Reply to the editor (hess-2014-400): Using measured soil water contents to estimate evapotranspiration and root water uptake profiles – a comparative study

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Dear Prof. Ursino,

We want to thank you for the handling of our manuscript and the guidance of the review process. We also would like to thank the anonymous referees for their very useful and constructive comments on our manuscript. We have carefully considered the reviewer's comments and implemented them into the revised version of the manuscript.
Please find below a point by point response to the comments of referee#1 and referee#2, which is similar to the author comments in the interactive discussion of the paper. The major changes in the paper are the restructuring of section *2.2.4 Inverse Model (im)* (P 68, L6; Comment 9 of referee#2) and the additional figure which is showing the evolution of the inverse procedure for a randomly selected calibration uncertainty (general comment of referee#2).
After the point by point response, we provide a revised version of the manuscript. All major changes of the manuscript were marked in yellow.

Authors point by point response to the referee report C5004 of the anonymous referee #1

First of all, we would like to thank the anonymous referee #1 for the very useful and constructive comments on the paper (hess-2014-400).

Comments 1: *The synthetic data of evapotranspiration and soil water uptake was used as reference in the manuscript (Sec 2.3). However, there is not enough statement on the reference data. For example, the accuracy of the synthetic values of evapotranspiration and soil water uptake, the frequency of the input data to get the reference data. I suggest that a more detailed introduction of the reference data should be added. Please make sure that the synthetic data is accuracy enough to be the reference.*

Response: We agree with the reviewer's comment that a more detailed introduction of the reference data is needed.
The used weather data to estimate evapotranspiration have a measurement resolution of 10 minutes. Before applying evapotranspiration and rainfall as input data to generate the synthetic reference soil moisture and root water uptake data, both data sets were aggregated to the temporal resolutions applied for the reference run (1 hour). Soil moisture and root water uptake were generated with the same temporal resolution. When translating the evapotranspiration to sink term profiles (precision 4 digits), rounding errors introduce a small in-accuracy. Thus, the sum of the sink term in the reference run deviates by 0.02% compared to the original evapotranspiration.

In-accuracies in our model are especially relevant for the inverse modeling procedure. We have avoided most of these errors, by using the same model set-up for the forward and backward simulations. This was done deliberately, in order to demonstrate that the inverse model performs excellently, when other errors are excluded. Besides the inverse modeling routine, rounding errors may introduce inaccuracies. We have estimated them by running the model forward for 1 to 24 hour steps (wet and dry periods) with rounded sink term profiles, where we reduced the accuracy to the one handled by our subroutine (4 digits for the sink term profiles). The resulting deviation of the volumetric water content from the non-rounded reference are very small (at the maximum on the order of 1e-5, but on average as small as 1e-9).

We agree that this is important to point it out in the manuscript and we will add the accuracy in the revised manuscript.

Comment 2: *The "evapotranspiration" in Figure 1, is the actual evapotranspiration or potential evapotranspiration?*

Response: The „Evapotranspiration“ in Figure 1 is the actual evapotranspiration. We will change the axis label accordingly in the revised manuscript.

Comment 3: *Line 15, Sect 3.1: "The Inverse Model (im) predicted the daily evapotranspiration for a measurement frequency of 24 h with a very small relative bias of 0.89 %" It seems that 0.89% is for the frequency of 12h in Table 2?*

Response: Yes, 0.89 % is for the frequency of 12 h (according to Table 2). We apologize for the typing error and we will change it to 12 h in the indicated sentence in the revised manuscript.

Comment 4: *Please make the captions for Table 2 and 4 more clear: the model performance for evapotranspiration or root water uptake?*

Response: Thank you for the useful suggestion. We will change the captions of Table 2 and 4 in the revised manuscript as follows:

<u>Old:</u>
Table 2: Comparison of the model performance of the four data-driven methods regarding time resolution of soil moisture measurements. The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. Days at which rainfall occurs were excluded for the data analysis.

Table 4: Comparison of the model performance of the Multi Step Multi Layer Regression and the Inverse Model regarding soil moisture measurement uncertainty. The model performance is expressed as correlation coefficient *R*, relative variability in simulated and reference values *RV* and relative bias (*b*) for the period 25 July to 26 August 2009. The precision uncertainty is abbreviated by prec err, the calibration uncertainty by cali err and the combined uncertainty by com err.

<u>New:</u>
Table 2: Comparison of the model performance of the four data-driven methods **for reproducing daily evapotranspiration for the particular time resolution** of soil moisture measurements. The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. Days at which rainfall occurs were excluded for the data analysis.

Table 4: Comparison of the model performance **with considering soil moisture measurement uncertainties for** the Multi Step Multi Layer Regression and the Inverse Model **for reproducing daily evapotranspiration and the mean depths where 25 %, 50 % and 90 % water extraction occurs.** The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. The precision uncertainty is abbreviated by prec err, the calibration uncertainty by cali err and the

combined uncertainty by com err. **The relative bias for reproducing evapotranspiration is abbreviated with b_{ET} and for reproducing mean depths where 25 %, 50 % and 90 % water extraction occurs is abbreviated with $b_{25\%}$, $b_{50\%}$ and $b_{90\%}$, respectively.**

Authors point by point response to the referee report C5106 of the anonymous referee #2

We would like to thank the anonymous referee #2 for the very helpful comments on our manuscript (hess-2014-400).

Comment 1: *Page 10861, line 13 (P61, L13): As the sink term is defined as water extraction, and increasing water extraction decreases water storage, it seems more appropriate to have the sign "-" in front of S(z,t).*

Response: We agree with the reviewer and we will change equation (1) (P61, L13) according to the reviewer's suggestion to:

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

Comment 2: *P62, L13: This method does not specifically neglect "vertical" soil water flow, it neglects soil water flow more generally.*

Response: Here, we also agree with the reviewer. The sentence will be changed as follows:

Old:
However, a disadvantage is that the depletion of soil water is assumed to occur only by root water uptake and soil evaporation, and vertical soil water fluxes are negligible (Hupet et al., 2002).

New:
However, a disadvantage is that the depletion of soil water is assumed to occur only by root water uptake and soil evaporation, and **soil water fluxes are negligible** (Hupet et al., 2002).

Comment 3: *P62, L27: The cited studies do not fit parameters of "time constant RWU profiles" as their RWU profiles are not time constant. Their RWU model parameters are time constant but as soil matric potential and transpiration vary, their RWU profiles change. The following ("whereas …" L27-29) does not contradict the cited studies then.*

Response: Yes, this is right fort he cited studies. We have changed the sentence accordingly and to show that the models implicitly assume relations between observables (like root distribution, soil water content) and root water uptake profiles, when uptake profiles depend on other biotic regulations as well.

Old:
Another problem is that the applied models for soil water flow ignore biotic processes. For example Musters et al. (2000) and Hupet et al. (2002) tried to fit parameters of time constant root water uptake

profiles, whereas empirical data strongly suggest that plants adjust the distribution of root water uptake dynamically depending on soil moisture storage (Green and Clothier, 1995; Lai and Katul, 2000; Li et al., 2002; Garrigues et al., 2006).

New:

Another problem is that the applied models for soil water flow potentially ignore biotic processes. For example Musters et al. (2000) and Hupet et al. (2002) tried to fit parameters for root distributions in a model determining uptake profiles from water availability **whereas empirical and modeling studies suggest that adjustment of root water uptake distribution may also be from physiological adaptations (Jackson et al., 2000; Zwieniecki et al., 2003; Bechmann et al., 2014)**.

Comment 4: *P64, L18: Here it could also be mentioned that a RWU model is used in addition of a soil water flow model.*

Response: Thank you for the useful hint. We will change the sentence as follows:

Old:

In this study, synthetic time series of volumetric soil water content generated by a soil water flow model (section 2.3), were treated as measured data and are used as the basis for all methods (section 2.2) estimating the sink term $\widetilde{S}(z)$ and total evapotranspiration $\widetilde{E}$.

New:

In this study, synthetic time series of volumetric soil water content generated by a soil water flow model coupled **with a root water uptake model** (section 2.3), were treated as measured data and are used as the basis for all methods (section 2.2) estimating the sink term $\widetilde{S}(z)$ and total evapotranspiration $\widetilde{E}$.

Comment 5: *P65, L20: During dry periods, non-null "q" may occur as capillary rise (q is then negative), especially if the water table is no deeper than 2 meters. A possible justification to prevent capillary rise from happening in the synthetic dataset would be to define the "water table" as the bottom of a lysimeter. Didn't capillary rise occur during dry periods in the synthetic dataset?*

Response: Yes, there is capillary rise in our synthetic dataset from the shallow water table, which is also realistic for our scenario. Overall, the capillary rise flux is smaller than drainage in magnitude, but it does introduce uncertainty to the method (Fig. AC2.1). However, our aim was to generate a scenario as realistically as possible to evaluate the particular methods and also show their drawbacks, and we therefore prefer to not make the proposed adjustment. It is true that this introduces an additional error to the ssml method, and we will point this out in the revision.

Comment 6: *P66, L2: A more precise definition of dry period should be provided here. I believe that later in the manuscript it is mentioned that the dry periods start 24 hours after the end of rain events. Was there no leaching later than that? I insist on these points (5 and 6) because they could be a major reason why the method ssml fails to predict accurate evapotranspiration.*

Response: We are aware that percolation can occur also up to several days after a rainfall event, especially in deeper layers. This is the case for the investigated summer period, which started one day after a rainfall event, and percolation was considerable for more than a week in the deep soil layers (Fig AC2.1 c). However, this period was chosen deliberately to investigate whether the particular data-driven methods can deal with leaching fluxes.

This is also discussed in section 4, P79, L13-20: "In those simpler soil water balance methods any change in soil moisture is assigned only to root water uptake (Rasiah et al., 1992; Musters et al., 2000; Hupet et al., 2002). However, even several days after a rainfall event the vertical matrix flow within the soil can be similar in magnitude to the root water uptake (Schwärzel et al., 2009) and this leads to considerable overestimation of the sink term, when soil water flow is not accounted for. This error sums up, when the sink term is integrated over depth and leads to a great bias in 20 the evapotranspiration estimate."
We agree with the reviewer's comment that a more precise definition of the applied dry period should be provided. We will change sentence P66, L2 accordingly:

<u>Old:</u>
Additionally, rainfall measurements are required to select dry periods.

<u>New:</u>
Additionally, rainfall measurements are required to select dry periods, where no percolation occurs. **These could start several hours up to several days after a rainfall event (Breña Naranjo et al., 2011), and the exact timing depends on the amount of rainfall and the site-location parameters like soil type and vegetation. In this study we waited 24 hours after the end of the precipitation event, before applying the model.**

We also approve that the statement in sentence P78, L22-24: "For the same reason, none of the water balance methods can be applied during times of fast soil water flow, for example during or shortly (one day) after a rainfall event.", could be confusing and we will edit the sentence to:

<u>New:</u>
"For the same reason, none of the water balance methods can be applied during times of fast soil water flow, for example **during or after a rainfall event**."

We agree that it is important to point the drawback of the ssml more out in the manuscript and we will specifically refer to the ssml in the above mentioned section in the revised manuscript.

Comment 7: *P67, L20: The assumption that mflow does not change significantly between day and night is interesting and could be directly illustrated from the synthetic dataset as mflow is known at all times.*

Response: Indeed, the manuscript would benefit from an illustration of the basic assumption of the msml method, that invariance of mflow during day and night. We correlated the mean fluxes in the nights before and after one particular day with the mean fluxes of the respective day, and found a strong correlation (R^2=0.99, p<0.001) (Fig. AC2.2). We will include this figure in the revised manuscript.

Comment 8: *P67, L21: Here it is not clear to me which nights are included in mflow. Is "antecedent and preceding nights" limited to two nights? In case daytime mflow would be correlated to night-time mflow, I would expect that the highest correlation would be with mflow from the most recent night. What additional pieces of information would other preceding nights provide?*

Response: Yes, "antecedent and preceding nights" is limited to one night before and after the considered day. We will make this more clear in the revised manuscript as follows:

Old:

The sink term can be calculated from Eq. (8a), assuming that m_{flow} can be estimated from Eq. (8b) and using the average of the antecedent and preceding nights $m_{flow,i}$.

New:

The sink term can be calculated from Eq. (8a), assuming that m_{flow} during the day can be estimated from Eq. (8b) and using the average of the **antecedent and the preceding night**.

Comment 9: P68, L22: I found the inverse model section quite confusing. It seems like the method of Zuo and Zhang is first explained, then for some reason a second method is explained. The first method would not be implemented though. I understand from the first sentences that the sink terms are optimized at each depth and each time step (while usually the RWU model parameters are optimized). Hopefully what follows can be clarified and made more concise.

Response: Obviously, this section leads to confusions and misunderstandings, for example that the method after Zuo and Zhang was not implemented. However, the method after Zuo and Zhang was implemented but we modified the termination process of the original iterative procedure. We agree that this section would benefit from a more concise and structured explanation. We restructured this section (Section 2.2.4 Inverse Model (im), P68, L6 - P70, L8) as follows (changes in bold letters) and will replace it in the revised manuscript.

