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Four Decades of Progress in Monitoring and Modeling of Processes in the Soil-Plant-Atmosphere System: Applications and Challenges

Estimating precipitation and actual evapotranspiration from precision lysimeter measurements

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Abstract

Large weighable lysimeters allow a precise determination of the soil water balance and the quantification of both water exchange at the soil-atmosphere interface and the flux below the root zone toward the groundwater. If well embedded into an equally-vegetated environment, they reach a hitherto unprecedented accuracy in estimating precipitation (P) by rain, dew, fog, rime and snow, and evapotranspiration (ET). Lysimeters largely avoid errors made by traditional measurement systems, such as the wind error of Hellmann rain gauges, the island error of class-A pans, or errors from soil-water measurements that are subject to subsurface heterogeneity. If the amount of seepage water is added to the lysimeter mass, temporal changes of the lysimeter mass can be used to solve the water balance equation for atmospheric fluxes. Increasing mass indicates P, decreasing mass ET. The determination of the net water balance (sum of P and ET) is accurate and robust. A problem arises in the separate estimation of the underlying P and ET fluxes, because weight differences in specified time intervals are affected by stochastic fluctuations due to mechanical vibration, which may be caused by wind or other factors. The aim of this study is to evaluate algorithms that aim on eliminating the effects of these fluctuations and to estimate actual fluxes across the soil-atmosphere boundary and the soil water balance from lysimeter measurements. We use synthetic and real measured data from large lysimeters to test which strategies of data evaluation can be applied, and which degree of accuracy can be reached.

Keywords: large lysimeter; ET measurement; precipitation measurement;

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1. Introduction

A correct and precise determination of water fluxes at the soil-plant-atmosphere (SPA) interface is of fundamental interest for agro-hydrological management purposes, as well as for basic scientific research, to improve the understanding of water and energy exchange processes between soil, plants and atmosphere. To date, many processes taking place at the soil-plant-atmosphere interface are still not fully understood. Studies on large lysimeters may help answer these questions. For a long time, large lysimeters have been recognized as tools for monitoring groundwater renewal fluxes [e.g. 1, 2]. Due to their relatively large surface they can be cultivated in a similar manner as the surrounding field [3]. Traditional lysimeter measurements were, however, prone to various errors. Weighable precision lysimeters have now evolved in a manner to reduce these errors to a minimum. They allow not only the determination of drainage water quantity and quality, but also the estimation of the water fluxes at the SPA interface.

Weighing lysimeters have been used to quantify precipitation (P) not only in the form of rain or snow, but also dew, fog and rime [4], and also to determine actual evapotranspiration (ET) [2]. While the calculation of P and ET by partitioning of a simple water balance equation is straightforward in theory, processing real data is error-prone because of data gaps, noise caused by mechanical vibration, outliers caused, e.g., by animals that touch the lysimeter, offset in mass after sampling of leachate, temperature dependence of the scale, crop growth and removal, and other factors. In recent years, hundreds of full-scale weighing lysimeters have been installed in Europe and all around the world in order to monitor SPA fluxes and soil moisture. For instance, in the context of the evolving Terrestrial Environmental Observatories in Europe (TERENO, [5]), changes in the hydrological cycle due to climate change are monitored at 12 sites in Germany with a total of 126 lysimeters [6]. Evaluation of the numerous measurement data, which will emerge by these measurement devices, is not trivial and raises the demand for clear technical guidelines.

A consortium of researchers in Germany and Austria, who are involved in the TERENO-SoilCan network or related to the international Lysimeter Research Group [7], is currently investigating whether an automated and objective interpretation of lysimeter data with respect to fluxes at the SPA interface is viable, while avoiding subjective parameter choices or manual interventions. In this paper, we first briefly look at typical data structures that are obtained from measurements at modern large lysimeters. This will illustrate some of the problems and pitfalls one encounters during the analysis of lysimeter weight data. Second, we present a strategy for development and testing of guidelines for the determination of P and ET from lysimeter measurements. Here, it is of particular interest to investigate the limits of an unbiased reconstruction of "true" time-series by removal of noise and outliers. Finally, we present a procedure to evaluate the accuracy of determining net P and ET fluxes from large precision lysimeters.

2. Material and Methods

2.1. Lysimeters

The data used to illustrate our methods are of two different types: (1) Synthetic data, either derived from real data or obtained from a numerical forward simulation. (2) True measured data from three lysimeter sites at Wagna (Austria), operated by the Joanneum Research Forschungsgesellschaft mbH, Graz, and at Wüstebach and Bad Lauchstädt (both located in Germany), operated by the TERENO-SoilCan network. The configuration of the lysimeters is shown in Fig. 1 exemplarily for the SoilCan lysimeters at Wüstebach and Bad Lauchstädt. An in-depth technical discussion is given by von Unold and Fank [3]. The Wagna lysimeter is, in principle, of similar experimental design.

