ (10)

where $\alpha$ is a fitting parameter, Tokunaga (2009) suggested $0 \leq \alpha \leq -1.5$, in our simulation we used a value of $\alpha = -1.5$.

When film flow is incorporated in the model the hydraulic conductivity declines far less in the dry range, above pF = 2.5 for the parameters shown here (Figure 5, bottom, right). This is well in accordance with experimental results, therefore the new model is better suited to describe evapotranspiration than the classical van Genuchten Mualem model (Peters, 2013).

### 2.2 Infrared Thermography Field Measurements

It is a common technique to employ infrared thermography (IRT) systems to assess evapotranspiration from land surfaces (Kalma et al., 2008). In my thesis I employed IRT to assess temperature differences of water repellent and artificially wettable top soil in a field study. The study took place on a former sewage farm in the north of Berlin. More details about the site and on the measurements can be found in the article manuscript given in Appendix 2.

In Figure 6 the measurement area is shown. For study set up grass was mown, plots were marked and half of them were treated using surfactant (Aqueduct, Aquatrolls Corp., USA) to render them wettable (Figure 6, left). After mowing water drop penetration time (WDPT) tests and TDR-surface water content measurements were conducted on several dates, this is described in detail in the manuscript.
Figure 6 Measurement area of the infrared thermography field study. Shortly after set up at the 2013-07-05 (left) and at the beginning of the camera recordings at the 2013-08-15 (right). Date format YYYY-MM-DD.

On the date of IRT recordings the soil surface temperature was not only recorded by IRT, but also with 5 temperature probes logged in one minute intervals. Air temperature and relative humidity in approximately 1.5 m height were recorded as well in one minute intervals. The surface temperature measurements from the probes were well in accordance with the IRT values, but showed far less variability. As these measurements did not reveal new conclusions they have not been included in the manuscript. The same applies to the humidity and air temperature measurements. If techniques to assess evapotranspiration from meteorological models were employed this information might be of use. Applicable techniques have been discussed by Kalma et al. (2008).

The mounted IRT camera is shown in Figure 7 (left). In Figure 7 (right) the recorded plot is shown. The wettable plot area can well be seen on the right sight of the right picture as grass is greener there. The border between water repellent and wettable starts at the wooden peg and goes up vertically. Part of the recorded plot was opened to study any effects of SWR on the water content in 10 cm depth (shown in Figure 7 (right), not shown in Figure 7 (left)). I did not observe any significant differences of water content between subsoil of the wettable and the water repellent area. Camera recordings for the opened area do exist, but have not been evaluated further.
2.3 Lysimeters

To determine the soil atmosphere energy balance precise measurements of the water balance and especially of evapotranspiration are needed. The most accurate devices to achieve this at a relatively large scale are weighable lysimeters. As lysimeters are highly precise weighing devices, they react to small changes of applied force. This leads to measurement errors often caused by wind (Vaughan and Ayars, 2009), but also other sources like traffic, construction work etc. For low temporal resolution measurements, with resolution of more than ~ 1 day, the errors can often be neglected. When temporal resolution is high, the measurement errors can add up and cause serious overestimations of precipitation and evapotranspiration. This is a relatively new problem as the advance of information technology systems enable much higher sampling rates, than were possible in the past. During my work for this thesis a new filter routine was developed to evaluate lysimeter measurements affected by noisy measurements. See Appendix 3 for the publication.

A measurement system equipped with sensors for soil and surface temperature, ground heat flux, soil moisture and in- and outgoing global and total radiation they can very well deliver long time high resolution measurements to solve the energy balance. Nonetheless a system stocked with these sensors would still not yield information on the sensible heat flux \( H \). As
discussed in Chapter 1.4 measurements of the sensible heat flux are rather complex and cost intensive.

In my research I made use of lysimeters, of which two were equipped in the above mentioned way, to solve the soil atmosphere energy balance for water repellent and wettable soils. All the lysimeters were filled with strongly water repellent substrate from a Dystric Arenosol under pine forest from Niederlehme (Brandenburg, Germany). The lysimeters are shown in Figure 8. The lysimeters were left water repellent for a measurement period of one year, after one year two of the lysimeters were made wettable by the use of surfactant (Aqueduct, Aquatrols Corp.).

Unfortunately major problems with the lysimeter weighing system did occur shortly after half of the lysimeters were treated with surfactant. Therefore we were not able to derive reliable conclusions on the effects of SWR on the energy balance from the lysimeter measurements. A comprehensive analysis of the lysimeter measurements, the associated uncertainties and possible conclusions despite the measurement problems was undertaken by Hoffmann (2014).
3 Overall Conclusion

In this chapter I will describe the outcomes of my work, give an overall conclusion and point to new and interesting questions that arose from my studies.

We were able to derive a filter algorithm for lysimeter measurements that aides precision measurements of precipitation and evapotranspiration. The new filter has the potential to be of major importance for future water balance and therefore also energy balance measurements, no matter if they are regarded to SWR or not. Other groups encountered similar problems in lysimeter measurements as we did (Schrader et al., 2013).

3.1 Water Balance

In order to assess the soil atmosphere energy balance it is necessary to determine the water balance of the soil. One of the main effects of SWR regarding the water balance and therefore the soil atmosphere energy balance are changes caused in evapotranspiration. I assessed these changes with my colleagues in a conceptual simulation study in which we predicted significant decreases in evapotranspiration. In our field study we measured temperature differences between water repellent and wettable soil of otherwise identical properties. Soil surface temperature differences of soils with otherwise similar properties are caused by differences in evapotranspiration (Kalma et al., 2008; Steiner and Hatfield, 2008). On the laboratory scale evaporation differences caused by SWR have been studied by Or et al. (2013) and Bachmann et al. (2001). To my knowledge the evapotranspiration differences between wettable and water repellent soil have not been measured yet on the field scale. I think it would be a promising endeavour to measure these in a broader context. I will elaborate this at the end of this chapter.

SWR results in heterogeneous properties of soils. Heterogeneity is not only important to understand SWR, but plays a part in many up to know poorly understood phenomena (Jury et al., 2011). Therefore the study of SWR might very well provide insights that also further the understanding of related fields. Heterogeneity of soils increases variations in water content, this leads to differences in evapotranspiration. Further studying heterogeneity caused by SWR will increase our understanding of heterogeneity in soils in general.

3.2 Soil atmosphere energy balance

Evapotranspiration contributes one important part to the soil atmosphere energy balance, but is obviously not the only balance element that needs to be measured to give a complete
description of the balance. As incoming energy remains constant a reduction in evapotranspiration has to increase other parts of the energy balance. From the experiences gained in my project I conclude that lysimeters are well suited to very accurately measure all parts of the energy balance, with the exception of sensible heat. As convective transport of sensible heat is strongly governed by dynamic, turbulent fluxes, I believe that scientists with a strong expertise in the theory and measurement of boundary meteorology would be needed to achieve the best possible measurements of sensible heat. This is a very important point and I want to stress that I am convinced an interdisciplinary approach is urgently needed to rigorously study these phenomena.

3.3 Possible Effects on Climate

The assessment of the impacts SWR might have on climate is not straightforward. Nonetheless one can try to assess the implications of a water repellent land surface for feedback with the atmosphere. It is straightforward to assume that SWR will lead to drier land surfaces. This in turn will i) increase the surface albedo, ii) lower the heat capacity of the topsoil and iii) decrease evapotranspiration. The increase in albedo comes to be, as dry surfaces tend to be brighter than wet surfaces.

In the following I will list some consequences of the two mentioned changes. The increased albedo of soil surfaces will increase the reflection of sunlight and the backscattered shortwave radiation from the atmosphere. This would be a cooling mechanism.

The lowered heat capacity of the soil will result in higher surface temperatures, which will lead to an increase of emitted thermal radiation and transport of sensible heat from the soil. As shown in the article on soil surface temperature (Appendix 2), the increase in thermal radiation is in the order of $10^8$ W m$^{-2}$, that is roughly 1% of incoming radiation and therefore very small. The radiation will partly be absorbed by the atmosphere and partly pass through it to outer space. The absorbed radiation would heat up the atmosphere. If all other variables were unchanged, a highly unlikely assumption for the very dynamic earth system, this would lead to a higher equilibrium temperature of the earth system.

The increase in sensible heat should heat up the atmosphere. This could increase thermal radiation from the atmosphere into space and change atmospheric wind systems. I am not able to assess the consequences of this.

On the other hand one could well argue that not the whole soil is affected by SWR, but very often only a water repellent top layer. Beneath this top layer can well hold moisture for a longer time span than under a wettable topsoil and therefore evapotranspiration could be
prolonged. This would imply a cooling effect that might well be of interest for optimisation of micro climate management in urban areas.

As SWR decreases evapotranspiration, I have to consider the effect of this. If the reduced evapotranspiration caused by SWR is not compensated by evapotranspiration at distant sites, the atmosphere will become drier. Water is the most potent greenhouse gas. This means that it is well possible that the heightened thermal radiation from water repellent soils may pass unhindered through the drier atmosphere as well as any other thermal radiation from the earth surface, therefore the postulated drier atmosphere would lead to a cooling effect on climate.

To assess the effect of SWR on climate I think it would be necessary to develop a robust data set for the surface energy balance effects of SWR under variable climatic conditions. With this data set it would be possible to derive quantitative assumptions that could be fed into climatic models. As climatic modelling is a very sophisticated and intricate business I cannot ascertain if it is probable that SWR surface energy effects have a significant impact on model results. Nonetheless I can imagine that SWR might be a feedback process that needs to be considered in climate models. In Figure 9 I visualized my discussion of the topic.

Figure 9 Possible consequences of SWR on climate mechanisms.

3.4 Future Studies

In order to assess the effects of SWR on a greater scale I am convinced it is necessary to establish a team of several scientists from soil physics, hydrology, meteorology and plant
physiology. I think it would be helpful to have some expertise on desert climate in the team, as desert soils have parallels to water repellent soils. Effects of SWR could be influenced by similar underlying mechanisms as effects in deserts, although it has to be pointed out that the quantitative effects are most probably in different orders of magnitude. A project that should assess effects of SWR using lysimeters should at least have a term of four years, as approximately one and a half years are needed to install the lysimeter and for the soil to consolidate and then a measurement period of at least two and a half years is needed to produce sound data.
References


Appendices
Appendix 1

Effect of Soil Water Repellency on Energy Partitioning Between Soil and Atmosphere:
A Conceptual Approach

H. SCHONSKY, A. PETERS and G. WESSOLEK

Department of Soil Conservation, Institute of Ecology, Technical University of Berlin, D-10587 Berlin (Germany)

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ABSTRACT

Water repellency (WR) is a phenomenon known from many soils around the world and can occur in arid as well as in humid climates; few studies, however, have examined the effect of soil WR on the soil-plant-atmosphere energy balance. The aim of our study was to estimate the effects of soil WR on the calculated soil-atmosphere energy balance, using a solely model-based approach. We made out evapotranspiration to have the largest influence on the energy balance; therefore the effect of WR on actual evapotranspiration was assessed. To achieve this we used climate data and measured soil hydraulic properties of a potentially water-repellent sandy soil from a site near Berlin, Germany. A numerical 1D soil water balance model in which WR was incorporated in a straightforward way was applied, using the effective cross section concept. Simulations were carried out with vegetated soil and bare soil. The simulation results showed a reduction in evapotranspiration of 30–300 mm year\(^{-1}\) (9%–76%) at different degrees of WR compared to completely wettable soil, depending on the severity degree of soil WR. The energy that is not being transported away by water vapor (i.e., due to reduced evapotranspiration) had to be transformed into other parts of the energy balance and thus would influence the local climate.