New:

The fourth approach is the most complex. The *i*nverse *m*odel (*im*) estimates the average root water uptake by solving the Richards' equation (Eq. 1) and iteratively searching the sink term profile for each time step, which produces the best fit between the numerical solution and measured values of soil moisture content (Zuo & Zhang, 2002). **The advantage of this method is the estimation of root water uptake without the a priori estimation of rooting profile function parameters since they are highly uncertain as elucidated in the introduction. We implemented the inverse water balance approach after Zuo and Zhang (2002) with the Fast Richard's solver (Ross, 2003), which is available as FORTRAN 90 code. We modified the original method by changing the convergence criterion. In the following section, we first introduce the iterative procedure as proposed by Zuo and Zhang (2002) and then explain the modification, which we conducted.**
The iterative procedure by Zuo and Zhang (2002) runs the numerical model over a given time step (Δt) in order to estimate the soil water content profile $\tilde{\theta}_{\mathrm{i}}^{(\mathrm{v}=0)}$ at the end of the time step, and assuming that the sink term ($\tilde{S}_{im,i}^{(v=0)}$) is zero over the entire profile. Here ~ depicts the estimated values at the respective soil layer i, and v indicates the iteration step. Next, the sink term profile $\tilde{S}_{im,i}^{(v=1)}$ is set equal to the difference between previous approximation $\tilde{\theta}_{\mathrm{i}}^{(\mathrm{v}=0)}$and measurements θ_{i} while accounting for soil layer thickness and length of the time step for units.

In the following iterations, $\tilde{S}_{im,i}^{(v)}$ is used with Richards' equation to calculate the new soil water contents $\tilde{\theta}_{\mathrm{i}}^{(\mathrm{v})}$. The new average sink term $\tilde{S}_{im,i}^{(v+1)}$ is then determined with Eq. (10).

$$\tilde{S}_{im,\mathrm{i}}^{(v+1)} = \tilde{S}_{im,\mathrm{i}}^{(v)} + \frac{\tilde{\theta}_i^{(v)} - \theta_i}{\Delta t} \cdot d_{z,i} \tag{10}$$

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

$$\varepsilon_{ZZ} \geq \frac{1}{n} \sum_{i=1}^{n} \left[\frac{\tilde{\theta}_i^{(v)} - \theta_i}{\theta_i} \right]^2 \quad , \tag{11}$$

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

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

(1) Calculate the difference between the estimated and measured soil water content (Eq. 12) and compare the change of this difference to the difference of the previous iteration (Eq. 13).

$$e_i^{(v)} = \left| \theta_i - \tilde{\theta}_i^{(v)} \right| \tag{12}$$

$$\varepsilon_{GH,\mathrm{i}}^{(v)} = e_i^{(v-1)} - e_i^{(v)} \tag{13}$$

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

(3) If $e_{\mathrm{i}}^{(v)} > 1.0\text{e-}4$: Calculate $\tilde{S}_{im,\mathrm{i}}^{(v+1)}$ according Eq. (10); else the current iteration sink term ($\tilde{S}_{im,\mathrm{i}}^{(v+1)} = \tilde{S}_{im,\mathrm{i}}^{(v)}$) is retained as it results in a good fit between estimated and measured soil water contents.

The iteration process continues until the convergence criterion $\varepsilon_{GH}^{(v)}$ (Eq. 13) does not change anymore between iterations (i.e. all layers have reached a satisfactory fit), or after a specified number of iterations (we chose 3000).

The required input information are besides the soil water content measurements and the rainfall, the soil hydraulic parameters.

Comment 10: *P70, L21: Here I did not find the spatial resolution of the simulation (1 cm?).*

Response: The spatial resolution of the simulation is according to the measurement depths 15-15-30-40-40-40-40 cm. The advantage of the applied soil water flow model is that the water fluxes are calculated with the matrix flux potential (Kirchhoff transformation), which allows a spatial discretization with large nodal spacing (Ross, 2006). The inversion of the soil model to estimate root water uptake benefits from this lower spatial discretization, which reduces computation times. This was the reason to choose this model.
We compared the model results for simulated soil water contents of the applied spatial discretization and one model with 1 cm spatial resolution. The obtained $R^2 = 0.98$ between both datasets justified the application of the coarse spatial resolution.
We will include a comment on the spatial resolution in the revised manuscript.

Old:
The model was set up for a one dimensional homogeneous soil profile, 220 cm deep. Measurement points were set in depths of 15, 30, 60, 100, 140, 180 and 220 cm. We used a maximum rooting depth of 140 cm, with 60% of root length density located in the top 15 cm of the root zone, which corresponds to mean values measured on the field site (Ravenek et al., 2014).

New:
The model was set up for a one dimensional homogeneous soil profile, 220 cm deep. Measurement points were set in depths of 15, 30, 60, 100, 140, 180 and 220 cm. **The spatial resolution of the soil model is according to the measurement points 15-15-30-40-40-40-40 cm. The advantage of the applied soil water flow model is that the water fluxes are calculated with the matrix flux potential (Kirchhoff transformation), which allows a spatial discretization with large nodal spacing (Ross, 2006).** We used a maximum rooting depth of 140 cm, with 60% of root length density located in the top 15 cm of the root zone, which corresponds to mean values measured on the field site (Ravenek et al., 2014).

Comment 11: *P72, L4-5: This sentence could be removed as its content is repeated in more detail in the next sentence.*

Response: Thank you for the useful hint. We will remove the indicated sentence in the revised manuscript.

Comment 12: *P74, L16: According to Table 2 the best result (b=0.89%) corresponds to the measurement frequency of 12h, not 24h. The captions of Table 2 and 4 do not specify what variable prediction is evaluated. From the rest of the text I believe it is the daily averaged ET though.*

Response: Yes, 0.89 % is for the frequency of 12 h (according to Table 2). We apologize for the typing error and we will change it to 12 h in the indicated sentence in the revised manuscript.

We will change the captions of Table 2 and 4 in the revised manuscript as follows:

Old:

Table 2: Comparison of the model performance of the four data-driven methods regarding time resolution of soil moisture measurements. The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. Days at which rainfall occurs were excluded for the data analysis.

Table 4: Comparison of the model performance of the Multi Step Multi Layer Regression and the Inverse Model regarding soil moisture measurement uncertainty. The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. The precision uncertainty is abbreviated by prec err, the calibration uncertainty by cali err and the combined uncertainty by com err.

<u>New:</u>

Table 2: Comparison of the model performance of the four data-driven methods **for reproducing daily evapotranspiration for the particular time resolution** of soil moisture measurements. The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. Days at which rainfall occurs were excluded for the data analysis.

Table 4: Comparison of the model performance **with considering soil moisture measurement uncertainties for** the Multi Step Multi Layer Regression and the Inverse Model **for reproducing daily evapotranspiration and the mean depths where 25 %, 50 % and 90 % water extraction occurs.** The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. The precision uncertainty is abbreviated by prec err, the calibration uncertainty by cali err and the combined uncertainty by com err. **The relative bias for reproducing evapotranspiration is abbreviated with b_{ET} and for reproducing mean depths where 25 %, 50 % and 90 % water extraction occurs is abbreviated with $b_{25\%}$, $b_{50\%}$ and $b_{90\%}$, respectively.**

Comment 13: *P75, L14: "The results show that lesser complex methods better reproduce ET". Isn't it the opposite, more complex methods (msml and im) better predict ET?*

Response: The reviewer is right, more complex methods better predict ET. The focus of the indicated sentence was more on the temporal resolution of the applied soil moisture data rather than a comparison between the methods. Lesser complex methods perform better when using soil water measurements with higher temporal resolution (e.g. of 1 and 3 h).

We rephrased this section to make this more obvious.

<u>Old:</u>

The results show that lesser complex data-driven methods, except the ssml, bet- 15 ter reproduce the actual evapotranspiration, when using soil water measurements with higher temporal resolution of 1 and 3 h.

<u>New:</u>

Our results also show that lesser complex data-driven methods, also perform better at higher temporal resolution (1 and 3 h), except for the ssml.

Comment 14: *P75, L27: It is explained that the standard deviation of z_25%, z_50% and z_90% from the synthetic dataset is almost 0. In consequence the RV index tends to values too high to be indicative, and its numerator (std dev of estimated z_25%, z_50% and z_90%) is used instead. Smaller std dev of estmations then become indicator of quality of fit, which makes sense. I am surprised though that the* *authors (i) insist in the introduction and discussion on the dynamism of RWU which adapts itself to soil moisture distribution, (ii) use a RWU model that has compensation implemented, but eventually generate a synthetic dataset that does not seem to have significant variations of RWU relative distribution…*

Response: Our aim was to generate a realistic scenario from a known experimental field site to evaluate the particular methods. In the case study there was no water stress and thus there was no redistribution of water uptake within the soil layers necessary although the applied model can reproduce different root water uptake patterns. Nevertheless, the uniformity of the root water uptake patterns has no technical influence on the application of the investigated data-driven methods. We will add this as a comment in the method section of the revised manuscript.

Comment 15: *P80, L17: The word "uptake" probably missing between "root water" and "model".*

Response: We apologize for the typing error and we will add "uptake" in the indicated sentence in the revised manuscript.

Comment 16: *P81, L12: The word "and" between "calibration error" and "but"…*

Response: Thank you for the hint. We will delete the word "and" in the indicated sentence in the revised manuscript.

Comment 17: *P95: More results could be provided in Table 4, if not within the body of the article, it could be added in appendix.*

Response: We will add the values of the mean relative bias between synthetic and predicted values of evapotranspiration and the depths where 25, 50, 90 % of water extraction occurs, according to Fig. 6 of the manuscript.

<u>New:</u>

Table 4: Comparison of the model performance with considering soil moisture measurement uncertainties for the Multi Step Multi Layer Regression and the Inverse Model for reproducing daily evapotranspiration and the mean depths where 25 %, 50 % and 90 % water extraction occurs. The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. The precision uncertainty is abbreviated by prec err, the calibration uncertainty by cali err and the combined uncertainty by com err. The relative bias for reproducing evapotranspiration is abbreviated with b_{ET} and for reproducing mean depths where 25 %, 50 % and 90 % water extraction occurs is abbreviated with $b_{25\%}$, $b_{50\%}$ and $b_{90\%}$, respectively.

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

Comment 18: *P98: If found the successive grey and white bands for respectively day and night to be sort of confusing as dark is commonly associated to night.*

Response: We agree that the distribution of the grey bands is confusing. Indeed, the figure would benefit from a change of the grey and white bands (grey=night, white=day). We will edit the figure accordingly in the revised manuscript (Fig. AC2.3).

Comment 19: *Page 10901: The coloured bands are not all visible due to overlapping.*

Response: We agree that Figure 5 does not show clearly the coloured bands. We adjusted the figure so that the bands for the precision error is now visible (Fig. AC2.4). The bands for the combined and the calibration error do really overlap almost completely. We will mention this in the figure legend to improve reading the figure.

General comment: *An illustration displaying what goes wrong with the im method for an isolated simulation would be helpful in addition to the confidence intervals of Fig. 5.*

Response: Thank you for the useful suggestion. We included a Figure showing the evolution of the inverse procedure (im) for the simulation with undisturbed soil moisture data (Fig. AC2.5) and for one isolated simulation with soil moisture data including a randomly selected calibration uncertainty (Fig. AC2.6). From figure AC2.6 it is evident that the inverse procedure is unable to close the water balance for the entire soil profile, especially if the sensors in the measurement transect have a different uncertainty range. The im fit the simulated soil moisture on the imprecise measured values at the expenses of the root water uptake, and thus overestimates the root water uptake in individually layers (Fig. AC2.6 d, e) and evapotranspiration. We will include figure AC2.6 as supplementary Figure S2 in the revised manuscript in addition to the discussion on page 88, line 27 to page 89, line 1 as follows.

<u>Old:</u>
This “calibration error” renders the evolution of the vertical potential gradients inconsistent with the evolution of the vertical sink term distribution, and thus introduces forbidding overestimation of evapotranspiration for the considered time steps

<u>New:</u>
This “calibration error” renders the evolution of the vertical potential gradients **and soil moisture profile** inconsistent with the evolution of the vertical sink term distribution, and thus introduces forbidding overestimation **of root water uptake and** evapotranspiration for the considered time steps **(Fig. S2)**.

Additional reference:

Bechmann, M., Schneider, C., Carminati, A., Vetterlein, D., Attinger, S., and Hildebrandt, A.: Effect of parameter choice in root water uptake models – the arrangement of root hydraulic properties within the root architecture affects dynamics and efficiency of root water uptake, Hydrol. Earth Syst. Sci., 18, 4189-4206, doi:10.5194/hess-18-4189-2014, 2014.

Breña Naranjo, J. A., Weiler, M., and Stahl, K.: Sensitivity of a data-driven soil water balance model to estimate summer evapotranspiration along a forest chronosequence, Hydrol. Earth Syst. Sci., 15, 3461-3473, doi:10.5194/hess-15-3461-2011, 2011.

Jackson, R. B., Sperry, J. S., and Dawson, T. E.: Root water uptake and transport: using physiological processes in global predictions, Trends Plant Sci., 5, 482–488, 2000.

Ross, P.J.: Fast Solution of Richards' Equation for Flexible Soil Hydraulic Property Descriptions, Land and Water Technical Report, CSIRO, 39/06, 2006.

Zwieniecki, M. A., Thompson, M. V., and Holbrook, N. M.: Understanding the Hydraulics of Porous Pipes: Tradeoffs Between Water Uptake and Root Length Utilization, J. Plant Growth Regul., 21, 315–323, 2003.