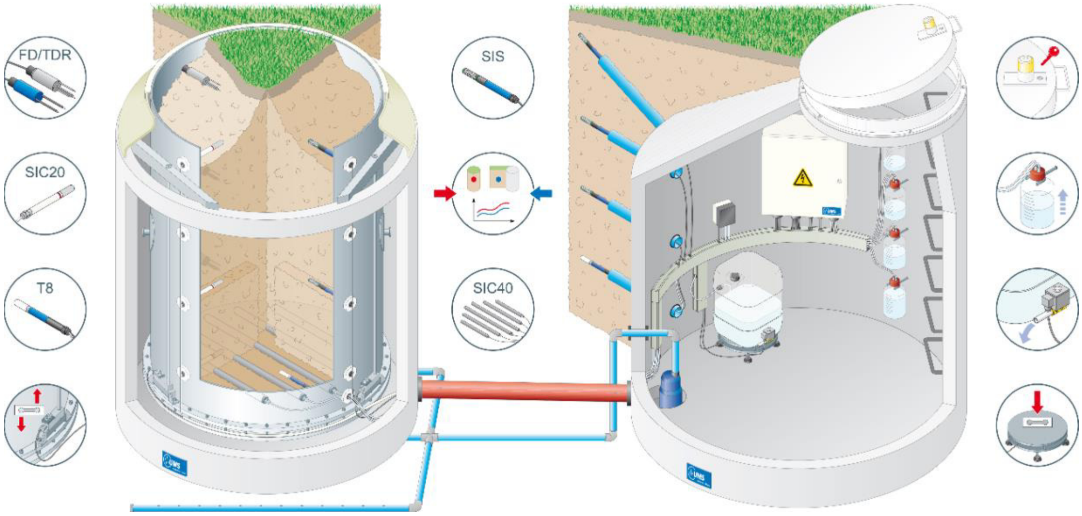

Fig. 1. Sectional drawing of a lysimeter with the central service pit, as used in the TERENO-SoilCan project. Main components are the soil monolith, weighing cells, and a suction cup rake connected to a pump and a weighed drainage water vessel (courtesy of UMS GmbH Munich, 2010, used by permission).

2.2. Data evaluation strategy

The data evaluation process, i.e. the calculation of ET and P fluxes from changes in lysimeter and seepage water weight, essentially consists of three major steps: (i) Correction of systematic errors and outliers in raw measured data, (ii) reduction or removal of random errors by smoothing, (iii) calculation of fluxes at the SPA boundary and cumulative ET and P.

2.2.1. Step (i): Correction of raw data

Typically, water fluxes are calculated from measurements of lysimeter and drainage water mass. Regardless whether the drainage is forced by extraction through a suction cup rake or passively through gravitational drainage, the time-series of lysimeter weight and drainage water quantity can be affected by a wide variety of singular disturbances, which add to the unavoidable measurement noise. Examples are withdrawal of water through suction cups, sudden changes in weight by harvesting, maintenance work on the lysimeters, impact of animals or persons entering or leaving the lysimeter surface, and so on. Detection and correction of such singular events can be partly automated by a plausibility control of data and suitable filters, but must be done manually in some cases.

2.2.2. Step (ii): Noise reduction by data smoothing

Data of the SoilCan and Wagna lysimeters are typically recorded in 1-minute intervals. Smoothing of the time-series in order to reduce noise is necessary. A variety of different smoothing procedures can be applied, which typically involve at least one parameter. Often, this parameter is directly related to the width of a moving window. Popular and easy-to-use smoothing methods are, for instance, the moving average, or methods based on local regression, such as the Savitzky-Golay filter. However, examples for the application of more advanced techniques on lysimeter data, like Wavelet filtering, can also be found in the literature [8]. In the results section, we will illustrate and discuss some of the advantages and disadvantages of selected smoothing procedures.