Key Words: climate, effective cross section, evapotranspiration, soil-atmosphere energy balance, soil hydraulic property, water balance

INTRODUCTION

The term water repellency (WR) is used to describe inhibited wetting behavior of surfaces. If the solid-water contact angle is greater than 90°, a surface is defined as water repellent or hydrophobic. Water repellency and hydrophobicity are used synonymously in soil science (Müller and Deurer, 2011), whereas WR is used more often (DeBano, 2000 and Doerr et al., 2000). In other fields, other definitions for WR exist. Reyssat et al. (2010) define WR as the bouncing back of a drop of water from a surface after impact; this definition is neither used in soil science nor by us. As WR is more commonly used, we do not use the term hydrophobicity from here on.

Water repellency is a phenomenon known from many soils in the world. It is widespread and can occur in humid climates as well as in arid climates (Doerr et al., 2000). The WR under field conditions is a function of soil water content, quantity and quality of soil organic matter and other, not yet fully understood, factors (Ellerbrock et al., 2005; Hardie et al., 2012). The hydrological implications of water-repellent soils such as surface runoff, water erosion and preferential flow have been studied relatively well up to date.

In many regions global warming will lead to drier land surfaces and thus increase the likeliness of WR for soils. We postulate that global warming can not only lead to an increase in WR of soils, but WR has an impact on the local energy balance between soil and atmosphere and thus, will lead to a feedback on global warming. The postulated mechanism is as follows. Water repellency leads to preferential flow (Wessolek et al., 2008); therefore less water is available in the upper soil horizons and less evapotranspiration does occur. The additional amount of energy that under wettable conditions vaporizes water has to appear in other parts of the energy balance. The parts of the soil-atmosphere energy balance that can be influenced are the sensible heat flux, longwave radiation emitted by the soil, reflected short wave radiation and the ground heat flux.

To our knowledge the effects of WR on the soil-atmosphere energy balance have not been studied yet. Müller and Deurer (2011) pointed out that changes of...
evaporation on water-repellent and surfactant-treated former water-repellent soils pose interesting questions for investigation. If enough water is available, e.g., in Central European climate, the main energy flow away from the soil surface is contributed by the latent heat flux (Hillel, 1998; Foken, 2008). Therefore, we expect the major contribution to the changes in the energy balance to originate from the reduction of evapotranspiration.

The aim of this study was to undertake a model-based estimation of differences in evapotranspiration between wettable and water-repellent soils with otherwise identical properties. To achieve our aim we used an established numerical water transport model to simulate actual evapotranspiration for a non-repellent soil as reference. We incorporate WR into the model assuming parts of the soil to be inactive for water transport due to WR.

MATERIALS AND METHODS

Hydraulic implications of soil water repellency

Soil WR changes the water budget of the soil-plant-atmosphere system and thus also has an influence on evapotranspiration. For our model we assume that plants on water-repellent regions become physiologically inactive and do not transpire any more; we neglect any adaptations of root growth or water redistribution through the root network by the plants. Typically, these plants become yellow and stop growth. Thus, only vaporization due to interception takes place. On wettable areas, vaporization originates from both transpiration and interception (Fig. 1). Increased surface runoffs from water-repellent areas as well as preferential flow are well known phenomena (Doerr et al., 2000). In this study we assume a plain soil surface, i.e., no surface runoff.

Soil WR is dynamic; i.e., it changes over the course of a year (Täumer, et al., 2006). Water repellency causes fingered flow of water in soils (Rutsem and Dekker, 2000; Wessolek et al., 2008). In order to describe the area of the soil that is contributing to water transport, i.e., the cross section that is not affected by WR, Täumer et al. (2006) established the effective cross section (ECS) concept, which we used in this study. The flow regimes in temperate climate, e.g., in Central Europe, for late summer, with a low ECS (Fig. 2a), and in early spring, with a high ECS (Fig. 2b), are schematically shown in Fig. 2. The ECS is described in more detail later on.

Conceptual model

The conceptual model is composed of four main parts: i) the core part of the modelling is the simulation of the water budget of the wettable fraction of the soil; ii) the upper boundary condition is given by meteorological data, collected at a site near Berlin, Germany, where precipitation and evapotranspiration are reduced by an interception model (Appendix A); iii) WR is taken into account by transforming infiltration data using the ECS concept of Täumer et al. (2006); and iv) at last the simulated evapotranspiration data is retransformed using ECS. Fig. 3 shows a schematic
overview of this concept. The single parts are explained in detail in the following paragraphs.

**Time-variable effective cross section**

Water repellency is incorporated into the model by using ECS (Täumer et al., 2006). The ECS values theoretically range from 0 to 1, describing the fraction of the soil cross section partaking in water transport. An ECS of 0.1 means that only 10% of the soil pores are transporting water, whereas 90% of the pores are not contributing to water transport (Fig. 2). The actual range of ECS under field conditions usually is between 0.1 and 0.9 (Täumer et al., 2006).

The spatial distribution of WR is not a static soil property but changes with time, usually having the largest extent in late summer and the lowest in late winter. Täumer et al. (2006) showed that the value of ECS follows a cosine-like function throughout a year. We choose the following functional relationship to describe the temporal dynamics of ECS:

$$
ECS(t) = B + A \left( \frac{\cos(2\pi t) + 1}{2} \right)^k
$$

where \( t \) (years) is the time; \( B \) (-) is the minimum value for ECS; \( A \) (-) is the amplitude and \( k \) (-) is a shape parameter. In this conceptual approach, ECS is only dependent on time. We think that this pure time dependence of ECS, reflecting the dependency of WR on temporal changing variables like water supply, is sufficient to estimate the order of magnitude of the evapotranspiration deficit. The site-specific factors influencing WR, such as quality and quantity of organic carbon and pH, can be reflected by varying \( A, B \) and \( k \). This creates different time courses of ECS, expressing different grades of severity of WR, which we used in this study (Fig. 4).

**1D water flow simulation**

We simulated the water budget of the wettable part with HYDRUS 1D (Šimůnek et al., 2013), which numerically solves the Richards equation:

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

where \( \theta \) (m\( ^3 \) m\( ^{-3} \)) is the volumetric water content; \( t \) (s) is the time; \( z \) (m) is the vertical coordinate (positive up); \( K \) (m \( s^{-1} \)) is the unsaturated hydraulic conductivity; \( h \) (m) is the water pressure head and \( S \) (m\( ^3 \) m\( ^{-3} \) s\( ^{-1} \)) is the sink term, representing root water uptake.

The simulations were run under isothermal conditions considering capillary, film and vapor flow. The model was run for bare soil without roots and vegetated soil with roots. Although bare soil does not transpire, we write evapotranspiration for both cases. The simulated soil column was 1.5 m deep with two horizons, the first horizon from 0 to 0.5 m and the second from 0.5 to 1.5 m depth. The root sink term in the vegetated case was set to a constant value in
the upper 0.5 m with a water stress function (default values of grass) (Feddes et al., 1978).

At the lower boundary, free drainage is assumed (unit gradient), simulating a soil without groundwater influence. The upper boundary condition was set as flux boundary condition with measured precipitation and potential evapotranspiration. In the case without plants, the minimal allowed pressure head at the top of the profile was $-106$ cm (representing equilibrium water pressure in air at 20 °C and 50% relative humidity). In the case with plants, the complete potential evapotranspiration was attributed to transpiration, simulating a complete coverage of the soil surface.

**Transformation of precipitation and evapotranspiration due to effective cross section**

First potential evapotranspiration ($E_{T0}$) of grass vegetation without water shortage was calculated using the FAO grass reference evapotranspiration formula according to Allen (2000). This equation is based on the Penman-Monteith approach and uses a constant formula according to Allen (2000). This equation is based on the Penman-Monteith approach and uses a constant formula according to Allen (2000). This equation is based on the Penman-Monteith approach and uses a constant formula according to Allen (2000). This equation is based on the Penman-Monteith approach and uses a constant formula according to Allen (2000).

$E_{Tact} = E_{T0} \times \text{ECS} + I$

where $E_{T0}$ (mm) is the measured precipitation and $I$ (mm) is the interception.

Again, transpiration by plants only takes place where the soil is wettable. Thus, the calculated ET of the model ($E_{Tsoil}$) was multiplied by ECS and the evaporation from interception was added, yielding the actual ET ($E_{Tact}$, mm):

$E_{Tact} = E_{Tsoil} \times \text{ECS} + I$

Note that this modeling approach assumes a vertically homogenous ECS.

**Reduction of evapotranspiration**

With this procedure the evapotranspiration deficit, $\Delta ET$ (mm), of a water-repellent soil compared to a wettable soil was calculated:

$\Delta ET = E_{Tact,phil} - E_{Tact,phob}$

where $E_{Tact,phil}$ (mm) is the actual evapotranspiration of the wettable soil (ECS = 1) and $E_{Tact,phob}$ (mm) is the actual evapotranspiration of the water-repellent soil, where the actual evapotranspiration rates are given by Eq. 4. If we take the heat of vaporization of water into account, we can calculate the evapotranspiration deficit in units of energy ($\Delta ET'$, kJ m$^{-2}$):

$\Delta ET' = \Delta ET - \frac{\rho}{M_{H_2O}} \Delta_{vap} H$

where $\rho$ (g L$^{-1}$) is the density of water at 20 °C ($\rho = 998.3$ g L$^{-1}$); $M_{H_2O}$ (g mol$^{-1}$) is the molar mass of water ($M_{H_2O} = 18$ g mol$^{-1}$) and $\Delta_{vap} H$ (kJ mol$^{-1}$) is the enthalpy of vaporization at 20 °C ($\Delta_{vap} H = 44.2$ kJ mol$^{-1}$). The temperature dependences of density and heat of vaporization for liquid water are very small and are therefore neglected here.

**Soil hydraulic properties**

In order to solve Eq. 2, the soil water retention function ($\theta(h)$) and the hydraulic conductivity function ($K(h)$) have to be known. To get the data for these functional relationships, we used evaporation method measurements (Peters and Durner, 2008a) from a typical water-repellent sandy soil. The measurements for the upper layer are from an organic A horizon (water drop penetration time of 7 h) and for the lower layer from a C horizon. Additionally, pressure plate data were taken for the C horizon. The water retention and unsaturated hydraulic conductivity data together with fitted hydraulic functions are shown in Fig. 5. We used rather realistic functional relationships for water retention and hydraulic conductivity accounting for capillary and adsorptive water retention and capillary, film and vapor conductivity (Peters, 2013) (Appendix B). These complex relationships are important since evaporation from a drying soil can be underestimated by orders of magnitude if the simple functions accounting only for capillary water retention (assuming residual water content) and conductivity are used (Peters, 2013).

**Meteorological data**

Meteorological data from a site near Berlin for the years 1997, 1998, 2002 and 2003 were used as boundary conditions for the model. We only used the results for the years 1998 and 2003 to make sure that the initial conditions do not influence the results. 1998 was a wet year, whereas 2003 was exceptionally dry. Interception
was subtracted from precipitation and evapotranspiration (see Appendix A for details).