Figures for „Author comment - response to referee #2"

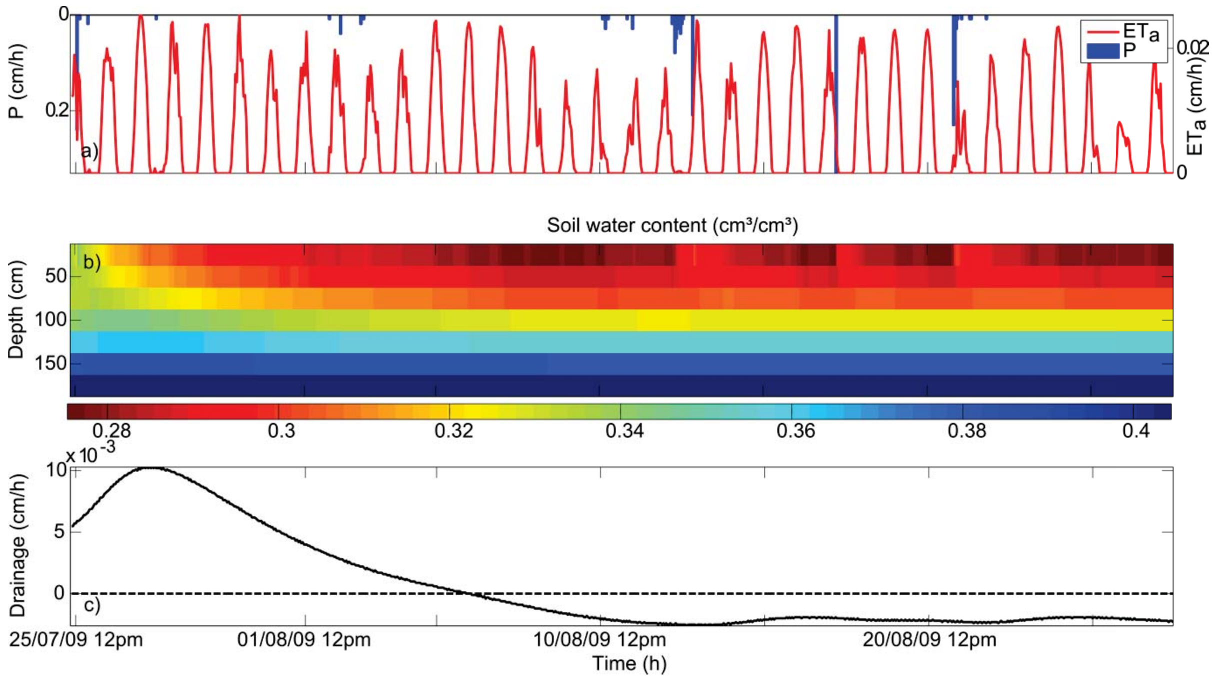

Figure AC2.1: Precipitation (P) and actual evapotranspiration (ET_a) from 25th July to 28th August (a), temporal and spatial evolution of soil water content (b) and drainage flux out of the soil column in 220 cm. Positive drainage indicate outflow and positive drainage indicate capillary rise.

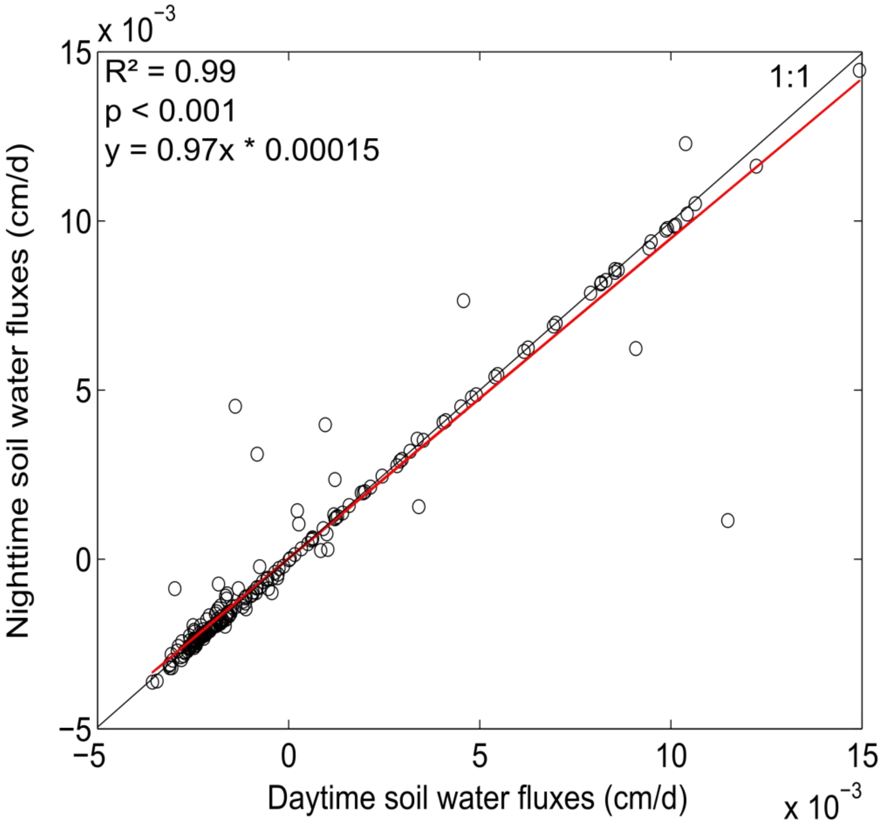

Figure AC2.2: Correlation between simulated mean fluxes of the respective day and the mean fluxes in the nights before and after one particular day. The solid red line is the regression line and the solid black line represents the 1:1 line. The analysis was conducted with the LinearModel.fit function of the Statistics toolbox in Matlab R2012.b.

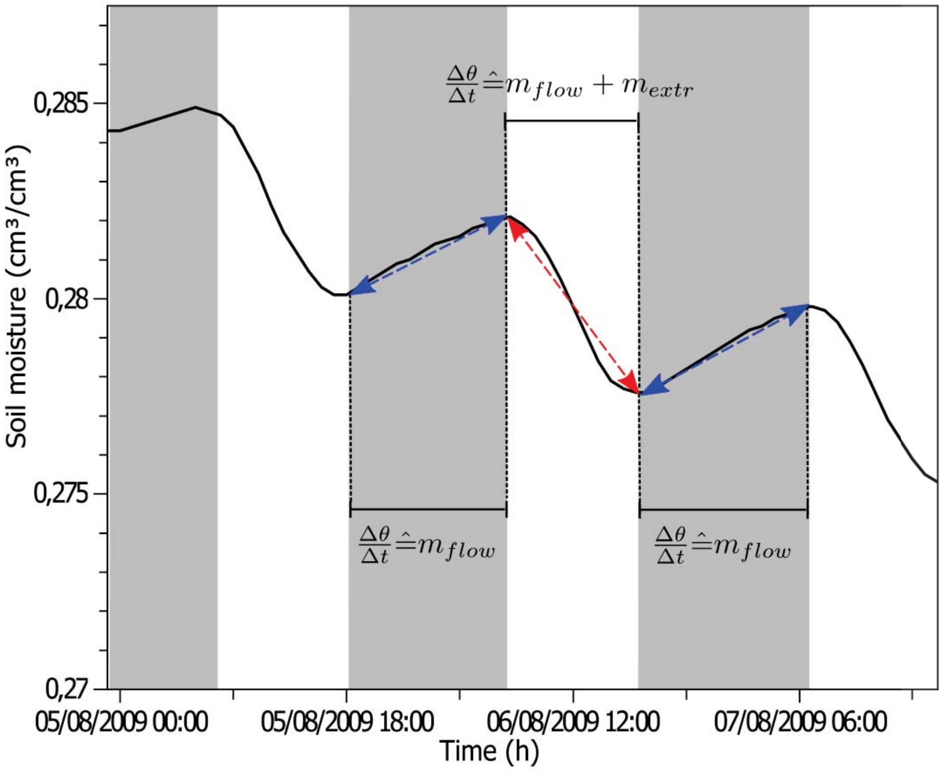

Figure AC2.3: Short term fluctuations of soil moisture in 15 cm depth during August 2009, showing the rewetting of soil at night times (blue line) and the water extraction at the day (red line); dashed lines depict the change between times with soil water extraction (white) and rewetting of soil (grey).

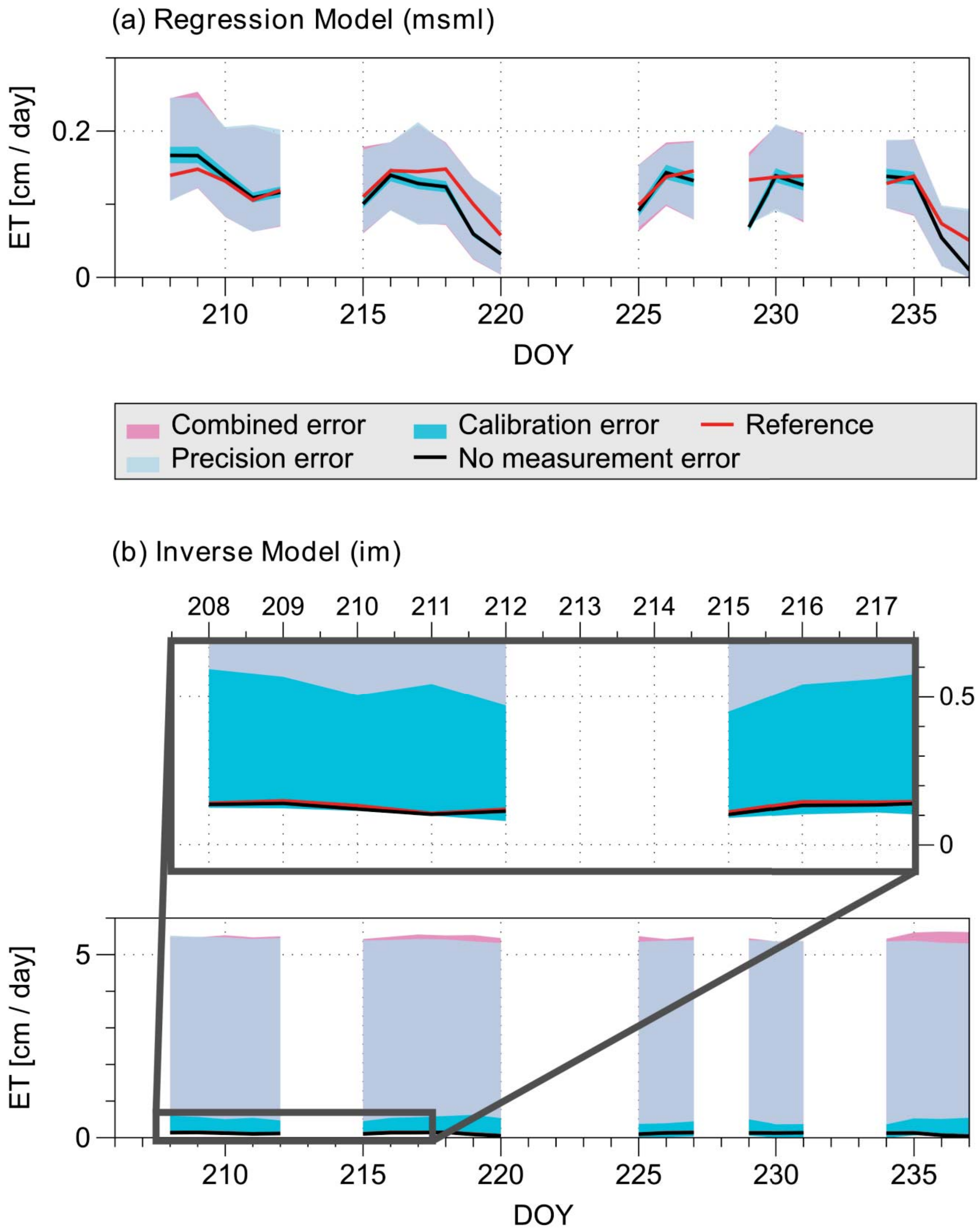

Figure AC2.4: Influence of soil moisture uncertainty on evapotranspiration estimated with the Multi Step Multi Layer Regression (Regression Model - msml) (a) and the Inverse Model (im) (b). The red line is the evapotransiration from the synthetic data (Reference). The colored bands indicate the 95% confidence intervals.