2.2.3. Step (iii): Calculation of fluxes and cumulative fluxes

Based on a data record of the lysimeter mass and an independent record of seepage water quantity (equal to the flux across the lower boundary), the flux at the SPA interface is easily calculated from a mass balance equation of the lysimeter: increasing mass shows precipitation (including interception and irrigation), decreasing mass is the effect of drainage and ET (including evaporation of intercepted water):

$$\begin{aligned} \Delta W &= \Delta w_{\mathrm{lys}} + \Delta w_{\mathrm{drain}} \\ \Delta P &= \begin{cases} \Delta W, & \Delta W > 0 \\ 0, & \Delta W \leq 0 \end{cases} \\ \Delta ET &= \begin{cases} 0, & \Delta W \geq 0 \\ \Delta W, & \Delta W < 0 \end{cases} \end{aligned} \tag{1}$$

In Eq. (1), Δw_{lys} [kg] is the mass change of the lysimeter between two time steps, $\Delta w_{\mathrm{drain}}$ [kg] is the mass change in the drainage sampling vessel, ΔP [kg] is the sum of precipitation that hit the lysimeter plus vegetation surface during the time interval and ΔET [kg] is the corresponding evapotranspiration, which includes interception loss. The mass difference in the evaluation period indicates a change of stored water volume. Assuming that the weight measurement by scales is without long-term drift, the soil water mass balance (P minus actual ET) is always accurate in lysimeter systems, and precise up to the resolution of the scale. In modern lysimeters, this resolution is in the magnitude of 10 g, which is equal to 0.01 mm of water equivalent for lysimeters with a surface area of 1 m² [3]. This illustrates that, for the determination of the net boundary flux at the SPA interface, lysimeters are measurement devices with unprecedented precision. However, the separate estimation of the underlying components P and ET is challenging, because increases and decreases in measured weight in specified time intervals are affected by fluctuations, which cannot be fully eliminated by smoothing procedures. Different strategies to filter raw data and to reconstruct P and ET are currently studied [e.g. 9]. One promising strategy is to define threshold values, which must be exceeded to interpret a measured weight gain as P and weight loss as ET.

2.3. Validation strategy

Validation of the procedure and quantification of resulting uncertainties is a crucial step in the development of an objective and optimal strategy to calculate net P and ET fluxes. A standard approach is to compare the evaluation results with results obtained from alternative methods, in particular micro-meteorological measurements. For example, one can define precipitation sampled by Hellmann rain gauges or Pluviometers as a reference measurement. Alternatively, eddy covariance system measurements can be used to validate lysimeter results. The general problem of these approaches is that virtually all meteorological methods suffer from own calibration problems, which are in part similar to those of the lysimeter evaluation. For example, weighing pluviometers, where rain is collected in a vessel on a scale, are by principle similar systems as weighing lysimeters, but have a smaller area, no vegetation, and show systematic errors due to wind. Ciach [10] found considerable errors in tipping-bucket rain gauges that are highly dependent on rainfall intensity and time scale. He further noticed a strong dependence of the errors on the data collecting and processing strategy.

A completely alternative validation strategy is based on virtual realities, i.e., constructed data series that mimic “true” lysimeter measurements. These (errorless) courses of lysimeter and drainage vessel weight data allow a perfect calculation of soil water balance. Superimposed on the errorless data are disturbances, which reflect fluctuation patterns as found in natural data. In this contribution we follow this strategy by (i) creating fully synthetic lysimeter data by numerical modeling with temporally highly resolved atmospheric boundary conditions, and (ii) by using measured lysimeter data to derive plausible data series that represent virtual truths. Disturbances are likewise constructed by two basic approaches: In the first approach, we compute noise just by statistical means, e.g. normally-distributed noise, with and without short-term autocorrelation, and with or without scaling components, e.g., based on wind speed. In the second approach, we use true measured data, extract the residual pattern between a smooth approximation and the measured minute-by-minute data, and add these patterns to “errorless” data. Using a wide variety of data with different noise characteristics and magnitudes, we investigate whether it is possible to find approaches for an automatic parameterization of the P and ET calculation procedure. Assessment of the suitability of the approaches will be based on the integral sums of rain and precipitation for given periods of time, and on the direct reconstruction of short term events.