RESULTS AND DISCUSSION

The model simulation setup consisted of bare/vegetated soil, four WR cases (wettable, slight, medium and severe WR) and two years (the wet year 1998 and the exceptionally dry year 2003). It resulted in 16 simulation runs.

The cumulative atmospheric boundary fluxes as well as interception are shown in Fig. 6. 1998 was a wet year with 602 mm precipitation and 661 mm potential evapotranspiration, whereas 2003 was extremely dry with 431 mm precipitation and 724 mm potential evapotranspiration. Especially, the precipitations of the two years were very different, while the differences in potential evapotranspiration were relatively small. The
temporal distribution of precipitation in both years was rather homogenous. The evapotranspiration showed the typical annual course with the steepest slope during summer. Note that approximately 20% of the precipitated water was intercepted for the cases with vegetation.

Fig. 7 shows the simulated cumulative evapotranspiration for the two years. The values give the range of evapotranspiration deficit to be expected from a sandy soil with different degrees of WR. For the wettable case, evapotranspiration was reduced from $ET_0$ to $ET_{act,phil}$ by 39% for the bare soil and 34% for the vegetated soil in 1998. In 2003, the reductions increased to 55% (bare) and 48% (vegetated) (Fig. 8). As expected, the reduction for the bare soil was larger than for the vegetated soil.

The additional reductions ($\Delta ET$) caused by slight and medium WR were rather small, whereas the severe WR case caused a drastic reduction of evapotranspiration, as the parameterization for the severe case resu-
ltered in a long period with very low ECS (Fig. 4). Note that the course of ECS determined in the study of Täumer et al. (2006) is in between our medium and severe case. This reduction of evapotranspiration is in accordance with the results of Shokri et al. (2009), who studied evaporation in different mixtures of wettable and water-repellent soil particles in laboratory experiments.

Interestingly, ΔET was larger in the wet year (1998) than in the dry year (2003). This effect is explained by the fact that the reduction from potential to actual ET was already very high for year 2003 (Fig. 8). However, as the time dependence of water repellency in real systems is mostly caused by low water supply in summer (Täumer et al., 2006; Wessolek et al., 2009), the temporal course of ECS would be slightly different for the two years. In all cases, ΔET was the highest in summer and lowest in the beginning and at the end of the year, which was in accordance with the temporal course of ECS (Fig. 4).

Under field conditions, the reduction of the wettable soil surface (i.e., ECS) will either lead to increased preferential flow or increased surface runoff. Biemelt et al. (2011) found increased surface runoff on the catchment scale for water-repellent soils. From our model we could estimate the amount of the so-called “excess water” using ΔET. The nonlinear increase of this water with decreasing ECS is illustrated in Fig. 9.

The evapotranspiration of the different WR cases at the end of the two simulated years are shown in Fig. 8. ΔET ranged from 29 mm (9% reduction) for bare soil with slight WR in 2003 to up to 304 mm (76% reduction) for bare soil with severe WR in 1998. These values can be directly converted into amounts of energy (Eq. 6). Therefore, we get ΔET′ ranging from 79 to 746 MJ m\(^{-2}\).

Foken (2008) stated that the latent heat flux of the soil-atmosphere energy balance ranges from 630 to 1,580 MJ m\(^{-2}\) per year; as the overall turnover of the energy balance can be estimated by net radiation, which is the main inflow of energy into the system, it can range from 630 to 3,150 MJ m\(^{-2}\). These values make clear that a reduction of 746 MJ m\(^{-2}\) of latent heat flux nearly halves the maximum latent heat flux normally encountered under field conditions and is more than a fifth of the energy turnover of the system. Thus, the reduction of evapotranspiration due to WR could well be an important alteration of the soil-atmosphere energy balance.

The energy not being transported away by ET has to appear in other parts of the energy balance, i.e., sensible heat flux, reflected and emitted radiation and ground heat flux. The sensible heat flux does normally contribute the second largest energy flux after latent heat flux away from the soil surface (Foken, 2006). Therefore, we expect the sensible heat to be the energy balance term most influenced by the change in latent heat.

CONCLUSIONS

The effect of soil WR on actual evapotranspiration, which is an important part of the soil-atmosphere energy balance, was assessed in this study. WR can decrease the volume of soil contributing to water transport. We expressed this in the model using the effective cross section concept. This resulted in 75% less actual ET calculated using HYDRUS as compared to completely wettable soil. The energy that does not evaporate water is still present, as the incoming energy due to short and long wave radiation is not affected by WR. Thus, other parts of the energy balance will be increased. We expect the most important effect of WR on the energy budget to be an increase of sensible heat flux towards the atmosphere. The predicted shift from latent to sensible heat flux due to WR might pose interesting questions for (micro-)meteorological research. The highest effect of WR on the energy balance was in the driest and hottest period of the year. In this time, the high temperatures in the upper layers of the soil and the atmosphere above the soil surface might lead to heat stress for plants and soil biota due to WR.

Our simulation study gave a general idea of the order of magnitude of effects we can expect from water-repellent soils. Its aim was not to be a process-oriented model. Further investigations on real soil-plant-atmosphere systems have to be carried out to com-
pare our results with experiments under field conditions. Such measurements should include measurements of all important energy flux terms, such as short and long wave outgoing radiation, sensible heat and ground heat flux. Another open question is when and to which extend plants reduce their transpiration in water-repellent soils. In our study we set the transpiration on these soil parts to zero which might be a too strong reduction at the beginning of the season.

APPENDIX A: INTERCEPTION

Interception decreases the amount of water reaching the soil surface. To take this into account we developed a simple bucket model for interception. The units are all given in mm and the temporal resolution is in days.

We first define the variables of the model and then introduce them in detail. ET$_0$ is the potential evapotranspiration. P is the precipitation. I$_P$ is the precipitation-dependent interception storage. I$_a$ is the actual interception storage. I$_I$ is the water remaining in interception storage at the end of a day. I$_{max}$ is the maximum interception storage. E$_a$ is the actual evaporated water from interception storage. P$_t$ is the fraction of precipitation which is retained by canopy due to interception. P$_n$ is the fraction of precipitation which infiltrates into the soil.

The precipitation-dependent interception storage for a daily resolution is given by (modified from Feddema et al., 1978):

$$I_{p,i}(P_i) = \begin{cases} P_i & (P_i \leq 0.25 \text{ mm}) \\ \frac{P_i}{a} & (0.25 \text{ mm} < P_i < 17 \text{ mm}) \\ \frac{I_{max}}{(P_i \geq 17 \text{ mm})} & \end{cases}$$

where $I_{p,i}$ is the precipitation-dependent interception storage at day $i$; $P_i$ is the precipitation at day $i$; $a$, $b$, $c$ and $d$ are fitting parameters and $I_{max}$ is the maximum amount of water that can be stored in the canopy. Parameter values (Feddema et al., 1978) are given as follows: $a = 55$; $b = 0.53$, $c = 0.0085$, $d = 5$ and $I_{max} = 1.85$ mm.

In some cases, the actual amount of water in the interception storage at day $i$ ($I_{a,i}$) may be higher than the ET$_0$ at that day (ET$_{0,i}$). The remaining part of the water intercepted in storage at day $i$ ($I_{r,i}$) is given by:

$$I_{r,i} = I_{a,i} - ET_{a,i}$$

Note that $I_{r,0} = 0$ mm. $I_{a,i}$ is the maximum of $I_{p,i}$ or $I_{r,i-1}$:

$$I_{a,i} = \max(I_{r,i-1}, I_{p,i})$$

The actual evaporated water from the interception storage at day $i$ ($E_{a,i}$) is ET$_{0,i}$ if $I_{a,i}$ is greater than ET$_{0,i}$; otherwise it is equal to $I_{a,i}$:

$$E_{a,i} = \min(I_{a,i}, ET_{0,i})$$

Interception-reduced potential evapotranspiration for plants at day $i$ ($ET_{r,i}$) is given by:

$$ET_{r,i} = ET_{0,i} - E_{a,i}$$

The fraction of the precipitated water which is retained in the canopy at day $i$ ($P_{r,i}$) is given by:

$$P_{r,i} = I_{a,i} - I_{r,i}$$

Finally, the fraction of the precipitated water which infiltrates into the soil at day $i$ ($P_{n,i}$) is given by:

$$P_{n,i} = P_i - P_{r,i}$$

APPENDIX B: HYDRAULIC FUNCTIONS

Especially in sandy soils, evaporation and transpiration can be largely underestimated by the usually used models accounting only for capillary water retention and conductivity (Peters and Durner, 2008b; Peters, 2013). Therefore, we used the suggested model combination of Peters (2013) accounting for adsorptive water retention as well as for film and vapor conductivity. The water retention is given by the sum of capillary- and adsorptive-held water:

$$\theta(h) = \theta_0[wS_{cap} + (1 - w)S_{ad}]$$

where $\theta$ (-) is the volumetric water content; $h$ (m) is the matric suction; $\theta_0$ (-) is the saturated water content; $w$ (-) is the weighting factor, subject to $w \leq 1$ and $S_{cap}$ and $S_{ad}$ are the saturation of the capillary and adsorptive fractions, respectively. Here $S_{cap}$ is expressed by the unconstrained van Genuchten function (van Genuchten, 1980):

$$S_{cap}(h) = [1 + (\alpha h)^n]^{-m}$$

where $\alpha$ (m$^{-1}$), $n$ (-) and $m$ (-) are the curve shape parameters. $S_{ad}$ is given by:

$$S_{ad} = \begin{cases} \frac{\ln[(h + h_a)/(h_0 + h_a)]}{\ln[(2h_a)/(h_0 + h_a)]} & (h > h_a) \\ 1 & (h \leq h_a) \end{cases}$$

where $h_0$ (m) is the suction at water content of 0 and
\( h_a \) (m) is the suction below which the adsorptive fraction is saturated.

The conductivity model is given by:

\[
K = K_s [(1 - \omega) K_{\text{rel}}^{\text{cap}} + \omega K_{\text{rel}}^{\text{film}}] + K^{\text{vap}} \tag{B4}
\]

where \( K_s \) (m s\(^{-1}\)) is the saturated liquid conductivity; \( \omega \) (-) is the weighting factor, subject to \( \omega \leq 1 \); \( K_{\text{rel}}^{\text{cap}} \) (-) and \( K_{\text{rel}}^{\text{film}} \) (-) are the relative capillary and film conductivities, respectively; and \( K^{\text{vap}} \) (m s\(^{-1}\)) is the isothermal vapor conductivity. \( K_{\text{rel}}^{\text{cap}} \) was calculated using the Mualem model (Mualem, 1976) as a function of \( S^{\text{cap}} \) by numerical integration and \( K_{\text{rel}}^{\text{film}} \) is given as a function of \( S^{\text{film}} \) (Peters, 2013):

\[
K_{\text{rel}}^{\text{film}}(S^{\text{film}}) = \frac{h_0}{K_a} a (1 - S^{\text{film}}) \tag{B5}
\]

where \( a \) (-) is a parameter which determines the slope of the unsaturated part of film conductivity as a function of suction on the log-log scale. See Peters (2013) for more details.