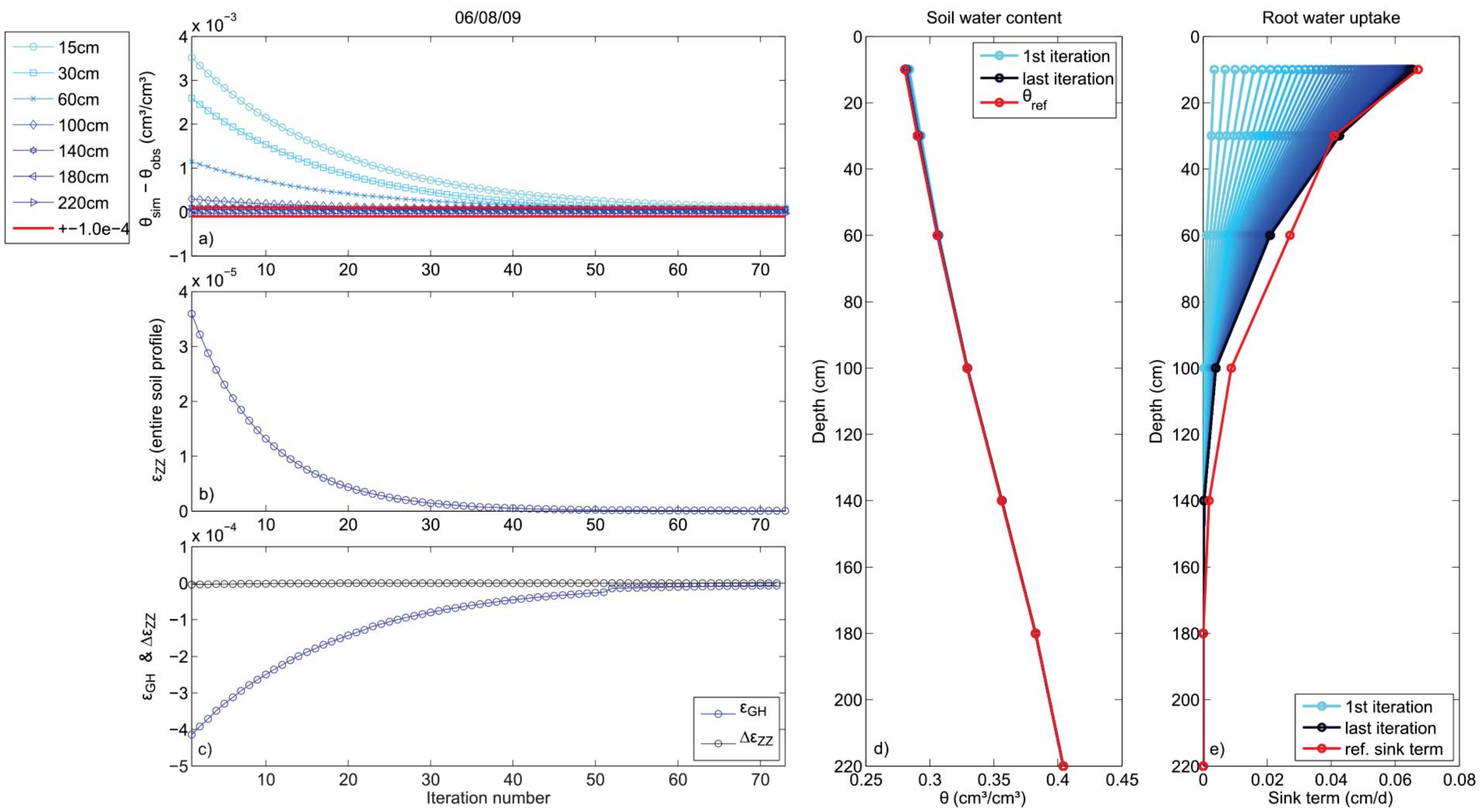

Figure AC2.5: Evaluation of the inversion process with undisturbed soil water content data of the im method (daily resolution). Subplot a) shows the difference of simulated (θ_{sim}) and observed soil water content (θ_{obs}) for each conducted iteration step in each depth. Suplot b) shows the evolution of the decision criteria ε_{ZZ} at each iteration step and c) depicts the convergence criteria $\Delta\ \varepsilon_{ZZ}$ and ε_{GH} for each iteration step until the reach their value for termination. Subplot d) shows the reference soil water content profile (θ_{ref}) which is in this case equal to θ_{obs} and the respective iterations. Subplot e) shows the reference sink term and the evaluation of the estimated sink term over depth for each conducted iteration.

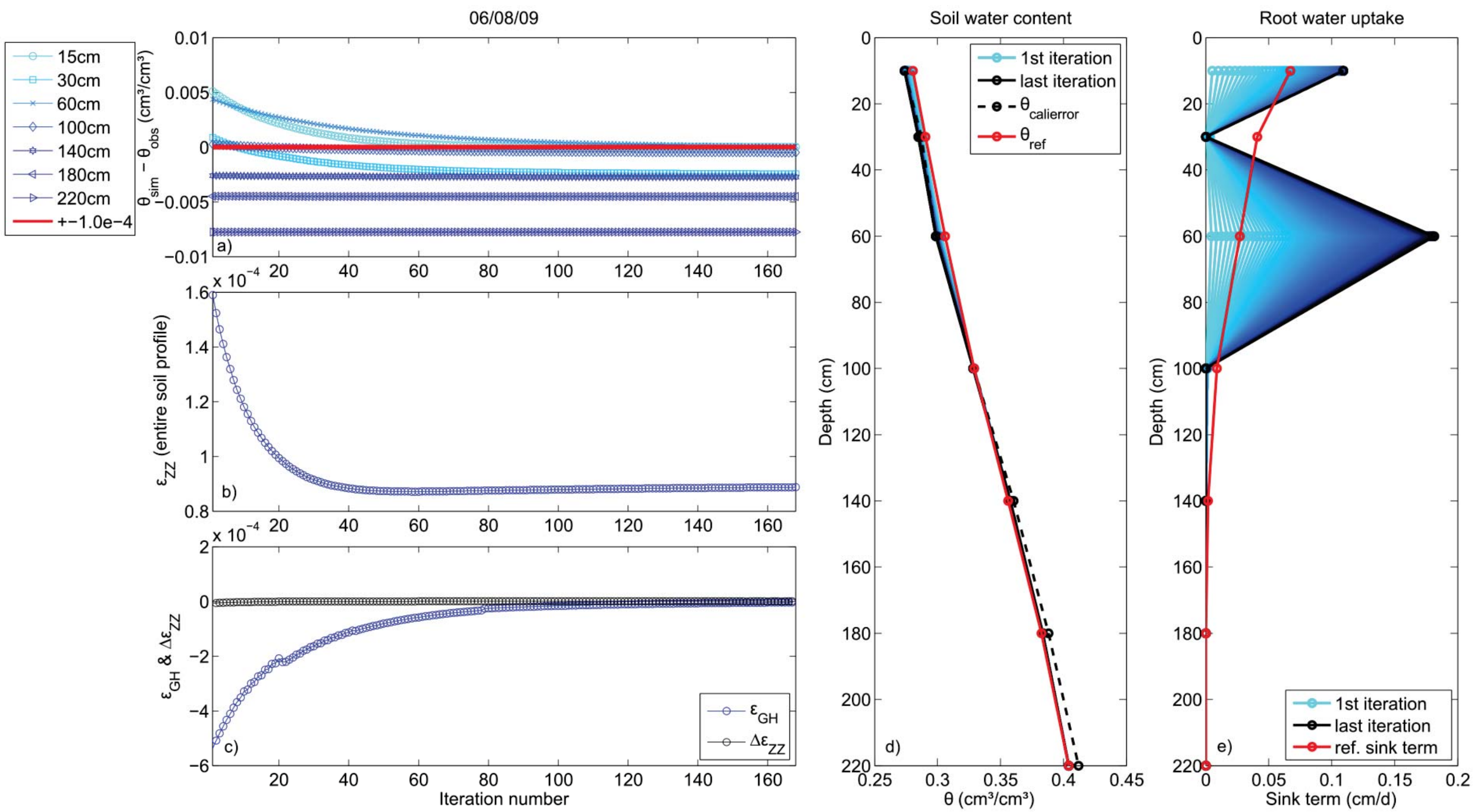

Figure AC2.6: Evaluation of the inversion process with disturbed soil water content data (calibration uncertainty) of the im method (daily resolution). Subplot a) shows the difference of simulated (θ_{sim}) and observed soil water content (θ_{obs}) for each conducted iteration step in each depth. Suplot b) shows the evolution of the decision criteria ε_{ZZ} at each iteration step and c) depicts the convergence criteria $\Delta\ \varepsilon_{ZZ}$ and ε_{GH} for each iteration step until the reach their value for termination. Subplot d) shows the reference soil water content profile (θ_{ref}), the perturbed soil moisture profile ($\theta_{calierror}$) and the respective iterations. Subplot e) shows the reference sink term and the evaluation of the estimated sink term over depth for each conducted iteration.

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

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Abstract

Understanding the role of plants for soil water relations, and thus for ecosystem functioning, requires information about root water uptake. We evaluated four different complex water balance methods to estimate sink term patterns and evapotranspiration directly from soil moisture measurements. We tested four methods: The first two take the difference between two measurement intervals as evapotranspiration, thus neglecting vertical flow. The third uses regression on the soil water content time series and differences between day and night to account for vertical flow. The fourth accounts for vertical flow using a numerical model and iteratively solves for the sink term. Neither of those methods requires any a priori information of root distribution parameters or evapotranspiration, which is the advantage, compared to common root water uptake models. To test the methods, a synthetic experiment with numerical simulations for a grassland ecosystem was conducted. Additionally, the time series were perturbed to simulate common sensor errors, like those due to measurement precision and inaccurate sensor calibration. We tested each method for a range of measurement frequencies and applied performance criteria to evaluate the suitability of each method. In general, we show that methods accounting for vertical flow predict evapotranspiration and the sink term distribution more accurately than the simpler approaches. Under consideration of possible measurement uncertainties, the method based on regression and differentiating between day and night cycles leads to the best and most robust estimation of sink term patterns. It is thus an alternative to more complex inverse numerical methods. This study demonstrates that highly resolved (temporal and spatial) soil water content measurements may be used to estimate the sink term profiles when the appropriate approach is used.

Nomenclature

b	relative bias (%)
d_T	length of active transpiration period over a day (h)
$d_{z,i}$	thickness of soil layer i (m)
DOY	day of year
e	difference in observed and estimated soil water content in the inverse model
E	evapotranspiration (mm h^{-1} or cm d^{-1})
E_s	bare soil evaporation (mm h^{-1})
E_t	transpiration (mm h^{-1})
$\tilde{E}$	estimated evapotranspiration (mm h^{-1})
h	soil matric potential (m)
i	soil layer index
j	time step index
$K(h)$	hydraulic conductivity (m s^{-1})
K_{sat}	saturated hydraulic conductivity (m s^{-1})
m_{tot}	slope of fitted linear function on $\theta(t)$
m_{extr}	slope of fitted linear function on $\theta(t)$ due to sink term
m_{flow}	slopes of fitted linear function on $\theta(t)$ due to vertical soil water flow
n_{vG}	van Genuchten parameter (-)
NSE	Nash-Sutcliffe efficiency criterion
P	precipitation (mm h^{-1})
q	percolation (mm h^{-1})
RV	relative variability
S	sink term in Richards equation (s^{-1})
S_i	discretized sink term in the soil layer i (m s^{-1})
$\tilde{S}$	estimated sink term (m s^{-1})
s	standard deviation
t	time (s)
Δt	time step (h)
v	iteration step number (-)
$\bar{x}$	mean value
x	observed (synthetic) value
$\tilde{x}$	estimated values
z	vertical coordinate (m)

z_r active rooting depth (cm)

$z_{25\%}$ depth up to which 25 % of root water uptake occur (cm)

$z_{50\%}$ depth up to which 50 % of root water uptake occur (cm)

$z_{90\%}$ depth up to which 90 % of root water uptake occur (cm)

α van Genuchten parameter (m^{-1})

θ Volumetric soil water content (m^3 m^{-3})

θ_r residual volumetric soil water content (m^3 m^{-3})

θ_s saturated volumetric soil water content (m^3 m^{-3})

$\tilde{\theta}$ estimated volumetric soil water content (m^3 m^{-3})

$\Delta\theta$ deviation in volumetric soil water content over time (m^3 m^{-3})

ε_{ZZ} decision criterion for termination of the iteration process (Inverse Model from Zuo & Zhang (2002))

$\varepsilon_{GH,\mathrm{i}}$ decision criterion for termination of the iteration process in the Inverse Model proposed here

1 Introduction

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

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

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

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

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

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

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

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

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

2 Material and Methods

2.1 Target variable and general procedure

The evapotranspiration E consists of soil evaporation E_s and the plant transpiration E_t (Eq. 2)

$$E = (E_s + E_t) \tag{2}$$

The distinction between soil evaporation and combined transpiration is not possible for any of the applied water balance methods. Therefore, the water extraction from soil by plant roots and soil evaporation is called sink term profile in the rest of the paper. The integrated sink term over the entire soil profile results in the total evapotranspiration (Eq. 3),

$$E(t) = \int_{z=z_r}^{0} S(t,z)dz \;\rightarrow E_{\mathrm{j}} = \sum_{\mathrm{i}=1}^{n} S_{\mathrm{i,j}} \cdot d_{z,\mathrm{i}} \;, \tag{3}$$

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

In this study, synthetic time series of volumetric soil water content generated by a soil water flow model coupled with a root water uptake model (section 2.3), were treated as measured data and are used as the basis for all methods (section 2.2) estimating the sink term $\widetilde{S}(z)$ and total evapotranspiration $\widetilde{E}$. In order to investigate the influence of sensor errors, the generated time series were systematically disturbed, as shown in section 2.4. Based on these estimations we evaluate the data-driven methods on predicting evapotranspiration $\widetilde{E}$ and sink term profiles using the quality criteria given in section 2.5. As in eco-hydrological studies it is often interesting up to which depth a given fraction of root water uptake occurred (e.g. Green & Clothier, 1999; Plamboeck et al., 1999; Ogle et al., 2004), estimated sink term profiles were compared accordingly. Specifically, we determined up to which depths 25 %, 50 % and 90 % ($z_{25\%}$, $z_{50\%}$ and $z_{90\%}$) of water extraction takes place.