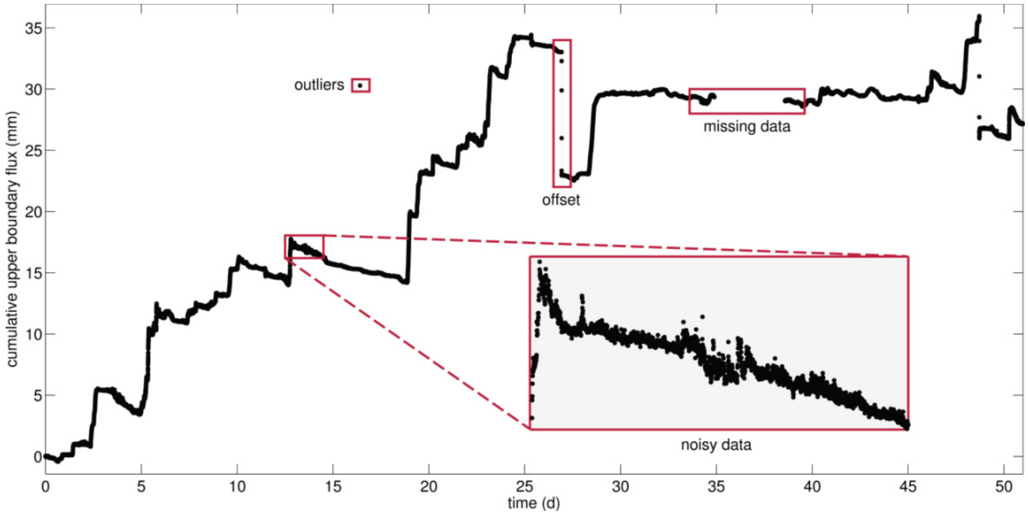

Fig. 2. Illustration of practical problems with data from weighing lysimeters. The figure shows the cumulative upper boundary flux of a lysimeter, calculated by adding cumulative weight and drainage. Positive values indicate a precipitation surplus. Data offsets at day 26 and day 48 indicate emptying of the drainage vessel. Example data were taken from the lysimeter at Bad Lauchstädt, Germany and slightly modified for illustrational purposes.

2.4. Synthetic data

Fully synthetic data were created by numerical solution of Richards’ equation using the simulation software HYDRUS-1D [11]. Atmospheric boundary conditions were measured in 10 minute intervals at the Wagna lysimeter site and kindly provided by Joanneum Research. We simulated 4.5 years of unsaturated water transport in a homogeneous 3 m profile consisting of a silt loam (soil hydraulic properties measured by Schelle et al. [12]). As an approximation of real transpiration rates, we modeled root-water-uptake from a constant grass cover with a leaf area index LAI = 3 m^2 m^{-2} using the approach of Feddes et al. [13] with parameters taken from a database included in the software. From these simulations, water fluxes across the soil-atmosphere boundary, actual transpiration, and flux density in 1.5 m depth, corresponding to the lower boundary of our virtual lysimeter, were used to derive error-free lysimeter mass data, based on the soil water balance equation. To evaluate the performance of different algorithms for different error structures and intensities, we created synthetic weighing data by disturbing the data with (a) normally distributed noise ($\sigma = 25$ g) and (b) noise scaled by wind speed up to five times the intensity of (a).

3. Preliminary results

3.1. Correction of raw data by elimination of singular and systematic errors

The first step in the data exploration is to check for crude and systematic errors in the data series. Figure 2 illustrates some of the most common singular events that occur in time series of lysimeter weight and drainage. These include data gaps due to failures of the data logging system, individual outliers caused by electronic disturbances or by added weight to the lysimeter, and sudden drops indicating data offsets. Automatic correction of the data can be done by plausibility filtering, which can be applied to the time series of drainage water weight, w_{drain}, and the time series of the cumulative upper boundary flux, obtained by adding (corrected) w_{drain} and lysimeter weight w_{lys}, which are typically recorded in minute intervals.

(1) Weight increase of the drainage vessel between two measurements must lie below a maximum value, which reflects a reasonable expected maximum drainage rate.

(2) Weight decrease of the drainage vessel is physically impossible in lysimeters with gravity drainage at the lower boundary, and thus any weight decrease of the drainage vessel is interpreted as water removal by emptying the vessel or sampling of leachate. In systems where water can be pumped back into the system, reflecting capillary uptake of water from deeper soil, plausible weight changes must be limited to maximum pumping rates.

(3) Similar considerations are applied to the cumulative upper boundary flux, which is reconstructed as the sum of lysimeter weight and the corrected weight of the drainage water vessel. An increase between two measurements must lie below a maximum value, which reflects an expected maximum P rate. If a maximum increase is exceeded, the new measurement is discarded. The procedure is repeated for each time step until the end of the record.

(4) A decrease of the cumulative upper boundary flux between two measurements must lie below a maximum value, which reflects an expected maximum ET rate. If this maximum decrease is exceeded, the new measurement is discarded. The procedure is, again, repeated for each time step until the end of the record.

The described data processing can be used to correct raw data as illustrated in Fig.3. The choice of plausible maximum rates is not trivial. P and ET rates in minute intervals may be much higher than expected daily rates. Proper handling of data gaps is not discussed here, because they request individual reconstruction of data, e.g., by using measurements from additional instruments. Simple interpolation would ignore changes in weight, both positive and negative, during the gap and would thus lead to an underestimation of P and ET.