\( K^{\text{vap}} \) was calculated according to Saito et al. (2006) as:

\[
K^{\text{vap}} = \frac{\rho_{sv}}{\rho_w} D \frac{M g}{RT} H_r \tag{B6}
\]

where \( \rho_{sv} \) (kg m\(^{-3}\)) and \( \rho_w \) (kg m\(^{-3}\)) are the saturated vapor density and the liquid density of water, respectively, and \( \rho_a = 1000 \) kg m\(^{-3}\); \( M \) (kg mol\(^{-1}\)) is the molecular weight of water and \( M = 0.018015 \) kg mol\(^{-1}\); \( g \) (m s\(^{-2}\)) is the gravitational acceleration and \( g = 9.81 \) m s\(^{-2}\); \( R \) (J mol\(^{-1}\) K\(^{-1}\)) is the universal gas constant and \( R = 8.314 \) J mol\(^{-1}\) K\(^{-1}\); \( T \) (K) is the absolute temperature; \( D \) (m\(^2\) s\(^{-1}\)) is the vapor diffusivity and \( H_r \) (-) is the relative humidity. \( D \) is dependent on water content and is calculated according to Saito et al. (2006):

\[
D = \xi \theta_a D_a \tag{B7}
\]

where \( \theta_a \) (-) is the volumetric air content; \( D_a \) (m\(^2\) s\(^{-1}\)) is the diffusivity of water vapor in air and \( \xi \) (-) is the tortuosity factor for gas transport, calculated according to Millington and Quirk (1961):

\[
\xi = \frac{\theta_a^{7/3}}{\theta_s^{2}} \tag{B8}
\]

\( D_a \) and \( \rho_{sv} \) are dependent on temperature:

\[
D_a = 2.14 \times 10^{-5} \left( \frac{T}{273.15} \right)^2 \tag{B9}
\]

\[
\rho_{sv} = 10^{-3} \exp \left( 31.371 - \frac{6014.79}{T} - 7.92495 \times 10^{-3} T \right) T^{-1} \tag{B10}
\]

\( H_r \) was calculated with the Kelvin equation:

\[
H_r = \exp \left( \frac{h M g}{RT} \right) \tag{B11}
\]

For simplicity, \( T \) was assumed to have a constant value of 293.15 K, *i.e.*, 20 °C.

**REFERENCES**


Appendix 2

Impact of soil water repellency (SWR) on moisture dynamics and outgoing long wave radiation – a field study
Separating precipitation and evapotranspiration from noise – a new filter routine for high-resolution lysimeter data

A. Peters, T. Nehls, H. Schonsky, and G. Wessolek
Fachgebiet für Standortkunde und Bodenschutz, Institut für Ökologie, Technische Universität Berlin, Berlin, Germany

Correspondence to: A. Peters (andre.peters@tu-berlin.de)

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Abstract. Weighing lysimeters yield the most precise and realistic measures for evapotranspiration (ET) and precipitation (P), which are of great importance for many questions regarding soil and atmospheric sciences. An increase or a decrease of the system mass (lysimeter plus seepage) indicates P or ET. These real mass changes of the lysimeter system have to be separated from measurement noise (e.g., caused by wind). A promising approach to filter noisy lysimeter data is (i) to introduce a smoothing routine, like a moving average with a certain averaging window, w, and then (ii) to apply a certain threshold value, δ, accounting for measurement accuracy, separating significant from insignificant weight changes. Thus, two filter parameters are used, namely w and δ. In particular, the time-variable noise due to wind as well as strong signals due to heavy precipitation pose challenges for such noise-reduction algorithms. If w is too small, data noise might be interpreted as real system changes. If w is too wide, small weight changes in short time intervals might be disregarded. The same applies to too small or too large values for δ. Application of constant w and δ leads either to unnecessary losses of accuracy or to faulty data due to noise. The aim of this paper is to solve this problem with a new filter routine that is appropriate for any event, ranging from smooth evaporation to strong wind and heavy precipitation. Therefore, the new routine uses adaptive w and δ in dependence on signal strength and noise (AWAT – adaptive window and adaptive threshold filter). The AWAT filter, a moving-average filter and the Savitzky–Golay filter with constant w and δ were applied to real lysimeter data comprising the above-mentioned events. The AWAT filter was the only filter that could handle the data of all events very well. A sensitivity study shows that the magnitude of the maximum threshold value has practically no influence on the results; thus only the maximum window width must be predefined by the user.

1 Introduction

Precise knowledge of the water fluxes between the soil–plant system and the atmosphere is of great importance for understanding and modeling water, solute and energy transfer in the soil–plant–atmosphere system. The water flux towards the soil–plant system within a certain time interval is precipitation (P [mm]), which can be rain, snow and dewfall, whereas the flux leaving the soil–plant system towards the atmosphere within a certain time interval is given by soil evaporation (E [mm]), evaporation of intercepted water (I [mm]) and transpiration (T [mm]), often summed up to evapotranspiration (ET [mm]).

The precipitation is usually measured by a standard gauge 1 m above the soil surface, which is prone to systematic errors due to its geometry, wind and other factors (Michelson, 2004). One method to determine the reference evapotranspiration (ET0 [mm]) is the use of a class-A pan. Due to differences in albedo between water and grass and island effects, among other factors, these measured data have to be corrected by a so-called pan coefficient (Irmark et al., 2002; Gundekar et al., 2008), which is location dependent (Howell et al., 1983). Actual evapotranspiration is even more difficult to measure under field conditions.

Weighing lysimeters yield the most precise and realistic measures for P and ET, as they avoid all the above-mentioned systematic errors. In order to precisely distinguish between P and ET, which might occur both in relatively small time intervals, the masses of lysimeter and seepage water have to be measured in high temporal resolution. This is of special importance if the energy balance of the soil–plant–atmosphere system is focused on, where a great fraction of total heat flux is given by latent heat flux (Foken, 2008). Note that for long-term water balances focusing on, for example, ground water recharge, where a precise discrimination
of \( P \) and ET is not needed, a high temporal resolution of measurements is not necessary.

Lysimeters have been used in agricultural studies to measure ground water recharge (Yang et al., 2000), solute transport towards the groundwater (Schoen et al., 1999) or water fluxes at the soil–plant–atmosphere interface (Meissner et al., 2007) as well as in urban sites to study surface runoff (Neils et al., 2011).

The early weighable lysimeters are instrumented with lever-arm counterbalance systems (Aboukhaled et al., 1982), and are still used to date (Nolz et al., 2013). Depending on the measurement system, these lysimeters can reach resolutions of \(< 0.1 \text{ mm}\).

In the last decades, resolution and precision of the weighing systems have been substantially improved, and thus modern lysimeters, resting on weighing cells (von Unold and Fank, 2008), can reach resolutions of up to 0.01 mm. They are regarded as the most precise measurement devices for rainfall, actual evapotranspiration or even dewfall (Meissner et al., 2007).

As the resolution of the weighing systems increased, small mechanical disturbances (e.g., caused by wind) became visible in the data as noise (Ramier et al., 2004; Nolz et al., 2013). Therefore, precision and accuracy of the lysimeter measurements depend not only on the precision of the weighing device but also on external conditions, which cannot be controlled or turned off. Moreover, as the wind speed varies with time, the measurement noise also varies with time. In the study of Nolz et al. (2013) the accuracy of the system was up to 3 times lower due to wind (wind speed range 0 to 13 m s\(^{-1}\)). Ramier et al. (2004) report a reduced accuracy of up to 5 times due to wind disturbance.

A mandatory requirement for the quantification of \( P \) or ET from lysimeter measurements is that in a reasonably small time interval, either \( P \) or ET is negligible; in other words, they do not happen simultaneously (Ramier et al., 2004; Schelle et al., 2012). Note that in the case of snow or rainfall, the air right above the soil surface need not necessarily be water saturated. Thus, ET and \( P \) may actually take place at the same time. However, it can be assumed that during such precipitation events evaporation is negligible (i.e., \( \text{ET} \ll P \)).

With this assumption, every increase in system weight (lysimeter mass + cumulative seepage mass) is interpreted as \( P \), whereas every decrease in system weight is interpreted as ET. To apply this concept correctly, the noise (e.g., due to wind) has to be separated from signals using a filtering routine. Such filtering can be carried out in two steps as outlined by Fank (2013) or Schrader et al. (2013). First, a smoothing routine with a certain window width \( w \) is applied. Such a routine can be the simple moving average or a more advanced routine, like the Savitzky–Golay filter (Savitzky and Golay, 1964). Second, all changes in weight smaller than a predefined accuracy threshold \( \delta \) are discarded.

Both the window width \( w \) and the allowed accuracy \( \delta \) have to be defined before using the filtering routine. The problem with this procedure is the choice of the optimal values for \( w \) and \( \delta \). If the averaging window is too small, noisy data might be interpreted as real system changes. If the window width is too wide, small weight changes in short time intervals might be disregarded. The same applies to too small or too large values for \( \delta \).

The general requirement for such filters is that they have to be applicable for very different meteorological conditions – like short, heavy rainfalls (strong signals) – smooth evaporation events with low wind speed (low noise) and for events with or low \( P \) or ET but strong winds (high noise). The former requires narrow averaging windows, whereas the latter requires wide averaging windows. Moreover, in periods with low wind speed, the data are more accurate than in periods with high wind speed (Nolz et al., 2013). Application of constant \( w \) and \( \delta \) leads either to unnecessary losses of accuracy or to faulty data due to noise. A new filtering approach should solve this dilemma.

The best way to test filter routines would be to conduct lysimeter experiments under defined conditions (precision irrigator, wind canal etc.). However, it is easier to use artificial data, where the “true” signals are known (Schrader et al., 2013), or to test the routines by applying them to real lysimeter data from very different events, like strong wind or heavy rainfall, and to judge the filters through expert knowledge. The disadvantage of real data is that the true system response is not known. However, artificially composed data might not comprise the same complex system and noise behavior as in reality.

The aim of this paper is to introduce a new filter routine that is appropriate for any event, including events with low disturbances as well as strong wind and heavy precipitation in small time intervals. The novel approach is based on (i) an adaptive window width, \( w \), which depends on the signal strength, i.e., intensity of \( P \) or ET, and on (ii) an adaptive threshold value, \( \delta \), that depends on noise severity. The filter is compared to other routines using real lysimeter data that comprise all above-mentioned events.

2 Material and methods

2.1 Lysimeter setup

The measurements were conducted at the lysimeter station Marienfelde, south of Berlin (52.396731° N, 13.367524° E). The lysimeter was 1.5 m deep with a surface area of 1 m\(^2\). A lever-arm counterbalance system was used in combination with a laboratory scale, which had a resolution of 0.01 g. The resolution due to the lever-arm mechanism was 80 g for the lysimeter mass. With a water density of \( \approx 1000 \text{ kg m}^{-3} \), this results in a resolution of 0.08 mm for the upper boundary fluxes. The outflow of water at the lower boundary was directly recorded with a scale with a resolution of 5 g. All data were logged in a 1 min time interval.
The soil material in the lysimeter was a packed sand from a partly hydrophobic Dystric Arenosol from Niederlehme (Brandenburg, Germany). No plants were on the lysimeter, so evapotranspiration was reduced to mere evaporation. The data used in this study were recorded from 25 May to 6 October 2012 under very different weather conditions.