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

In the following we introduce the four investigated methods. They are summarized in Table 1.

Single Step Single Layer Water Balance (*sssl*)

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

$$\widetilde{E}_{sssl} = P - q - z_r \frac{\Delta\theta}{\Delta t} \quad , \tag{4}$$

where z_r is the active rooting depth, which is also the depth of the single soil layer, and is taken equal to the measurement depth of volumetric soil water content, θ. Δt indicates the length of the considered single time step. P is the rainfall and q the percolation out of the soil layer during the same time step. When rainfall occur infiltration as well as soil water flow takes place. It is assumed that percolation occurs only during this time and persists only up to several hours after the rainfall event (Naranjo et al., 2011). Since the percolation flux is unknown, the methods cannot be applied during these wet times. During dry periods q is set to zero and Eq. (4) simplifies to Eq. (5) (Naranjo et al., 2011)

$$\widetilde{E}_{sssl} = z_r \frac{\Delta\theta}{\Delta t} \, . \tag{5}$$

We applied Eq. (5) to estimate evaporation (in the single layer method equal to the sink term) from artificial soil water contents in 30 cm. Required input information are thus only time series of soil water content and active rooting depth $z_{r.}$ Additionally, rainfall measurements are required to select dry periods, where no percolation occurs. These could start several hours up to several days after a rainfall event (Breña Naranjo et al., 2011), and the exact timing depends on the amount of rainfall and the site-location parameters like soil type and vegetation. In this study we waited 24 hours after the end of the precipitation event, before applying the model.

Single Step Multi Layer Water Balance (*ssml*)

This method is similar to the *sssl* introduced above. It calculates the sink term based on two observation times (*s*ingle *s*tep), but is extended to several measurement depths (*m*ulti *l*ayer). The water balance during dry periods of each layer is the same as in Eq. (5), and uptake in individual layers is calculated by neglecting vertical soil water fluxes and therefore assuming that the change in soil water content is only caused by root water uptake (Hupet et al., 2002)

$$\widetilde{S}_{ssml,i} = d_{z,i}\frac{\Delta\theta_i}{\Delta t} \quad , \qquad (6)$$

where $\tilde{S}_{\mathrm{ssml,i}}$ is the estimated sink term in soil layer i, $\Delta\theta_{\mathrm{i}}$ is the change of soil water content in the soil layer i over the single time step (Δt) and $d_{z,\mathrm{i}}$ is the thickness of the soil layer i. Actual evpotranspiration (E_{ssml}) is calculated by summing up $\widetilde{S}_{\mathrm{ssml,i}}$ over all depths in accordance with (Eq. 3). The application of the *ssml*-method is restricted to dry periods. It requires time series of volumetric soil water content and rainfall measurements as input to select dry periods.

Multi Step Multi Layer Regression (*msml*)

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

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

Here, the basic assumption is that the soil water flow does not change significantly between day and night (Fig. S1). The slope of the fitted linear functions gives the rate of root water extraction and vertical flow. This can also be shown mathematically by disassembling the Richards' equation (Eq. 1) in vertical flow (subscript flow) and sink term (subscript extr) (Eq. 7), whereas the change of soil water content over time ($\partial\theta / \partial t$) integrates both fluxes:

$$\frac{\partial\theta}{\partial t} = \frac{\partial\theta}{\partial t}\Big|_{\mathrm{flow}} + \frac{\partial\theta}{\partial t}\Big|_{\mathrm{extr}} = m_{tot} \, , \qquad (7)$$

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

$$m_{tot} = m_{\mathrm{flow}} + m_{\mathrm{extr}} \qquad \text{day} \tag{8a}$$

$$m_{tot} = m_{\mathrm{flow}} \qquad \text{night} \tag{8b}$$

The sink term can be calculated from Eq. (8a), assuming that m_{flow} can be estimated from Eq. (8b) and using the average of the antecedent and the preceding night. A similar procedure has been applied in diurnal groundwater table fluctuations (Loheide, 2008). Also there, the extraction will be overestimated if day and night fluxes are not separately considered. Taking into account the soil layer thickness of the respective layer i ($d_{z,i}$), the mean daily sink term of soil layer i ($\tilde{S}_{msml,i}$) is obtained:

$$\tilde{\mathrm{S}}_{\mathrm{msm},i} = (\mathrm{m}_{\mathrm{tot},i} - \overline{m}_{\mathrm{flow},i}) \cdot \mathrm{d}_{\mathrm{z},i} \tag{9}$$

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

Inverse Model (*im*)

The fourth approach is the most complex. The *i*nverse *m*odel (*im*) estimates the average root water uptake by solving the Richards' equation (Eq. 1) and iteratively searching the sink term profile which produces the best fit between the numerical solution and measured values of soil moisture content (Zuo & Zhang, 2002). The advantage of this method is the estimation of root water uptake without the a priori estimation of rooting profile function parameters since they are highly uncertain as elucidated in the introduction. We implemented the inverse water balance approach after Zuo and Zhang (2002) with the Fast Richard's solver (Ross, 2003), which is available as FORTRAN 90 code. We modified the original method by changing the convergence criterion. In the following section, we first introduce the iterative procedure as proposed by Zuo and Zhang (2002) and then explain the modification, which we conducted.

The iterative procedure by Zuo and Zhang (2002) runs the numerical model over a given time step (Δt) in order to estimate the soil water content profile $\tilde{\theta}_{\mathrm{i}}^{(\mathrm{v}=0)}$ at the end of the time step, and assuming that the sink term ($\tilde{S}_{im,i}^{(v=0)}$) is zero over the entire profile. Here ~ depicts the estimated values at the respective soil layer i, and v indicates the iteration step. Next, the sink term profile

$\tilde{S}_{im,i}^{(v=1)}$ is set equal to the difference between previous approximation $\tilde{\theta}_{\mathrm{i}}^{(\mathrm{v}=0)}$ and measurements θ_{i} while accounting for soil layer thickness and length of the time step for units.

In the following iterations, $\tilde{S}_{im,i}^{(v)}$ is used with Richards' equation to calculate the new soil water contents $\tilde{\theta}_{\mathrm{i}}^{(\mathrm{v})}$. The new average sink term $\tilde{S}_{im,i}^{(v+1)}$ is then determined with Eq. (10).

$$\tilde{S}_{im,\mathrm{i}}^{(v+1)} = \tilde{S}_{im,\mathrm{i}}^{(v)} + \frac{\tilde{\theta}_i^{(v)} - \theta_i}{\Delta t} \cdot d_{z,i} \tag{10}$$

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

$$\varepsilon_{ZZ} \geq \frac{1}{n} \sum_{i=1}^{n} \left[\frac{\tilde{\theta}_i^{(v)} - \theta_i}{\theta_i} \right]^2 , \tag{11}$$

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

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

(1) Calculate the difference between the estimated and measured soil water content (Eq. 12) and compare the change of this difference to the difference of the previous iteration (Eq. 13).

$$e_i^{(v)} = \left| \theta_i - \tilde{\theta}_i^{(v)} \right| \tag{12}$$

$$\varepsilon_{GH,\mathrm{i}}^{(v)} = e_i^{(v-1)} - e_i^{(v)} \tag{13}$$

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

(3) If $e_{\mathrm{i}}^{(v)} > 1.0\mathrm{e}{-4}$: Calculate $\tilde{\mathrm{S}}_{im,\mathrm{i}}^{(v+1)}$ according Eq. (10); else the current iteration sink term ($\tilde{\mathrm{S}}_{im,\mathrm{i}}^{(v+1)} = \tilde{\mathrm{S}}_{im,\mathrm{i}}^{(v)}$) is retained as it results in a good fit between estimated and measured soil water contents.

The iteration process continues until the convergence criterion $\varepsilon_{GH}^{(v)}$ (Eq. 13) does not change anymore between iterations (i.e. all layers have reached a satisfactory fit), or after a specified number of iterations (we chose 3000).

The required input information are besides the soil water content measurements and the rainfall, the soil hydraulic parameters.

2.3 Generation of synthetic reference data

We used synthetic time series of volumetric soil water content with a measurement frequency of 1h, 3h, 6h, 12h and 24h. The time series of soil water content and also the sink term profiles were generated with a soil water flow model (Fast Richards Solver, Ross, 2003, same as used in section 2.2 for the Inverse Model). They were treated as measured data and are used as the basis for all methods. The synthetic data are based on meteorological and soil data from the Jena Biodiversity Experiment (Roscher et al., 2011). Root water uptake was calculated using a simple macroscopic root water uptake model, which uses an exponential root distribution with water stress-compensation (Li et al., 2001). Soil evaporation is taken as 20% of total evapotranspiration.

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

Upper boundary conditions are derived from measured precipitation and potential evapotranspiration calculated after Penman-Monteith (Allen et al., 1998) from measurements of the climate station at the experimental site (Weather Station Saaleaue, Max Planck Institute for Biogeochemistry - http://www.bgc-jena.mpg.de/wetter/). The used weather data have a measurement resolution of 10 minutes. Before applying evapotranspiration and rainfall as input data to generate the synthetic reference soil moisture and root water uptake data, both data sets were aggregated to the temporal resolutions applied for the reference run (1 hour). Soil moisture and root water uptake were generated with the same temporal resolution. When translating the evapotranspiration to sink term profiles (precision 4 digits), rounding errors introduce a small inaccuracy. Thus, the sum of the sink term in the reference run deviates by 0.02% compared to the original evapotranspiration.

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

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

The described forward simulation produces time series of soil water contents and root water uptake. Soil water content time series were used instead of measured data (synthetic measurements) as input for the investigated methods, while evapotranspiration and sink term profiles were used to evaluate them, based on the quality criteria described in section 2.5.

2.4 Influence of soil moisture sensor uncertainty

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

In this paper, we investigated the uncertainty of the applied methods stemming from calibration error (accuracy) and precision. For this we superimposed the original synthetic soil water content measurements generated in section 2.3 with artificial errors. ~~The precision error is taken as Gaussian noise with zero mean. The calibration error was taken as a wrong slope parameter on a linear calibration function.~~ Three types of errors were implemented, as follows (i) precision error: The time series for each soil layer were perturbed with Gaussian noise of zero mean and standard deviation of 0.067 Vol.% corresponding to a precision of 0.2 Vol.%; (ii) Calibration error: The perturbed time series were realigned along a new slope, which pivoted around a random point within the measurement range and a random intercept between ± 1.0 Vol.%, (iii) Calibration and precision: Perturbed series were created as a random combination of (i) and (ii), which is a common case in field studies (Spank et al., 2013). Errors were applied independently to all soil depths and 100 new time series were created for each of the error types. We determined the quality of the estimation methods using the median of 100 ensemble simulations with the 100 perturbed input time series, respectively. The values for the applied calibration uncertainty and precision are taken from the technical manual of the IMKO TRIME©-PICO32 soil moisture sensor (http://www.imko.de/en/products/soilmoisture/soil-moisture-sensors /trimepico32).

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

2.5 Evaluation criteria

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

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

$$R = \frac{Cov(\tilde{x},x)}{s_x \cdot s_{\tilde{x}}} \tag{15}$$

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

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

$$RV = \frac{s_{\tilde{x}}}{s_x} \tag{16}$$

RV values around one indicate a good estimation procedure.

Third, we use the relative bias (b) to describe the mean systematic deviation between estimated (~) and observed (synthetic) values, which is not captured by R:

$$b = \frac{\bar{\tilde{x}} - \bar{x}}{\bar{x}} \cdot 100\ (\%)\,, \tag{17}$$

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

3 Results

In total, we compared synthetic evapotranspiration rates from 33 consecutive days in July/August 2009. Evapotranspiration could not be estimated at days with rainfall for the Single Step Single Layer Water Balance (*sssl*) and the Single Step Multi Layer Water Balance (*ssml*) as well as for the Multi Step Multi Layer Regression (*msml*). Therefore, we excluded all days with rainfall from the analysis for all considered methods. We first consider in sections 3.1 and 3.2 the performance of the estimation methods on undisturbed synthetic time series, this is we ignore measurement errors or assume they do not exist. The influence of measurement errors is investigated in section 3.3.

3.1 Evapotranspiration derived by soil water content measurements

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

The Inverse Model (*im*) predicted the daily evapotranspiration for a measurement frequency of 12h with a very small relative bias of 0.89 %, which is the best for all investigated methods. Additionally, the *im* reaches the best R value (R=0.99) for all measurement frequencies (Tab. 2), and follows closely the 1:1 line between synthetic and estimated evapotranspiration (Fig. 3a and 3b). However, the relative variability (RV) and the relative bias indicate a better prediction with decreasing measurement frequency.

The second best method is the Multi Step Multi Layer Regression (*msml*), in particular when

applied for high temporal resolution measurements (1 and 3 hours). There, the bias is comparatively small (± 20%) and the correlation between synthetic (observed) and estimated values relatively high (R=0.58 and R=0.71 for 1h and 3h resolution respectively). Also, the *msml* results match well the 1:1 line between synthetic and estimated evapotranspiration (Fig. 3a and 3b).
The Single Step Single Layer Water Balance (*sssl*) and the Single Step Multi Layer Water Balance (*ssml*) show a weaker performance compared to the more complex methods *im* and *msml*. Neither of them follows well the 1:1 line between synthetic and estimated evapotranspiration (Fig. 3a and 3b). Regardless, they could reproduce the synthetic evapotranspiration with a relatively high linear correlation (Tab. 2), and comparable bias to the regression method, in particular for the range of intermediate measurement frequencies. However, values for the relative variability (*RV*) are comparatively large, in particular for the Single Step Multi Layer Water Balance (*ssml*). Interestingly, the model performance criteria of the simpler *sssl* show only minor differences between the particular temporal resolutions and performs overall better than *ssml*. Note that both water balance methods (*sssl* & *ssml*) overestimate the evapotranspiration at the beginning of the study period (Fig. 3c & 3d), which was marked by greater vertical flow between top soil and deeper soil due to preceding rainfall events.
Our results also show that lesser complex data-driven methods, also perform better at higher temporal resolution (1 and 3 h), except for the ssml. In contrast, the Inverse Model is better in predicting evapotranspiration when a coarse measurement frequency is used. Further, the results indicate that the estimated actual evapotranspiration becomes more accurate with increasing model intricacy and that is with accounting for vertical flow.

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

The Single Step Multi Layer Water Balance (*ssml*), the Multi Step Multi Layer Regression (*msml*) and the Inverse Model (*im*) are appropriate for determining root water uptake profiles by inclusion of all available measurements over depth. Table 3 summarizes the model applicability to estimate the depths at which 25 %, 50 % and 90 % of water extraction occurs (later stated as $z_{25\%}$, $z_{50\%}$ and $z_{90\%}$). Here, we used the standard deviation $s_{\tilde{x}}$ instead of the relative variability to evaluate the observed variance. This criterion was chosen because the standard deviation of the synthetic reference values is approx. zero and thus, the relative variability (*RV*) is getting very large, which is not practical for the method evaluation. The criteria are shown for the respective best achieved model performance (1h – *ssml* and *msml*; 24h – *im*).
Again, the quality of predicting the sink term distribution depends on the method complexity and increases with increasing complexity. The most complex *im* delivers the best prediction of sink term

distribution for a temporal resolution of 24 hours. The depths up to which 50 % of water extraction occur ($z_{50\%}$) could be predicted with a bias of less than 2 % (Tab. 3) and for $z_{90\%}$, the relative bias increased only slightly to approx. 3 %. Indeed, these comparatively accurate results are to be expected due to the two intrinsic assumptions: (1) the required soil hydraulic parameters for the implemented soil water flow model are exactly known and (2) the measurement uncertainty of the soil sensors is zero.

The regression method (*msml*) also delivers good estimations of sink term profiles over the entire soil column (Tab. 3 and Fig. 4), although it gets along without any intrinsic assumptions. Fig. 4 shows that the *msml* overestimates the sink term in the intermediate depths. The maximum relative bias is about -21% at $z_{50\%}$. Overall, the *msml* is applicable for determining the mean sink term distribution with an acceptable accuracy.

The *ssml* estimated sink terms correspond only weakly to the synthetic ones, and the relative bias is lowest for $z_{25\%}$ with 33% but increases strongly for $z_{50\%}$ and $z_{90\%}$ (Tab. 3). Moreover, the standard deviations of the predictions are substantial in most measurement depths (Tab.3, Fig. 4). Because of these large variations in sink term distribution, the prediction of sink term profiles becomes imprecise. Thus for the chosen simulation experiment, the *ssml* is not applicable for deriving the sink term from soil water content measurements.

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

We only evaluated the influence of measurement errors for two methods (*msml* and *im*). The single layer approach was omitted, since it does not allow the estimation of the sink term profile and *ssml* was omitted, since the estimation of the sink term profile was already inappropriate when ignoring measurement errors (see section 3.2).

The influences of soil moisture sensor uncertainties differ considerably among the investigated methods. The Multi Step Multi Layer Regression (*msml*) predicted the median daily evapotranspiration with precision uncertainty, calibration uncertainty and a combination of both reasonably well (Fig. 5). For all three types of uncertainty the correlation between synthetic (observed) and estimated values is relatively high (around R=0.9, Table 4). Also with respect to the median relative bias (%) the three cases differ only marginally (|b| = 7%, Tab. 4). Interestingly, the calibration uncertainty showed the lowest impact on the predicted evapotranspiration with a median bias of about -5% for the respective 100 ensemble calculations (Fig. 5).

Additionally, the bias is also used to compare the predicted relative water extraction depths ($z_{25\%}$, $z_{50\%}$ and $z_{90\%}$) (Fig. 6). The uncertainty caused by the calibration of the sensor shows the least differences to the observed values below 10%. These results are similar to these from simulations with soil moisture without any introduced measurement uncertainty. Further, the uncertainties caused by the precision of the sensors have the highest impact on predicted root water uptake patterns. It turns out that the relative uncertainty increases with increasing depth (decreasing sink term or rather water extraction) (Fig. 6 (a)).

Interestingly, the Inverse Model (*im*) shows worse model performances than the *msml* for all three types of uncertainty. Although, the predicted evapotranspiration from soil moisture with precision uncertainty is close to the observed values (Fig. 5), it differs around days where rainfall occurs (DOY 225, DOY 230 and DOY 234). This results in underestimation of evapotranspiration during these times, a weak correlation (Tab. 4), but an acceptable relative bias of about -10%. In contrast, for the calibration uncertainty it is the other way around. Here, the correlation is relatively high (R=0.85), but evapotranspiration is greatly overestimated (b=498%). A combination of both uncertainty sources does not further increase the overall error; but it combines both weaknesses to an overall poor estimation (Tab. 4).

The sensitivity to the type of uncertainty concerning prediction of sink term patterns is shown in Fig. 6b and Table 4. Similar to the *msml* the *im* is able to handle uncertainties in sensor precision to predict root water uptake depths whereas uncalibrated sensors lead to considerable increases in relative bias. Overall, the simpler *msml* shows a higher robustness against measurement uncertainties than the more complex *im*.

4 Discussion

We tested the application of several methods deriving based on the soil water balance how much water was extracted from the soil by evapotranspiration and how the extraction profile (sink term profile) changed with soil depth. The basis for all methods are time series of volumetric soil water content derived from measurements, although some methods require more information on soil properties, in particular the Inverse Model (*im*). None of the methods relies on a priori information on the shape of the sink term profile, or makes any assumptions on it being constant with time. This is the great advantage of these methods to others (Dardanelli et al., 2004; McIntyre et al., 1995; Hopmans & Bristow, 2002; Zuo et al., 2002). Since only changes in soil water content are considered, none of the investigated methods distinguish between soil evaporation and root water uptake. For the same reason, none of the water balance methods can be applied during times of fast soil water flow, for example during or after a rainfall event.

We used synthetic soil water content "observations" to validate the model results. This procedure has the great advantage that the "true" water flow and sink term profiles are perfectly known, including the nature of data uncertainty with regard to calibration error and sensor precision.

However, our model only accounts for vertical matrix flow, notably neglecting horizontal heterogeneity, which may be an additional challenge for deriving evapotranspiration in real world situations. Thus, additional tests of the methods in controlled field conditions, like in large lysimeters, and comparison with additional data, like isotope profiles, are necessary to confirm our results.

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

This distinction between vertical soil water flow and water extraction is the major challenge when applying water balance methods, because these fluxes occur concurrently during daytime (Gardner, 1983; Feddes and Raats, 2004). The regression method (*msml*) avoids this problem by considering vertical soil water fluxes, estimated from change in soil water content during nighttime. Li et al. (2002) used a similar approach to derive transpiration and root water uptake patterns from soil moisture changes between different times of the day. This direct attribution of nighttime change in soil water content to soil water flow inherently assumes that both nighttime evapotranspiration and hydraulic redistribution are negligible. Li et al. (2002) measured nocturnal sap flow, in order to ensure that nighttime transpiration was insignificant. Also in lysimeters, the weight changes can be used to validate the assumption. This assumption is the main drawback of this method, which however compares to the great advantage that it requires very limited input data, especially no a priori information about the soil properties. In contrast, the inverse modeling (*im*) approach inferred evapotranspiration and sink term patterns with greater quality, when soil water content measurements were free of error. However, because our analysis uses model generated time series of soil water content in order to mimic measurements, the soil properties of the original "experiment" are completely known, which is not usually the case in natural conditions. Usually, soil hydraulic parameters have to be estimated by a calibration procedure. This process is nontrivial and limited by the non-uniqueness of the calibrated parameters (Hupet et al., 2003), which results in uncertainties in simulated soil water fluxes and root water uptake rates (Duan et al., 1992; Musters and Bouten, 2000; Musters et al., 2000; Hupet et al., 2002; Hupet et al., 2003). This reliance of the inverse model approach on precise knowledge of the soil environment is the main drawback of that approach.

Several studies on estimation of root water uptake profiles focused on uncertainties related to calibrated parameters of soil and the root water uptake models (Musters and Bouten, 2000; Musters et al., 2000; Hupet et al., 2002; Hupet et al., 2003). While using data and models, uncertainties arise not from soil parameter uncertainty, but already evolve during the measurement process of the environmental data (Spank et al., 2013). Thus, in the second part of this paper, we investigated how measurement noise (precision), wrong sensor calibration (accuracy) and their combination reflect on the derivation of evapotranspiration and sink term patterns from soil water content measurements. We only performed this analysis for the two methods which performed satisfactory without sensor errors: The regression method (*msml*) and Inverse Model (*im*). In this more realistic setting, the simpler regression method (*msml*) performed much better than the Inverse Model (*im*). The latter was strongly affected by inaccurate or lack of site-specific calibration. This "calibration error" renders the evolution of the vertical potential gradients and soil moisture profile inconsistent with the evolution of the vertical sink term distribution, and thus introduces forbidding overestimation of root water uptake and evapotranspiration for the considered time steps (Fig. S2). Generally, the prediction of the inverse model improves when longer evaluation periods are considered (also compare Zuo & Zhang (2002)) and therefore the calibration error may become less prominent when considering time steps of several days as done in Zuo & Zhang (2002). Compared to the effect of calibration, the sensor precision had a much smaller effect. Thus, the Inverse Model may be applicable and should be tested in situations where all sensors in the profile are well calibrated. A further improvement of the Inverse Model could be achieved by smoothing the measured soil water content profiles via a polynomial function to get an accurate and continuous distribution of soil water contents as done in Li et al. (2002) and Zuo and Zhang (2002).

The regression model (*msml*) was overall more robust towards the investigated measurement errors. It was barely affected by calibration error ~~and~~ but was somewhat affected by sensor precision. This is expected, since the sensor calibration only improves the absolute values of the measurements, but does not affect the course of the soil moisture desiccation. The case is different for uncertainty due to sensor precision, which result in higher deviations between observed and predicted sink term uptake patterns (Fig. 6). As this method uses linear regression on the temporal evolution of soil water contents, the quantity of root water uptake depends on the gradient of the slopes. Those slopes are strongly influenced by the random scatter of data points, which is characteristic for sensor noise.

Using the smallest time step of 1h, we could estimate the relative depth where 50% of water extraction occurs with a bias less than 30%. Using higher time resolution with several measurements per hour or several minutes and noise reducing filters (Li et al., 2002; Peters et al., 2013) would likely further improve this result. This method should be further evaluated in lysimeters, to test its application in controlled but more realistic environments.

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

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

Our results show that water balance methods have potential to be applied for derivation of water extraction profiles, but they also suggest that their application may be challenging in realistic conditions. In particular, the Inverse Model (*im*) has great potential, in theory, but obtaining information of the soil environment with sufficient accuracy may be unrealistic. The regression method (*msml*) is particularly promising, as it requires little input and is comparably robust towards measurement errors. Further tests in controlled environments and ideally in concert with isotope studies should be conducted to further test the application of these methods in real world conditions. The great advantage of all considered methods is that they do not require a priori information about total evapotranspiration or the shape of the root water uptake profiles. Root water uptake moves up and down depending on soil water status (Lai & Katul, 1998; Li et al., 2002, Doussan et al., 2006; Garrigues et al., 2006), and many existing approaches are unable to account for this dynamic of root water uptake. Root water extraction profiles are central topics in ecological and eco-hydrological research on resource partitioning (e.g. Ogle et al., 2004; Leimer et al, 2014; Schwendenmann et al., 2014) and drivers for ecosystem structure (Arnold et al., 2010). Water balance methods are potential tools for comparing those extraction profiles between sites and thus contributing to ecohydrological process understanding.

5. Conclusions

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

Layer Water Balance (*sssl*) and the Single Step Multi Layer Water Balance (*ssml*).

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

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

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Figure captions

Figure 1: Actual evapotranspiration (ET_a) and precipitation (P) (cm/d) in the growing season (from March 2009 to September 2009) (a) and synthetic time series of soil water content (b) with daily resolution.

Figure 2: Short term fluctuations of soil moisture in 15 cm depth during August 2009, showing the rewetting of soil at night times (blue line) and the water extraction at the day (red line); dashed lines depict the change between times with soil water extraction (grey) and rewetting of soil (white).

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List of tables

Table 1: Overview of the four applied data-driven methods, the acronym of the methods for further use and the required input data.

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

Table 2: Comparison of the model performance of the four data-driven methods for reproducing daily evapotranspiration for the particular time resolution of soil moisture measurements. The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. Days at which rainfall occurs were excluded for the data analysis.