2.2 Data processing

The total mass of the system, \( M \) [kg], is the sum of the masses of the lysimeter, \( M_{\text{Lys}} \) [kg], and of the outflow, \( M_{\text{out}} \) [kg]:

\[
M = M_{\text{Lys}} + M_{\text{out}}. \tag{1}
\]

Beginning at a certain time, \( t_0 \), the cumulative water mass flux at the upper boundary is given by \( M - M_0 \), where \( M_0 \) [kg] is the mass of the lysimeter system at \( t_0 \). Note that with the lysimeter geometry outlined above, a water storage change in kilograms is equal to a change in millimeters. Therefore, all water storage changes are given in millimeters in the following.

In order to evaluate the new filter, we focus on three very different benchmark events, including a day of smooth evaporation (6 July 2012), a heavy rainfall event with an intensity of approximately 1 mm min\(^{-1}\) (21 August 2012) and a day with strong wind and low evaporation (23 September 2012) (see Fig. 1). In the following these three events are denominated as “smooth evap”, “heavy prec” and “strong wind”. There was no precipitation on 23 September 2012 (detected by rain gauge). In the time between 1 July and 3 July 2012 a power breakdown led to data loss.

As mentioned above it is assumed that either ET or \( P \), but not both, take place within the same time interval. With this assumption and with perfect (i.e., non-noisy) data a change in \( M \) is either precipitation or evapotranspiration. Thus, \( P \) and ET can be calculated by (Schrader et al., 2013):

\[
P = \begin{cases} 
\Delta M & \text{for } \Delta M > 0 \\
0 & \text{for } \Delta M \leq 0 
\end{cases} \tag{2}
\]

\[
ET = \begin{cases} 
\Delta M & \text{for } \Delta M < 0 \\
0 & \text{for } \Delta M \geq 0 
\end{cases}
\]

where \( \Delta M \) [kg] is a change in cumulative upper boundary mass flux in the according time interval. However, lysimeter data are usually noisy to some extent, and thus \( \Delta M \) might be possibly noise due to wind or other external disturbances. Thus, Eq. (2) is only valid after an appropriate data-filtering procedure is applied. Such a procedure must be a compromise between too “strong” and too “weak” filtering. If noise is filtered not at all or too little, both \( P \) and ET are overestimated. If the data filter is too “strong”, both processes might be underestimated (Schrader et al., 2013). An appropriate filter routine must take this into account for a wide range of very different conditions, as will be discussed in the following.

3.2 Separating \( P \) and ET from noise – general approach

A promising approach to filter noisy lysimeter data is (i) to introduce a smoothing routine, like a moving average with a certain averaging window \( \omega \), and then (ii) to apply a certain threshold value \( \delta \), accounting for measurement accuracy, separating significant from insignificant weight changes (Fank, 2013; Schrader et al., 2013). In Fig. 2, the implementation of these two steps is illustrated for the case of the strong wind event (23 September 2012).

The simplest form of a smoothing routine is the simple moving average, hereafter denoted as MA. In the MA
routine a certain window width \((w \ \text{[min]})\) is chosen and then the arithmetic mean of the data in the time window of \(t_i - (w - 1)/2\) to \(t_i + (w - 1)/2\) is calculated for each point in time \(t_i \ \text{[min]}\). Another, more complex smoothing routine is the Savitzky–Golay filter (Savitzky and Golay, 1964), which has been used in several lysimeter studies (Vaughan et al., 2007; Vaughan and Ayars, 2009; Huang et al., 2012; Schrader et al., 2013). The Savitzky–Golay filter, hereafter denoted as SG filter, is based on a local least-squares polynomial approximation. With either an MA or SG filter, the data are smoothed to a large extent, depending on the smoothing window width.

After smoothing, there is usually still some noise left (Fig. 2, center panel), which would lead to an overestimation of both \(P\) and ET. Therefore, a threshold value, \(\delta \ \text{[mm]}\), is introduced to reduce the fluctuations (Fig. 2, right panel). The threshold approach, which might more correctly be named “thresholding with memory”, makes sure that significant weight changes are separated from insignificant changes in a way that all changes in weight smaller than a predefined accuracy threshold \(\delta\) are discarded. As long as a change from \(t_{i-1}\) to \(t_i\) is smaller than \(\delta\), the value for \(t_{i-1}\) is kept. Such a threshold value should be at least as high as the scale resolution.

Data with small noise (“smooth evap” in Fig. 1) need a relatively small value for \(\delta\), whereas data with large noise (strong wind) need larger values for \(\delta\). Moreover, if small or no changes happen, \(w\) should be large, whereas it should be small in the case of a strong signal, like the heavy precipitation event in Fig. 1. Therefore, an optimal separation of ET and \(P\) cannot be achieved with constant values for \(w\) and \(\delta\). In other words, an appropriate filter must have different properties for the “strong wind”, the “heavy rain” and the “smooth evap” events (Fig. 1). In conclusion, time-variable window widths for averaging and threshold values are required, where the window width should depend on signal strength and the threshold value on the amplitude of the data noise.

### 3.3 Adaptive window and adaptive threshold (AWAT) filter routine

We solve the above-mentioned problem in three steps (Fig. 3): first, a maximum window width, \(w_{\text{max}}\), is defined in which information for signal strength and data noise is collected for each data point, \(i\). This information is derived from simple statistical measures by fitting a moving polynomial to the data within \(w_{\text{max}}\). Second, a moving average with an adaptive window width is applied, where the window width is a function of signal strength. Third, an adaptive threshold value is applied, where the threshold value depends on the measurement noise (the software is available from the authors). These three steps will be explained in detail in the next paragraphs.

---

**Fig. 3.** Scheme of adaptive window and adaptive threshold (AWAT) filter.

#### 3.3.1 Derivation of measures for signal strength and noise

For each data point, \(i\), a polynomial of \(k\)th order (Eq. 3) is fitted to the neighboring data within a time window of a certain constant width, \(w_{\text{max}}\) (for example 31 min) by minimizing the residual sum of squares. The polynomial for data point \(i\), \(Y_i(t)\), is given for the time interval \(t_i - w_{\text{max}}/2\) to \(t_i + w_{\text{max}}/2\):

\[
Y_i(t) = \sum_{j=0}^{j=k} a_j t^j \quad \text{for} \quad t_i - w_{\text{max}}/2 \leq t \leq t_i + w_{\text{max}}/2. \tag{3}
\]

The order of the polynomial must be high enough to guarantee that it can describe the data in the time window reasonably well. However, it should be low enough to avoid the noise being described by the polynomial as well. To select the optimal order, we use an extension of Akaike’s information criterion (Akaike, 1974) as suggested by Hurvich and Tsai (1989):

\[
\text{AICc} = r \ln(\text{SSQ}/r) + 2n + \frac{2n(n + 1)}{r - n - 1} \tag{4}
\]

where SSQ is the sum of squared residuals, \(n = k + 1\) is the number of adjustable parameters and \(r\) is the number of data within the time window. Note that \(r\) must be odd. The first term of Eq. (4) penalizes a poor fit, the second term the number of parameters and the third term is the correction term for small values of \(r/n\). The polynomial with the smallest AICc is selected as the best one. If no or low \(P\) or ET take place, \(k\) is low, since the data might be best described by a straight line. In the case of strong changing signal response in the time window, e.g., strong \(P\) followed by ET or vice versa, \(k\) is high. Figure 4 shows the fitted polynomials and the order \(k\) as selected by the AICc for three points in time in each of the three benchmark events. Although the AICc is a well-suited and much-used identification tool for the best model, there...
is a possibility of “overfitting”, e.g., if some kind of outlier is within the data. Therefore, we chose a maximum allowed order $k_{\text{max}}$ of 6. As can be seen in Fig. 4, $k_{\text{max}}$ is only reached for the heavy precipitation event.

Note that the polynomial is not a “perfect” model as can be seen for the heavy precipitation event. However, the required information can be derived. For each data point $i$, $s_{\text{res},i}$ and $s_{\text{dat},i}$ are calculated:

$$s_{\text{res},i} = \sqrt{\frac{1}{f} \sum_{j=1}^{f} [y_j - \bar{y}_j]^2}, \quad (5)$$

and

$$s_{\text{dat},i} = \sqrt{\frac{1}{f} \sum_{j=1}^{f} [y_j - \bar{y}_j']^2}, \quad (6)$$

where $y_j$, $\bar{y}_j$ and $\bar{y}_j'$ are the measured data, the mean of the data within the time window and the fitted values, respectively. Considering the polynomial to be a good approximation for the system behavior, the value of $s_{\text{res},i}$ is a measure for the noise, i.e., the accuracy of the measurements. This accuracy is not a single value and an intrinsic property of the used scales but also depends on the wind conditions and thus is time dependent.

The quotient $B_i = s_{\text{res},i}/s_{\text{dat},i}$ is a measure of how much of the variation in the data is explained by the polynomial model and thus a measure of the signal strength. Note that $B_i = \sqrt{1 - R^2_i}$, where $R^2_i$ is the coefficient of determination. The values for $s_{\text{res},i}$ and $R^2_i$ are also given in Fig. 4.

Note that the polynomial regression is solely used to get information for data noise and signal strength. Other models, like splines with fixed or even variable knots, could be used as well to get the required information. We chose the polynomials because the parameters and thus the required information can be found by linear regression. This is especially important when the amount of data to be filtered is large. In this study we used approximately $2 \times 10^6$ data points, meaning that with $k_{\text{max}} = 6$, approximately $1.2 \times 10^6$ polynomial fits had to be conducted.

### 3.3.2 Calculation of adaptive width of moving window

The window width at time step $i$, $w_i$ [min], in which the data are smoothed by the moving average is now a function of $B_i$ and is thus time dependent. We use a simple linear relationship for $w_i(B_i)$:

$$w_i(B_i) = \max(w_{\text{min}}, B_i \cdot w_{\text{max}}), \quad (7)$$

where $w_{\text{min}}$ and $w_{\text{max}}$ are the minimum and maximum allowed window widths. Since $B_i$ has a value of 0 if the polynomial explains the complete data variation and a value of 1 if the polynomial explains nothing of the variation, the window width varies between $w_{\text{min}}$ for evaporation and/or precipitation events with no noise and $w_{\text{max}}$ for events with no evaporation or precipitation. Since $w_i$ must be an odd number, $w_i$ is rounded to the nearest odd integer. Figure 5 left illustrates the dependency of $w_i(B_i)$. We suggest to use the temporal resolution of the measurements (1 min) for $w_{\text{min}}$, so that for $B_i = 1$ the data are not smoothed at all. Note that $w_{\text{max}}$ is the time window in which the complete information for data point $i$ is gained (see above). Table 1 shows

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**Table 1.** Calculated variables for the depicted times of Fig. 4. The letters refer to the subplots in Fig. 4.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
<th>i</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B$</td>
<td>–</td>
<td>0.525</td>
<td>0.487</td>
<td>0.496</td>
<td>1.000</td>
<td>0.990</td>
<td>0.994</td>
<td>0.127</td>
<td>0.130</td>
<td>0.108</td>
</tr>
<tr>
<td>$s_{\text{res},f97,5,r}/w$</td>
<td>mm</td>
<td>0.074</td>
<td>0.069</td>
<td>0.070</td>
<td>0.530</td>
<td>0.533</td>
<td>0.545</td>
<td>1.078</td>
<td>1.262</td>
<td>1.036</td>
</tr>
<tr>
<td>$\delta$</td>
<td>mm</td>
<td>0.081</td>
<td>0.081</td>
<td>0.081</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
</tr>
</tbody>
</table>

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www.hydrol-earth-syst-sci.net/18/1189/2014/

Hydrol. Earth Syst. Sci., 18, 1189–1198, 2014
The dynamic impact of external mechanical disturbances on the accuracy of the system is taken into account by introducing a linear functional relationship between the threshold value, $\delta$, on fitting accuracy of the polynomial, $s_{res,i} \cdot b_{7.5,r}$, and the threshold value, $\delta$, on fitting accuracy of the polynomial, $s_{res,i} \cdot b_{7.5,r}$ (right panel). See text for further explanations.