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

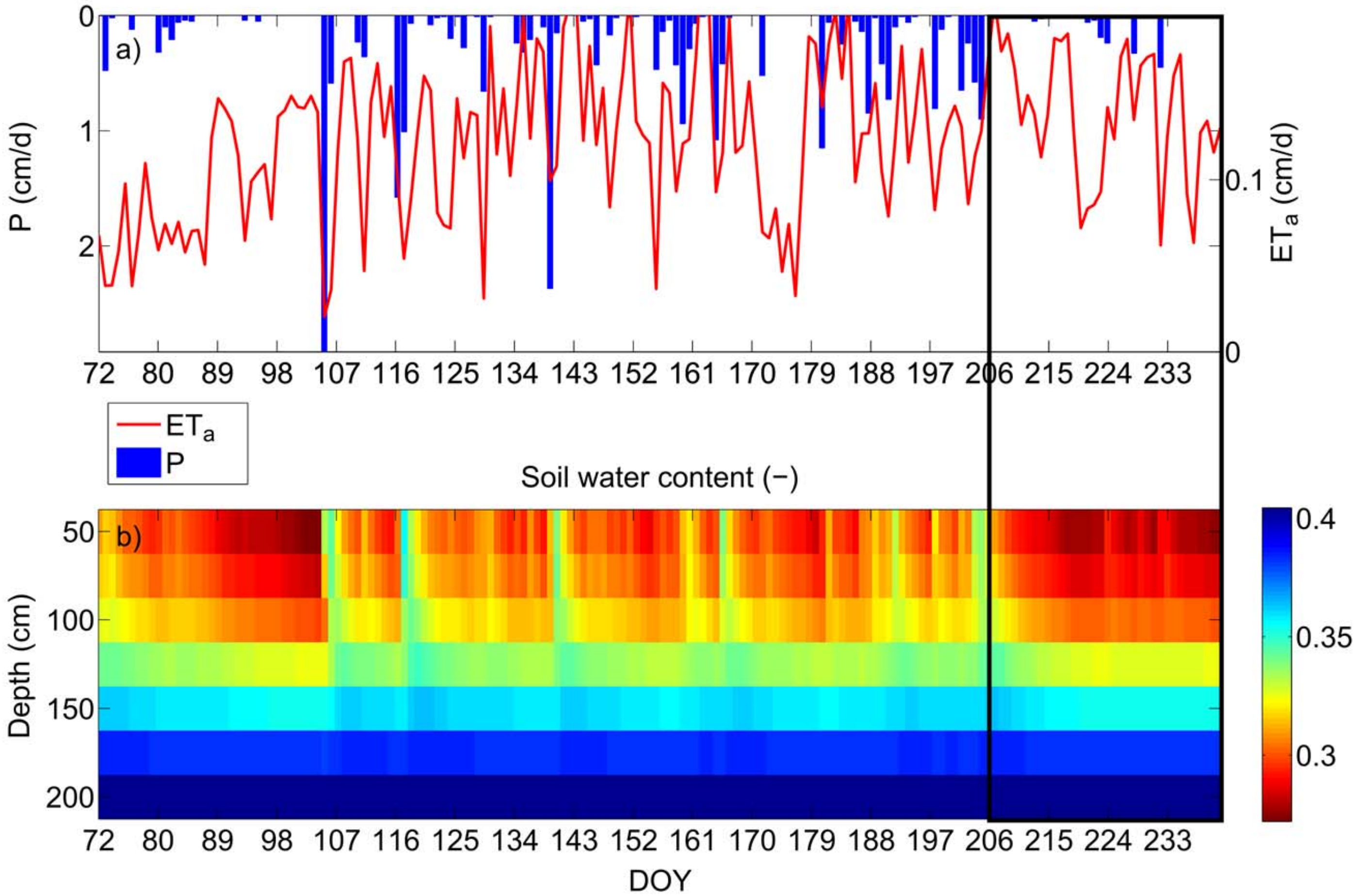
Table 3: Comparison of model performance for reproducing the sink term profile (Single Step Multi Layer Water Balance, Multi Step Multi Layer Regression and Inverse Model). Depths where 25 %, 50 % and 90 % water extraction occurs were regarded. Mean synthetic (syn.) depth and mean estimated (est.) depth describe the mean depth over 33 days, where water extraction occurs. *b* is the relative bias and $\tilde{s}$ is the standard deviation of the estimated values. Larger width of the black arrow denotes higher accuracy of the model results.

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

Table 4: Comparison of the model performance with considering soil moisture measurement uncertainties for the Multi Step Multi Layer Regression and the Inverse Model for reproducing daily evapotranspiration and the mean depths where 25 %, 50 % and 90 % water extraction occurs. The model performance is expressed as correlation coefficient R, relative variability in simulated and reference values RV and relative bias (b) for the period 25 July to 26 August 2009. The precision uncertainty is abbreviated by prec err, the calibration uncertainty by cali err and the combined uncertainty by com err. The relative bias for reproducing evapotranspiration is abbreviated with bET and for reproducing mean depths where 25 %, 50 % and 90 % water extraction occurs is abbreviated with b25%, b50% and b90%, respectively.

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

List of figures



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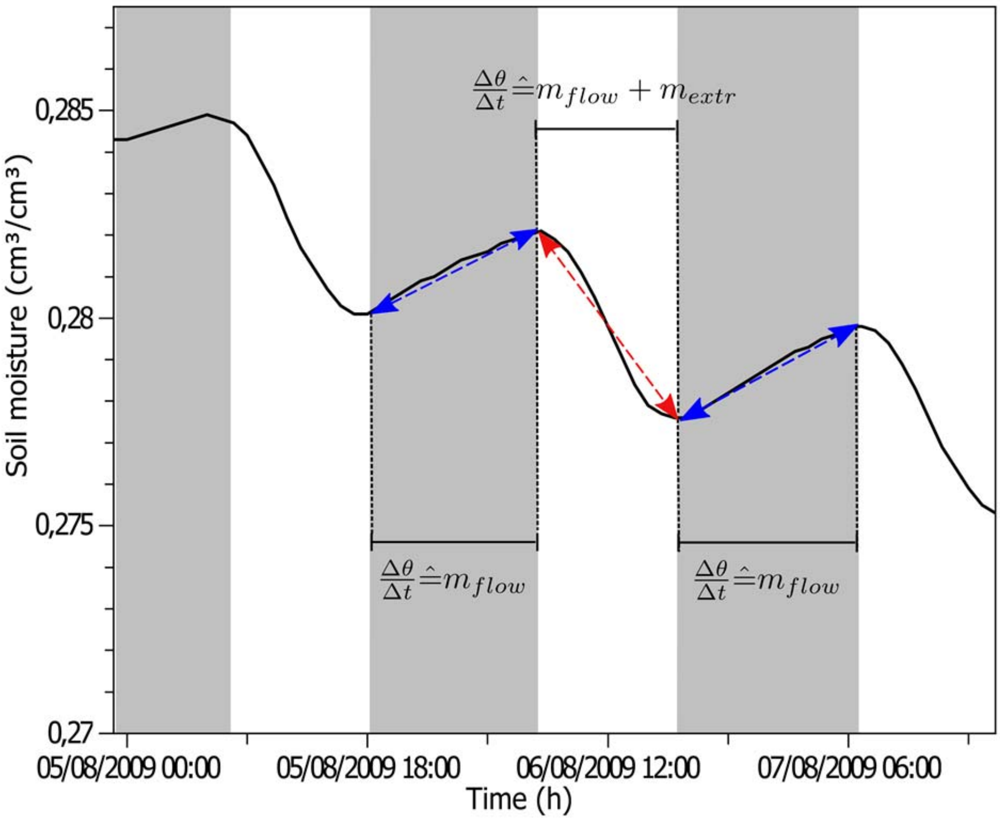

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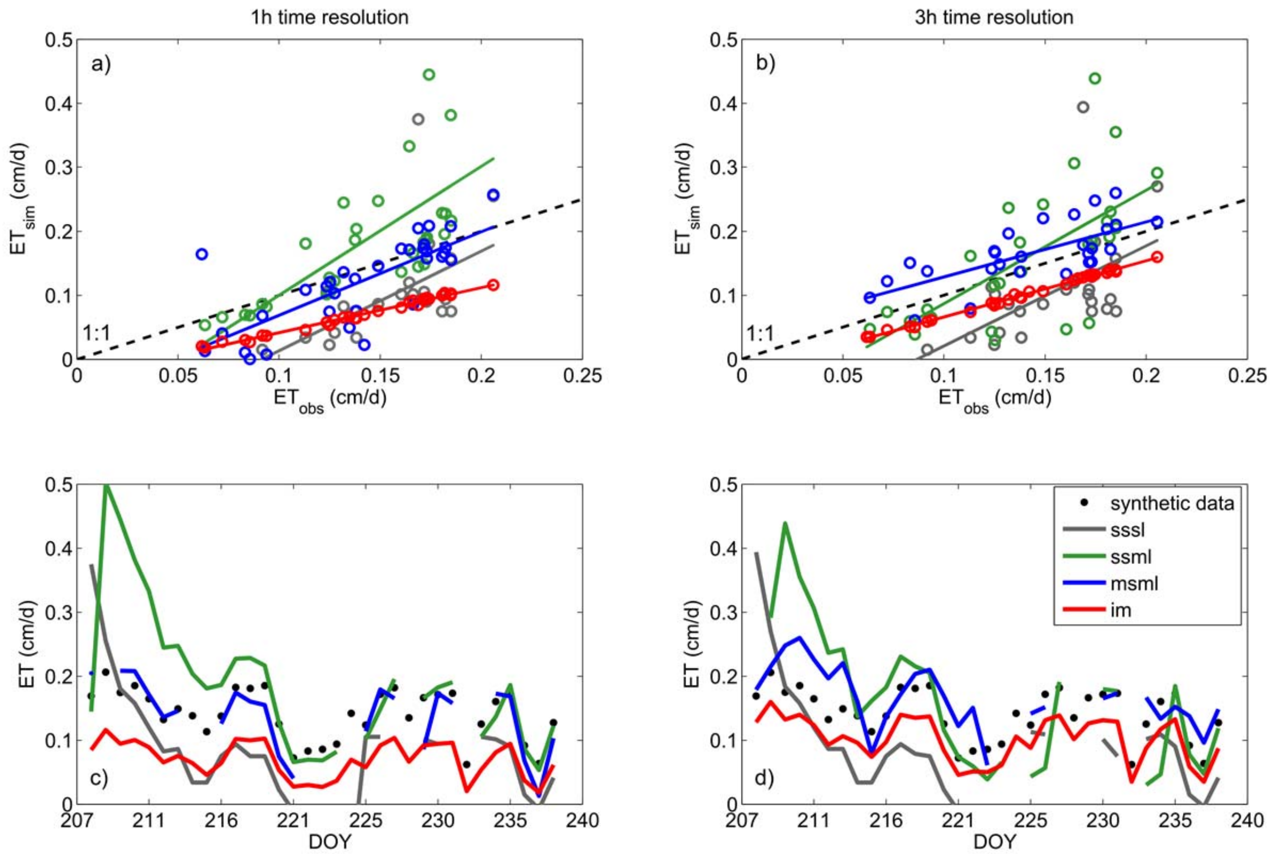

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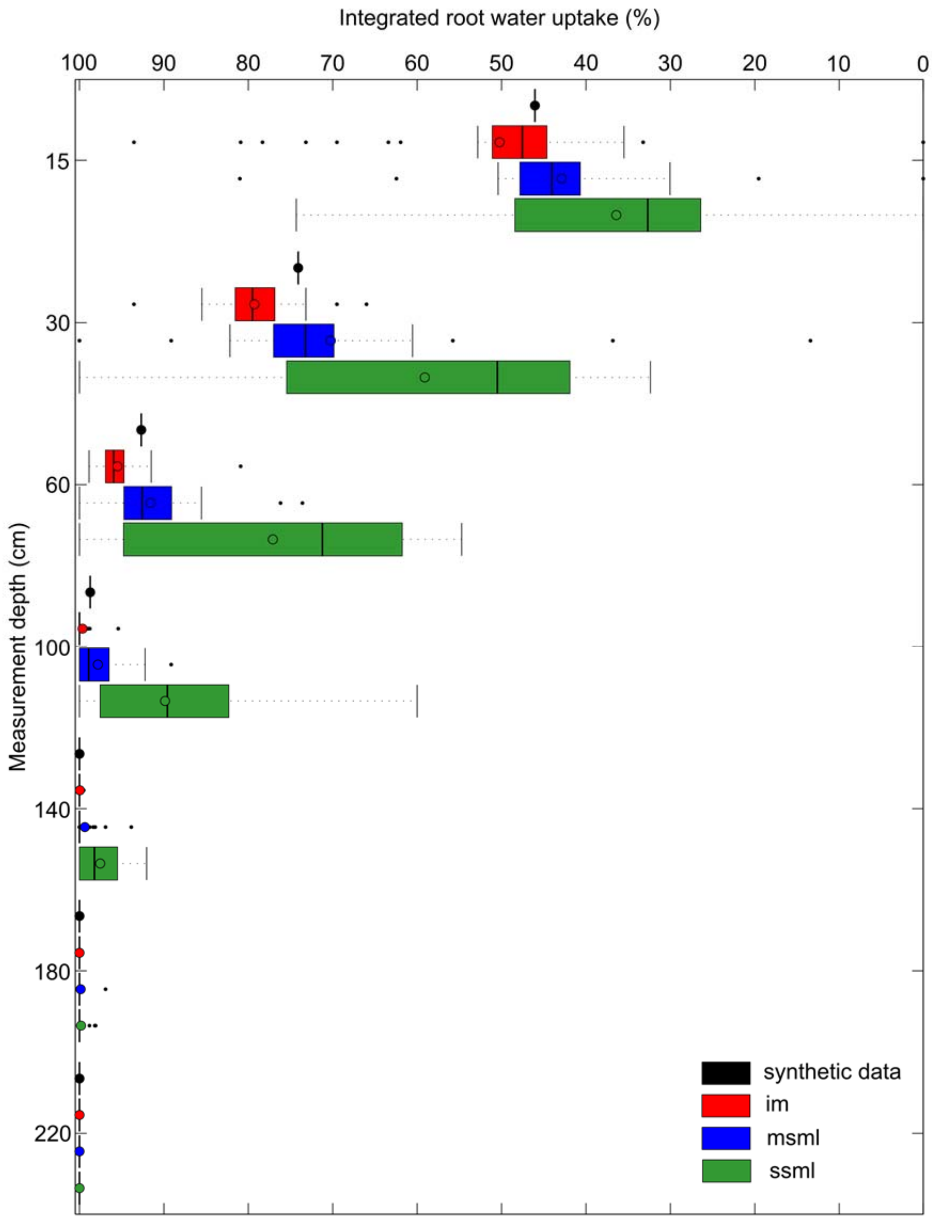