In the following we will compare the performance of the new adaptive width and threshold filter (denoted as AWAT) to that of the MA and second-degree SG filters with fixed $w$ and $\delta$.

### 4 Results – test on data

The MA and SG filters were applied with three fixed window widths, namely 11, 31 and 61 min, and two threshold values, 0.081 and 0.24 mm. These values were also used as $w_{max}$ and $\delta_{max}$ for the AWAT filter. In summary, three filter routines with three window widths and two threshold values were applied, yielding a total of 18 variants.

#### 4.1 Test of AWAT filter with variable $w$ and fixed $\delta = 0.081$ mm

In Fig. 6, the upper boundary fluxes of the three events are shown together with the applied filters. For all three filters, the threshold value was 0.081 mm and the window width was 11, 31 and 61 min.

In the case of a narrow window width of 11 min the smooth evaporation (left) and the heavy rainfall event (right) can be described reasonably well with the SG and MA filters. However, the data with strong wind (center) would be interpreted as a series of small evaporation and precipitation events. Since there was no precipitation at 23 September 2012 (detected with rain gauge), this is a misinterpretation and thus a wider window width is required. If the width is increased to 31 or 61 min, the data noise is reduced but still visible to some extent for that day. However, this noise reduction is done at the cost of the accuracy for the heavy rain event, where the narrow window is optimal. For the event with smooth evaporation, the window width has no significant impact on the results.

The SG filter does not smooth the heavy precipitation data as much as the MA filter does, but it tends to oscillate, which will lead to an overestimation of both precipitation and evapotranspiration. This oscillation behavior of SG filters was also reported by Bromba and Ziegler (1981).

Using the new AWAT filter leads to a better description of the data. Again, the smooth evaporation event is well described. Moreover, the heavy precipitation event is also very well described, with $w_{max}$ being either 11 or 31 min. Even with $w_{max} = 61$ min, the data are described reasonably well.

The strong wind event is better described by the AWAT filter than by the SG filter and equally well as by the MA filter. Thus, the noise for the strong wind event is greatly reduced but in none of the cases completely erased. It is obvious from the data that the measurement accuracy is worse than the scale accuracy in that time interval. Therefore, $\delta$ or $\delta_{max}$ must be increased, as shall be discussed next.
4.2 Test of AWAT filter with variable \( w \) and \( \delta \)

In Fig. 7, the threshold value for the MA and SG filters was now 0.24 mm, whereas for the AWAT filter, \( \delta_i \) is given by Eq. (8), with \( \delta_{\text{min}} = 0.081 \) mm and \( \delta_{\text{max}} = 0.24 \) mm.

Increasing \( \delta \) for the MA and SG filters leads to better filtering in the middle of the strong wind event, where \( \delta = 0.24 \) mm might better represent the low measurement accuracy in that time interval. However, this large value is unsatisfactory for the beginning and the end of that day, when low noise and thus higher accuracy is observed. Moreover, with \( \delta = 0.24 \) mm the smooth evaporation event is no longer well described. Thus, the quality increase in the middle of the strong wind event leads to an accuracy loss for the smooth evaporation event, where the measurement accuracy is actually better than 0.24 mm. Using a constant value of \( \delta = 0.24 \) mm for the AWAT filter leads to the same disadvantages as for the MA and SG filters (not shown). For the heavy precipitation event, the higher value for \( \delta \) does not significantly influence the results.

In contrast, the AWAT filter with variable \( \delta_i \) leads to very good results if \( w_{\text{max}} = 31 \) min. Even in the case of \( w_{\text{max}} = 61 \) min, the new filter is well suited, although the data of the heavy precipitation event are now filtered slightly worse. Obviously the AWAT filter with variable window width and accuracy is better suited to separate evaporation and precipitation from noise than compared to the MA and SG filters. In the following, this statement is underlined by an analysis of residuals.

4.3 Analyzing residuals

Figure 8 shows the frequency distributions of the residuals between filtered and measured data for the case with \( w \) and \( w_{\text{max}} = 31 \) min for the three filters. The blue bars show the residual distribution for filtering without threshold values. In that case the residuals are more or less symmetrically distributed with zero mean. However, as has been discussed above, omitting the threshold value would lead to an overestimation of both \( P \) and \( ET \).

If a threshold value (red bars) of \( \delta = \delta_{\text{max}} = 0.081 \) mm is introduced, all filters show a slight tendency towards negative residuals. Since a value of 0.081 mm for \( \delta \) is too small (see above), a value of 0.24 mm is favored. Now the tendency of MA and SG filter towards negative residuals is strongly increased, whereas the increase is only slight for the AWAT filter. The mean of the residuals for the AWAT filter is \(-0.021\),
which is \( \approx 25\% \) of the scale resolution. The means of the residuals for the MA and SG filters are \(-0.066\) and \(-0.060\).

The tendency towards negative residuals for the filtered data when applying the threshold values is explained as follows: as long as a change from \( t_{i-1} \) to \( t_i \) is regarded as insignificant, the value for \( t_{i-1} \) is kept (see Figs. 6 and 7). This leads to an underestimation, and thus to negative residuals for evaporation events, as well as to an overestimation, and thus positive residuals for precipitation events. In temperate climates, in which our data were measured, evaporation periods exceed periods with precipitation.

4.4 Comparison of estimated cumulative fluxes at upper boundary

The estimated cumulative evaporation for the time period from 5 July 2012 to 7 October 2012 is shown in Fig. 9. The window width \( w = w_{\text{max}} = 31\text{ min} \). If \( \delta \) (for MA and SG) or \( \delta_{\text{max}} \) (for AWAT) was 0.24 mm, the estimated cumulative fluxes are highest for the AWAT filter and lowest for the MA filter, which predicts approximately 11% less evaporation. The SG filter predicted approximately 5% less evaporation. If \( \delta \) was 0.081 mm, the estimated evaporation was considerably higher for the MA and the SG filter than compared to
δ = 0.24 mm. For the AWAT filter the estimated fluxes are only slightly greater if δmax = 0.081 mm.

In general, the influence of the magnitude of δmax on the estimated fluxes is only minimal for the AWAT filter (Fig. 10, left panel). From δmax = 0.081 to 0.24 mm, the estimated cumulative fluxes are reduced by ≈ 1.3 mm. For δmax > 0.24, there is no influence on estimated cumulative fluxes anymore. This is different for the MA and SG filter, where the magnitude of δ has a drastic influence on the estimated evaporation and precipitation.

Varying w or wmax has a great influence on estimated fluxes for all three filters, with the highest fluxes being estimated for the smallest window widths. As expected, greater w or wmax lead to lower fluxes in the complete range of variegated widths for the AWAT and the MA filters. The fluxes estimated with the SG filter can even increase as w increases. This might be due to the fact that the SG filter tends to oscillate depending on signal strength and w (see Figs. 6 and 7).

5 Summary and conclusions

A new filter routine for lysimeter data with adaptive averaging window width and threshold value was introduced. A test with benchmark events, including strong wind as well as smooth evaporation and heavy rainfall, showed that neither a simple moving average nor the more sophisticated Savitzky–Golay filter were able to meet all three events with high accuracy. In contrast, the new filter was able to meet the data of all three events very well. Thus, the new filter can greatly help to separate precipitation and evapotranspiration from noise with much better precision for different atmospheric conditions.

Although not perfectly matching the data, a moving polynomial was sufficient to yield the required information for window width and threshold value. The usage of spline functions with k knots might be more precise than a polynomial of 4th order. However, such spline functions must be fitted by nonlinear regression, which would consume more computer resources by far. This would particularly limit the procedure for large data sets. The suggested routine with polynomial regression requires approximately 30 s to 1 min on a regular personal computer for the analyzed time of approximately 140 days, including ≈ 2 × 10^5 data points in 1 min resolution.

Using the Savitzky–Golay filter led to oscillation in the filtered output for the heavy precipitation event resulting in an overestimation of both precipitation and evapotranspiration. As such events occur in most climates, it is not recommended to use the Savitzky–Golay filter for evaluating lysimeter data.

The SG and MA filter require two filter parameters, namely the window width w and the threshold value δ. The selected value for δ has a drastic influence on the estimated fluxes for the SG and MA filter. For the AWAT filter, the maximum threshold value, δmax, had practically no influence if greater than 0.16 mm. Figures 6 and 7 show that δmax = 0.24 mm was a much better choice than δmax = 0.081 mm. Thus, it is concluded that δmax can be set to any reasonably high value. The value for w and wmax had great influence on the results for all three filters. Thus, if δmax is given a reasonably high value, only one filter parameter, wmax, remains. Choosing wmax carefully through expert knowledge should result in high-quality filtering of lysimeter data with respect to precipitation and evapotranspiration estimations. For our benchmark events, including very different atmospheric conditions, wmax = 31 min led to the best results.

It is worthy of mention that noise caused by wind is not necessarily symmetric around the mean signal. Wind might lead to temporally different air pressures above the lysimeter compared to the lysimeter cellar, which in turn might lead to slightly systematic lower or higher values for lysimeter weights in such wind events. However, strong wind events do lead to greater noise, which leads to higher threshold values. In the strong wind event (Figs. 6 and 7), a systematic effect is barely visible, whereas the noise is very high. Lower wind speeds will lead to lower noise but also to lower systematic
effects. Thus, a small systematic effect due to wind will not be accounted for in the analysis.

The new filter should be tested with other data sets and with artificial data (Schrader et al., 2013) to prove its general applicability and to figure out whether 31 min is a generally applicable maximum window width.

Acknowledgements. This study was financially supported by the Deutsche Forschungsgemeinschaft (DFG grants WE 1125/29-1 and FOR 1736 UCaHS – WE 1125/30-1). We thank Michael Facklam, Reinhold Schwartengräber, Björn Kluge, Joachim Buchholz and Steffen Trinks for their assistance with the lysimeter construction and maintenance. Finally, we thank our reviewers Johann Fank and Frederik Schrader as well as our editor Wolfgang Durner for their insightful comments and suggestions.

Edited by: W. Durner

References


Appendix 3

Separating precipitation and evapotranspiration from noise – a new filter routine for high-resolution lysimeter data
Impact of soil water repellency (SWR) on moisture dynamics and outgoing long wave radiation – a field study

in preparation: Publication planned in Geoderma.

Authors: SCHONSKY Horst\textsuperscript{a}, KLUGE Björn\textsuperscript{a}, WESSOLEK Gerd\textsuperscript{a} and PETERS Andre\textsuperscript{a*}
\* Corresponding author: Andre PETERS, Phone: +49 30 314 73539

Affiliation:
\textsuperscript{a} Department of Ecology, Soil Conservation, Technische Universität Berlin, Ernst-Reuter-Platz 1, 10587 Berlin, GERMANY

E-Mails: schonsky@mailbox.tu-berlin.de, bjoern.kluge@tu-berlin.de, gerd.wessolek@tu-berlin.de, andre.peters@tu-berlin.de

Graphical Abstract

Abstract

Soil water repellency (SWR) is known to occur in many soils all around the world. Up to date the effects on soil water dynamics have been studied extensively, but only a few studies highlight the role SWR plays in the soil atmosphere energy balance.

The objective of our study was to determine the effect of SWR on dynamics of water content distribution and outgoing long wave radiation.

Therefore, a field experiment on a naturally extremely water repellent former sewage farm was conducted. Seven measurement plots (2.5 by 1.5 m) were established, of which three were made wettable by applying surfactant. Water contents in the top soil
were repeatedly measured during summer season. In Mid-August, outgoing long wave radiation was measured in high spatial and temporal resolution via infrared camera recordings for 24 hours on a subplot containing wettable and water repellent parts of two plots.

After precipitation events, mean water contents were lower and variability in water contents were higher for water repellent topsoil. After long periods of drying, no differences in water contents and variability between treatments were observed. At the 24 h measurement campaign, water repellent areas were warmer during day times and cooler during night times. The mean outgoing long wave radiation from the water repellent soil was 3.7 W m$^{-2}$ larger than from the wettable soil over the course of a day. The overall effect of SWR may well be able to cause significant changes to the soil atmosphere energy balance, where less energy is transported from the soil surface by latent heat flux and more by long wave radiation as well as by sensible heat flux. This in turn may have an effect on energy partitioning in the atmospheric boundary layer.

Keywords: Soil water repellency; energy balance; long wave surface radiation; soil water dynamics

1. Introduction

Soil water repellency (SWR) plays an important role for many soils around the world. SWR prevents a homogenous wetting and reduces the retention of water caused by hydrophobic coatings on soil particles.

Several researchers found that SWR does occur in arid as well as in humid climate (e.g. Doerr et al., 2006; Jaramillo et al., 2000). The hydrological implications have been and are still studied (Jordán et al., 2013; Oostindie et al., 2013; Stroosnijder et al., 2012). Effects of SWR are for example increased surface runoff and erosion (Leighton-Boyce et al., 2007), increased occurrence of preferential flow (Wessolek et al., 2008) and wilting of vegetation (Kostka, 2000).

The causes for SWR are manifold, such as influences of vegetation, wild fires, high acidity or soil contamination (Doerr et al., 2000; Müller and Deurer, 2011). The latter may occur due to waster water irrigation, which led to extreme levels of SWR on a former sewage farm site in the vicinity of Berlin, Germany (Täumer et al., 2005).

Soil water repellency under natural conditions is no static property of the soil. SWR dynamics are to a large extend governed by variations of water contents and soil
temperature (Bayer and Schaumann, 2007) as well as wetting history, which lead to distinct seasonal dynamics of SWR, with high SWR in summer and low SWR in winter (Täumer et al., 2006).

On the catchment scale Biemelt et al. (2011) have studied the effect of SWR on runoff and evapotranspiration, but did not compare this to wettable conditions. Soil water repellency is very likely to have a significant influence on the energy balance. Effects of SWR on the soil atmosphere energy balance have been studied in a conceptual frame for the field scale (Schonsky et al., 2014). They hypothesized that SWR leads to lessened evapotranspiration, thereby increasing the sum of latent, sensible and ground heat fluxes. To our knowledge no field scale measurements on the implications of SWR on the energy balance have been published yet.

The soil atmosphere energy balance in closely linked to water balance via latent heat transport due to vaporization. The main components of the soil atmosphere energy balance are incoming short- and longwave radiation, outgoing short- and longwave radiation, sensible heat flux, latent heat flux and ground heat flux. The incoming shortwave radiation outside of the earth atmosphere is determined by the sun. The other parts of the energy balance are responding to the incoming radiation tending to acquire thermodynamic equilibrium. If one part of the energy balance is changed, the other parts will be influenced by this. As a change in SWR will influence water dynamics and thus latent heat transport, this will most likely have an influence on the soil atmosphere energy balance (Schonsky et al., 2014) and the atmospheric boundary layer.

Infrared thermography (IRT) is a non-invasive technique that measures thermal, i.e. longwave, radiation from surfaces. It has been used in large scale applications to assess soil water content and evapotranspiration (Sandholt et al., 2002). On smaller scales it has been used to study soil surface evapotranspiration (Qui and Ben-Asher, 2010; Shahraeeni and Or, 2010) as well as to detect different metabolic rates of bacteria in soil (Kluge et al., 2013).

The aim of this study is to assess the impact of soil water repellency on (i) outgoing long wave radiation and (ii) the water dynamics on the field scale under atmospheric conditions. We hypothesized that SWR leads in summer to less water in the topsoil and thus less heat capacity and less outgoing latent heat flux at daytime, leading to higher surface temperatures and outgoing long wave radiation at daytime. As the energy balance terms at daytime are usually much larger than at night times, we furthermore hypothesized that total energy loss due to long wave radiation is higher for SWR soils.
In order to test our hypothesises, a field study on a water repellent former sewage farm was conducted, where some plots were treated with a surfactant to make the soil wettable. This guaranteed that the water repellent and wettable soil had otherwise identical properties.

2. Material and methods

2.1. Study site

The study site is in the north of Berlin, Germany (52°39'52.1"N, 13°28'45.8"E) located on a former sewage farm. After the sewage farm use ended, an afforestation attempt failed, most probably due to summertime water shortage, nutrient deficiencies and heavy metal toxicity (Täumer et al., 2005; Schweiker et al., 2014). For afforestation the ground was levelled, resulting in slightly wavy terrain with wavelength of approx. 3 m and amplitude of 10-15 cm. The main vegetation now is couch grass (Elytriga repens) and the dominant soil type hortic anthropsol. The topsoil has high and variable organic matter content, mainly between 0.04 and 0.06 g g⁻¹, occasionally up to 0.3 g g⁻¹; it is 0.4-0.6 m thick, underlain by non-calcareous, medium sized, fluvial sand. The top soil exhibits high SWR during summer; even 50% of samples taken in winter (January 2003) by Täumer et al. (2005) were extremely water repellent, with water drop penetration times > 1 h. A comprehensive description of the study site and soil properties was given by Täumer et al. (2005) and Wessolek et al. (2009).

To get information on meteorological quantities in our study area we used data recorded by the Tegel meteorological station of the Deutscher Wetterdienst (DWD, Germany's National Meteorological Service, station number 430). The station is 13 km away from our field site.

2.2. Experimental setup

An area of approx. 40 m² was mowed to a grass height of 5 cm at 2013-05-07 [YYYY-MM-DD]. On this area seven plots were established (Figure 1). Three of the plots (2, 4 and 6) were made wettable by use of the surfactant Aqueduct by Aquatrols Corporation (USA). Four plots (1, 3, 5 and 7) were kept water repellent. The plot length of 2.5 m was enough to cover one wavelength of the terrain.
Figure 1: Sketch of the seven field plots; wettable plots are indicated by structured grey background; the area recorded by IRT is indicated by smooth grey background; transect measurements of water content are indicated by dotted lines.

The wettable plots were regularly treated with a water-surfactant mixture. In order to have identical external boundary conditions for the three water repellent plots, they were watered at these dates with the same amounts of water as the wettable plots. Except from mowing, we left plot 7 untreated as a reference. In Table 1 the dates of mowing, water and surfactant application and measurements are shown.

Table 1: Experiment related work steps; water and surfactant applications. The producer recommends minimum surfactant application of 2.5 mL m\(^{-2}\).

<table>
<thead>
<tr>
<th>Date</th>
<th>Work step/ measurement</th>
<th>Water [mm] Plots 1-6</th>
<th>Surfactant [mL m(^{-2})] Plots 2, 4, 6 (wettable)</th>
</tr>
</thead>
<tbody>
<tr>
<td>YYYY-MM-DD</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2013-05-07</td>
<td>Mowing</td>
<td>4.8</td>
<td>9.6</td>
</tr>
<tr>
<td>2013-05-14</td>
<td></td>
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<td>9.6</td>
</tr>
<tr>
<td>2013-06-06</td>
<td>top soil water content</td>
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<td></td>
</tr>
<tr>
<td>2013-06-20</td>
<td>top soil water content</td>
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<td>2.7</td>
</tr>
<tr>
<td>2013-07-11</td>
<td>top soil water content</td>
<td>0.9 (plots 2, 4, 6)</td>
<td>5.3 (plots 1, 3, 5)</td>
</tr>
<tr>
<td>2013-08-15</td>
<td>24 h IRT recording; top soil water content</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2014-04-01</td>
<td>top soil water content</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Note that in July (2013-07-11) slightly less water (1.8 mm less) was applied to the wettable plots in comparison to the water repellent plots due to technical reasons. As we expect the water repellent plots to be less moist than the wettable plots, this mistake in
watering of the plots would not artificially increase the differences between the treatments and thus this will not affect the results in an unfavourable way.

2.2.1. Measurements

Top soil water content was measured on 2.2 m transects (Figure 1) with a 0.2 m interval at 5 dates (Table 1) using a TDR probe (rod length 100 mm, rod spacing 15 mm; FOM/mts – field operated meter for soil moisture (TDR), salinity and temperature; EasyTest, Poland).

To assess the persistency of SWR we conducted Water Drop Penetration Time (WDPT) tests (Letey, 1969); for feasibility reasons WDPT measurements were terminated if the drop had not penetrated after 5 min. We measured WDPTs on the soil surface at several times in the measurement campaign to test the effect of the surfactant. WDPTs for the surfactant treated plots were in the order of tens of seconds, whereas the untreated plots mainly showed WDPTs above 5 min.

In order to investigate the influence of SWR on the energy balance, a 24 hour measurement campaign was conducted at 2013-08-15 and 2013-08-16 at a part of the study area (grey area in Figure 1). At that time no precipitation occurred. Minimum and maximum air temperatures were 9.8°C and 22.7°C at 2013-08-15 and 16.8°C and 26.6°C at 2013-08-16. Sunshine duration at the two days was 10.35 and 11.13 hours, respectively. During this campaign, long wave radiation from the surface was determined with a spatial resolution of approximately 6 mm and temporal resolution of 1 minute with an infrared camera. For the IRT recordings we used an infrared thermography camera system (Infratec variocam head hr; Jenoptic, Germany). The spectral range was 7.5-14 μm, the temperature resolution 0.05 K and the control accuracy: ± 1 °C. As we are comparing temperatures, the absolute temperature and therefore the control accuracy is of minor importance. The camera was mounted on an approximately 4 m high tripod. The evaluated area (Figure 2) was on a summit of the terrain.

Concomitant to the measurements shown here, we removed parts of the topsoil (left side parts of both pictures in Figure 2) and also recorded the area with IRT (not shown).
To analyse the surface temperature, we chose rectangles on screen. Due to distortion by viewing angle, these images represent quadrilaterals on the physical surface. For these we calculated mean temperatures and standard deviations. The quadrilaterals were chosen to cover as much area as possible without causing border effects. The projection of the upper rectangles covers an area of slightly less than 0.44 m² and the lower of slightly more than 0.37 m².

The measured precipitation at the weather station is shown in Figure 3. In the three weeks previous to our camera recordings, 15th and 16th of August, a rather high amount of 78.5 mm of rainfall was detected.