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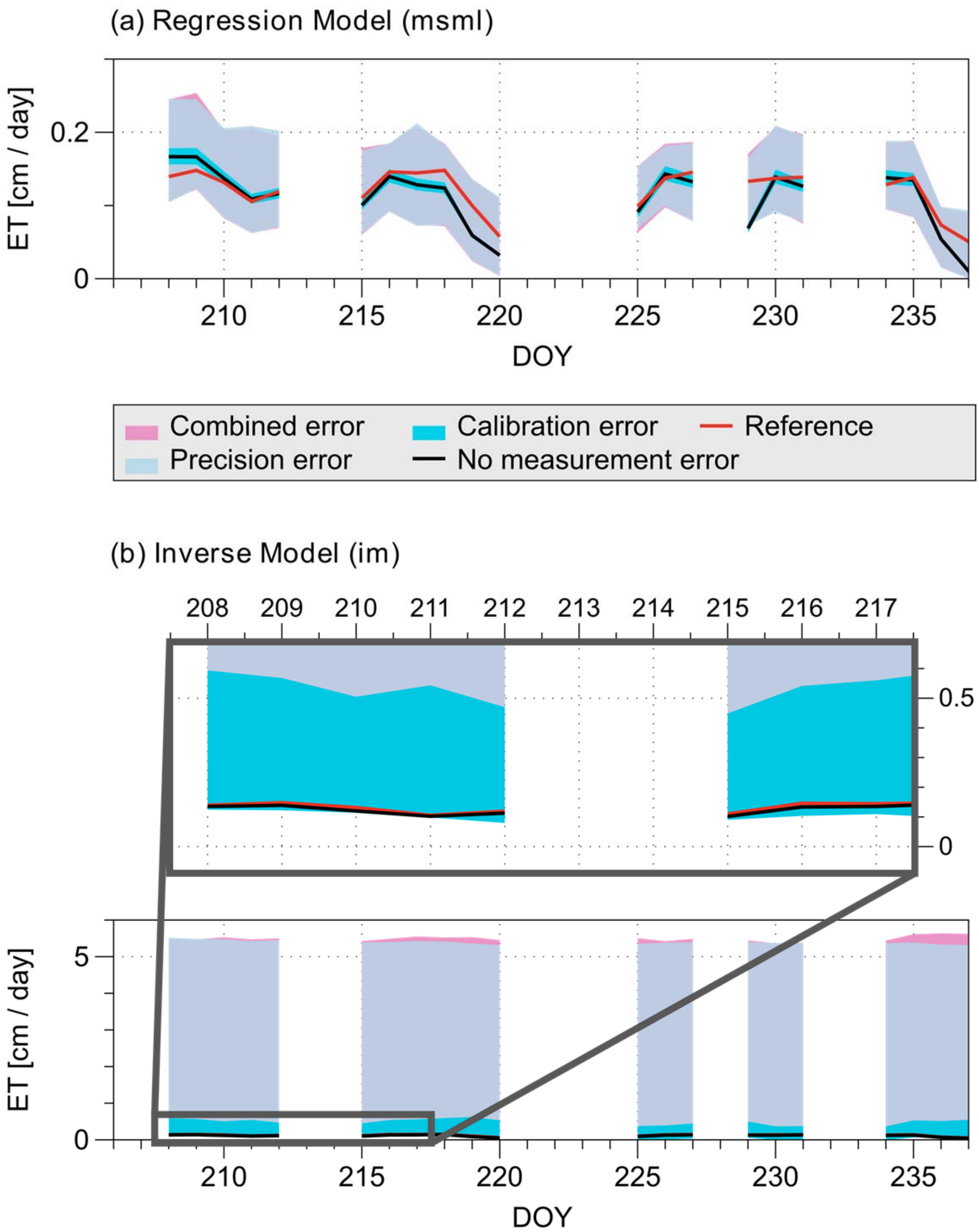

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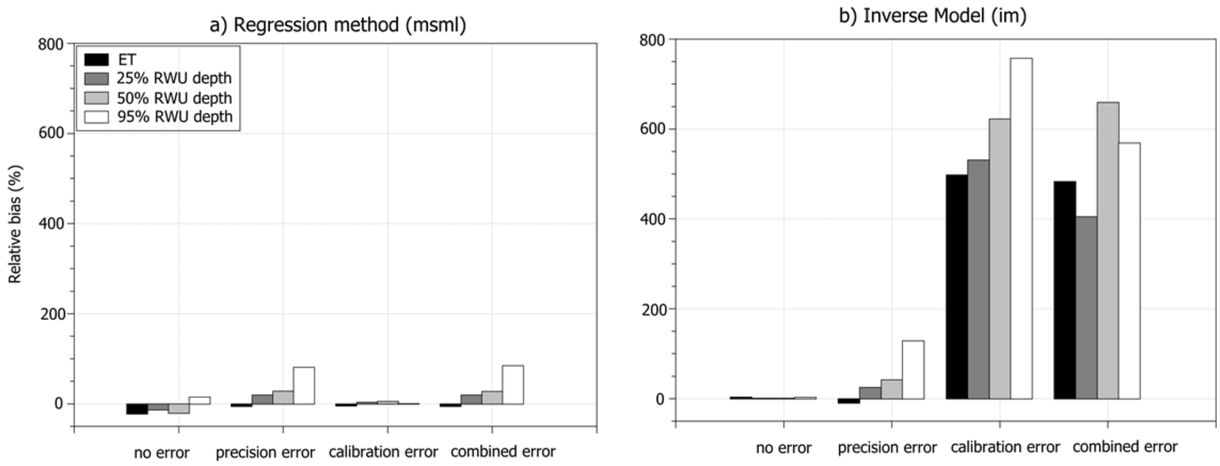

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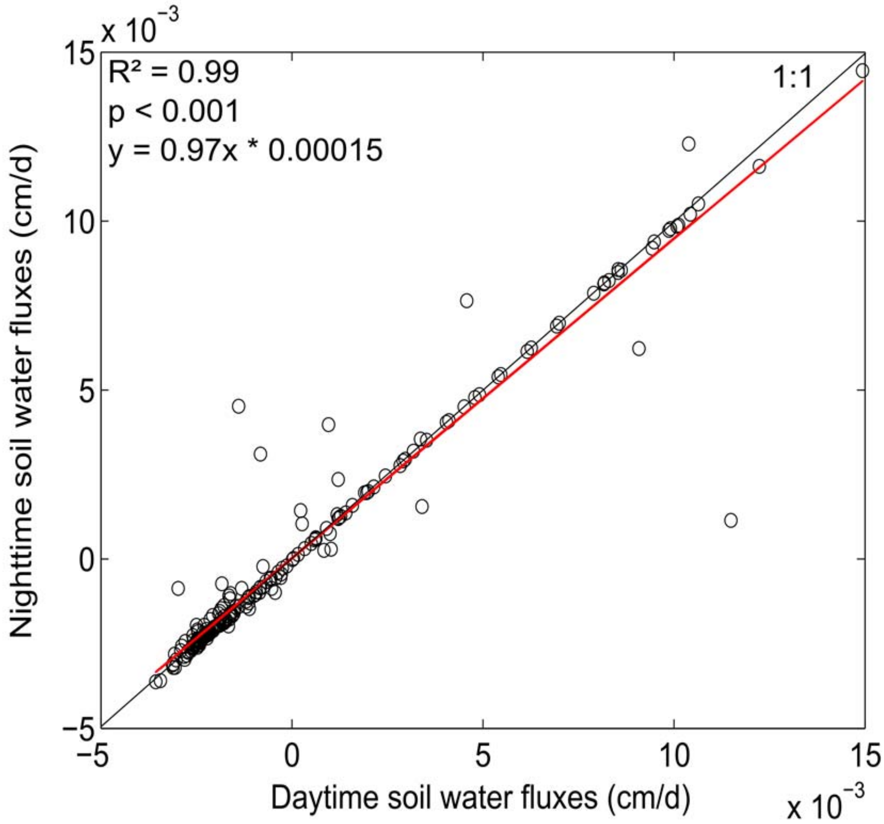
Supplementary figures:



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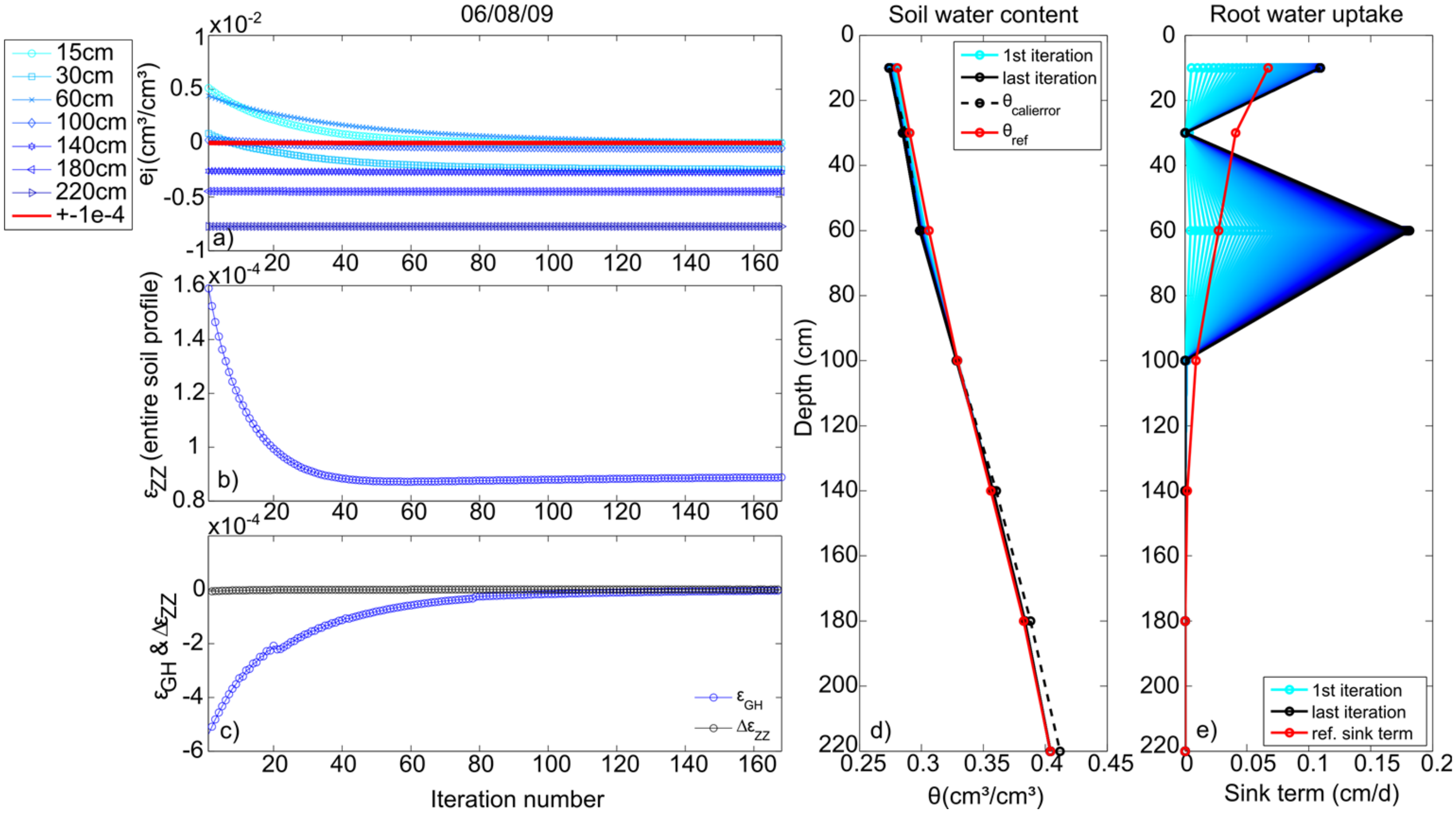

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