2.3. Analysis of IRT measurements

The soil temperature, $T$ [K] is measured via longwave radiation. The temperature-radiation flux relationship is described by the Stefan-Boltzmann law.
where $J$ is the radiation flux [W m$^{-2}$], $\varepsilon$ is the emissivity coefficient [-] and $\sigma$ the Stefan-Boltzmann constant [W m$^{-2}$ K$^{-4}$]. Van de Griend and Owe (1993) reported emissivities for long grass ranging from 0.949 to 0.958. Therefore we used a value of 0.95 for $\varepsilon$ in our study. The mean radiation flux $\bar{J}$ [W m$^{-2}$] for a certain time interval $t_0$ [s] to $t_{end}$ [s] is given by:

$$\bar{J} = \frac{\int_{t_0}^{t_{end}} J \, dt}{t_{end} - t_0}$$

(2),

which was calculated by numerical integration using the trapezoidal method.

3. Results and discussion

3.1. Temporal dynamics of water content

In Figure 4 water content transects of all seven plots are shown at four different dates in summer season of 2013 and one in spring 2014; precipitation before the first four measurements is shown in Figure 3. It is interesting to note that no major water content differences occur between the depression and the summit of the profile. At the beginning of June (I) and in mid-August (IV) mean water content was high due to precipitation in the time before the measurements. In mid-June and mid-July (II and III) mean water content was low as no precipitation occurred in the days before those measurements. Note that on 20$^{th}$ of July (II) rainfall occurred after we measured the water content. In times when soil water content was high water repellent soil parts had lower overall water contents than wettable parts, whereas no differences in water content were observed when soil water content was low. These findings imply that the effect of SWR on water dynamics is pronounced under wet conditions, while it is less important under dry conditions. Under dry conditions, soil water is largely depleted and the water content is close to the wilting point for all plots; thus no differences are detectible at those times. Under wet conditions, the non-repellent soil stores water relatively homogeneously and close to field capacity, whereas the water repellent soil stores available water only in small non-repellent subregions; this larger heterogeneity in water content distribution of water repellent soil plots in comparison to the non-repellent plots is also expressed in the much higher variation coefficients at wet times (Table 2). These SWR induced dynamics of water distribution on a three month time
scale within the summer season should not be confused with temporal dynamics of SWR itself, where SWR is more pronounced in the dry season (summer) and less in the wet season (winter) (Täumer et al., 2006).

At the beginning of April 2014 (V), the year following the measurements, no significant differences between plots were observed anymore (Figure 4). This underlines that the soil plots show similar characteristics, which we only altered by surfactant application. It also reinforces the assumption that the surfactant we used has no long-lasting effects on SWR.

Figure 4: Water content at different times for transects from depression (0 m) to summit (2.5 m) of the seven plots. In August (IV) for the two plots on which IRT was conducted we measured water content only from 1 – 2.4 m.
Table 2: Mean, standard deviation and variation coefficient for the water content measurements shown in Figure 4.

<table>
<thead>
<tr>
<th>Date</th>
<th>Mean [vol.-%]</th>
<th>Standard deviation [vol.-%]</th>
<th>Variation coefficient [-]</th>
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<tbody>
<tr>
<td></td>
<td>water repellent</td>
<td>wettable</td>
<td>water repellent</td>
</tr>
<tr>
<td>2013-06-06</td>
<td>12.7</td>
<td>16.8</td>
<td>4.5</td>
</tr>
<tr>
<td>2013-06-20</td>
<td>6.3</td>
<td>6.4</td>
<td>2.9</td>
</tr>
<tr>
<td>2013-07-11</td>
<td>4.9</td>
<td>5.1</td>
<td>2.2</td>
</tr>
<tr>
<td>2013-08-15</td>
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<td>14.9</td>
<td>3.1</td>
</tr>
<tr>
<td>2014-04-01</td>
<td>13.7</td>
<td>15.6</td>
<td>2.7</td>
</tr>
</tbody>
</table>

Figure 5 shows the water content distribution on the subplots for IRT measurements just before IRT recordings were taken. The wettable upper part displays high water contents, whereas the water repellent lower part has lower water contents. The measurements on the grid points in Figure 5 illustrates a similar water content distribution as the transect measurements for all plots on the 15th of August in Figure 4.

Figure 5: Water content (TDR) readings on a grid at the beginning camera recordings, time format [DD.MM. hh:mm CEST (Central European Summer Time)]. Measurement points are shown by red circles. Values between the measurement points were interpolated by kriging (Golden Software, 2002). Note that the y-axis starts at 0.2 m and ends at 1.3 m as we did not measure directly at the lower plot border. The black boxes indicate areas for which temperature was evaluated (see also Figure 2, right); the lower evaluation area expands further than the TDR readings. The dashed line at 0.6 m indicates the border between water repellent (at the bottom) and wettable (at the top).
3.2. Diurnal course of surface temperatures

Figure 6 exemplarily shows three thermograms of the evaluated area for three different time steps in the 24 h measurement campaign at the 15th and 16th of August 2013; the evaluated area is indicated by a shaded rectangle in Figure 1. The left image shows the surface temperature distribution at the afternoon of the first day, the image in the centre the temperatures at midnight and the right image temperatures at noon of the second day. During daytimes the wettable upper part of the area is cooler and the lower water repellent part is warmer; during nighttime this pattern reverses. This is well in accordance with our expectations; our reasoning goes as follows. Under moist conditions SWR decreases the average water content of the topsoil (Figure 4), which will lead to less energy loss due to evapotranspiration, decreased thermal conductivity and heat capacity. When the soil is heated by solar radiation, i.e. a net radiation flux towards the soil occurs, the temperature of the water repellent soil will be raised more for the same amount of energy than the temperature of the wettable soil. During nighttime the situation is reversed. Then evapotranspiration is negligible and outgoing long wave radiation leads to an energy loss, which has a higher impact on temperature for the water repellent soil with lower heat capacity and thermal conductivity. The recording time of the IRT picture of Figure 6 (left) corresponds to the time of TDR measurements shown in Figure 5. We see roughly similar patterns where the wettable upper part of the area shows higher water content and lower temperatures and the lower water repellent part lower water content and higher temperatures. On a smaller scale the similarities between the thermogram and the TDR measurements are not very pronounced, which is probably caused by the different measurement techniques. The IRT records surface temperatures, whereas the TDR probe measures mean water contents in an approximately 0.1 m deep surface layer. Redistribution of water from the point of withdrawal to the evaporating plant leaves further blurs the picture.
Figure 6: Three camera screenshots from the IRT recordings. The time of the screenshot is given above the pictures [DD.MM. hh:mm CEST]. Top rectangle: non-repellent; bottom rectangle: water repellent. Please note the different temperature scales next to each sub-figure.

Figure 7 (top) depicts the diurnal course of mean surface temperatures and standard deviation of the temperatures in the evaluated area for the water repellent and the wettable area. The temperature difference at day time is much more pronounced than at night time. The standard deviation during daytimes is higher for the water repellent area, indicating a more heterogeneous temperature distribution, which corresponds well with the higher variation coefficient for the water content distribution at that time (Table 2). During night times the standard deviation for the water repellent area is slightly lower (approximately 0.1 °C).

Figure 7: Top: Diurnal temperature course and standard deviation (SD) of temperature for the two evaluated areas. Bottom: Temperature difference ($T_{\text{water repellent}} - T_{\text{wettable}}$) and SD difference ($SD_{\text{water repellent}} - SD_{\text{wettable}}$).
The temperature difference, $\Delta T$, between the water repellent and the wettable soil parts is shown in Figure 7 (bottom). During night times $\Delta T$ does not vary much although the surface temperatures of both areas do change, i.e. both areas show similar thermal behaviour. Before dusk, from 16:18 to 17:17 [hh:mm], the water repellent area was up to 4.6 °C cooler than the wettable area; this was caused by the shadow of a tree that moved through the recorded area as the sun was setting. To analyse the differences in radiation emitted from the soil we therefore excluded that period from data evaluation. The difference in mean radiation flux from the wettable and water repellent soil was calculated using Equation (2). This difference contains information on the difference in the energy balance between wettable and water repellent soil. Energy that is transported away from the soil via thermal radiation will not show up in the other parts of the energy balance, i.e. the sum of ground heat flux, sensible heat and evapotranspiration. We analysed the emitted radiation for periods when the soil was directly hit by radiation from the sun and periods when no direct sunlight influenced it, i.e. roughly day- and nighttimes. The measurement time with direct sunlight was 10.3 h (evaluated intervals: 13:08–16:17, 17:16–18:59, 15th, and 8:01–13:25, 16th) and without 13.0 h (evaluated interval 19:00–8:00 15th to 16th). In Table 3 the mean energy fluxes are shown. Over all the mean outgoing long wave radiation is 3.7 W m$^{-2}$ greater for the water repellent soil, which means 320 kJ m$^{-2}$ d$^{-1}$. As the measurement period in direct sunlight was shorter than the period without direct sunlight the longwave radiation difference for the whole period is most likely underestimated. Although this energy difference in outgoing long wave radiation is small (equivalent to 0.13 mm vaporization at 20°C), the influence of SWR on energy partitioning is clearly detectable by IRT and well in agreement with the concept of Schonsky et al. (2014). We expect the difference in evapotranspiration to be much larger than 0.13 mm and assume that a large part of the energy, which is not lost due to latent heat in the water repellent soil, is lost by sensible heat flux.
Table 3: Mean energy fluxes, $\overline{J}$ [W m$^{-2}$], in direct sunlight and without direct sunlight as well as energy flux for the whole measurement period.

<table>
<thead>
<tr>
<th></th>
<th>wettable</th>
<th>water repellent</th>
<th>difference water repellent – wettable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct sunlight</td>
<td>424.9</td>
<td>435.5</td>
<td>10.6</td>
</tr>
<tr>
<td>No direct sunlight</td>
<td>369.8</td>
<td>368.1</td>
<td>-1.7</td>
</tr>
<tr>
<td>Whole measurement period</td>
<td>394.1</td>
<td>397.8</td>
<td>3.7</td>
</tr>
</tbody>
</table>

4. Summary and conclusion

In summer time SWR leads to less water in the top soil, when moist conditions occur, whereas under dry conditions there are no distinct differences in water contents between water repellent and non-repellent soils. Less water in the top soil will lead to less evapotranspiration as pointed out by Schonsky et al. (2014). This in turn leads to higher surface temperatures and thus to higher amounts of long wave outgoing radiation at day time and lower at night times. These effects could be experimentally shown in this study. It could be further shown that under such moisture conditions the overall energy loss due to long wave radiation is higher for water repellent soils. As under dry conditions there are no differences in water contents, the energy balance is most likely also alike. As soil water plays an important role as temperature buffer, SWR will lead to much higher temperature fluctuations and radiative fluxes as compared to non-repellent conditions. We have shown that SWR can be detected via IRT measurements, when other soil properties and boundary conditions are similar.

The overall effect of SWR may well be able to cause significant changes to the soil atmosphere energy balance, where less energy is transported from the soil surface by latent heat flux and more by long wave radiation as well as by sensible heat flux. It might well be that changes in partitioning the energy balance terms due to SWR has an effect on energy partitioning in the atmospheric boundary layer and thus on local climate.

Long term energy balance measurements for water repellent and wettable soils should be conducted to get information on the annual effect of SWR on the energy flux partitioning.
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References