3.2. Noise reduction by data smoothing, and calculation of fluxes and cumulative fluxes

Raw data of the SoilCan lysimeters, that are stored every minute, are already averaged from instantaneous measurements on a scale of seconds. Further smoothing of these data aims at the separation of signal changes that are caused by noise from those that are caused by true atmospheric fluxes. While this is easy in some situations, e.g. a calm day with sunny weather, it becomes completely different in

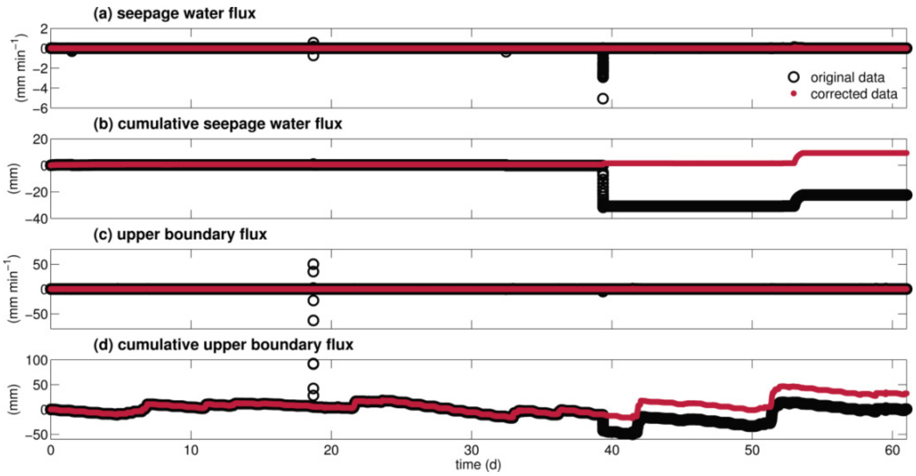

Fig. 3. Reconstruction of the upper boundary flux from corrupted time-series. Data are from the lysimeter at Wagna, Austria.

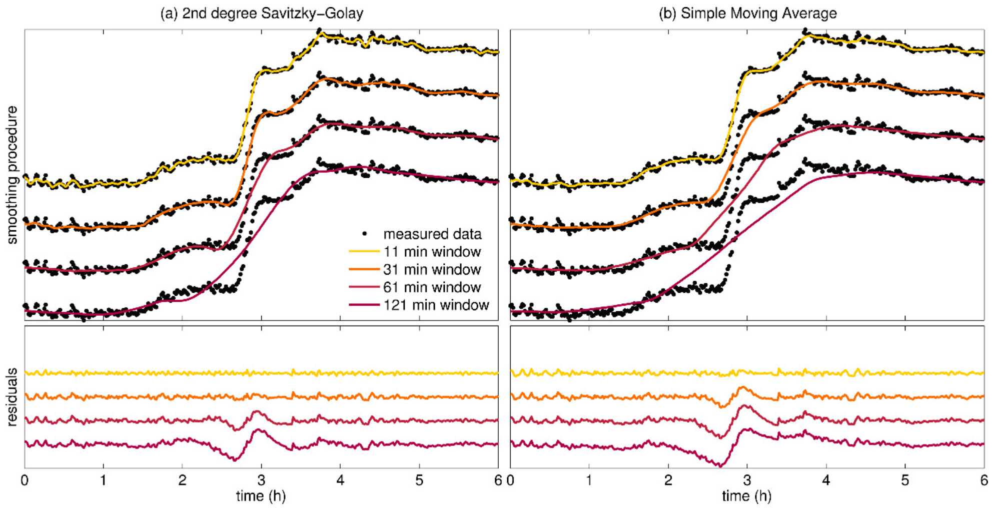

Fig. 4. Effect of smoothing algorithm and smoothing window on the reconstruction of lysimeter weight changes. Upper part: Black dots indicate original measurements of lysimeter weight from the Wagna lysimeter. Colored lines represent smoothed lines with smoothing windows from 10 minutes (=11 data points) to 2 hours (=121 data points). Lower part: Plot of the residuals.

situation with capricious weather, where short but intense precipitation events are followed by interception with cooling and sunny spells. It is thus difficult to find a simple smoothing procedure, which can properly handle data from completely different meteorological situations without external adjustment of smoothing parameters [8, 9, 14]. Figure 4 exemplarily shows a comparison of two popular low-pass filters, namely the so-called simple moving average (SMA) and a second degree Savitzky-Golay (SG) filter, applied to a 6 hour time-series of lysimeter weight measurements, with a short rain shower. Results for four different smoothing window widths are shown. For given smoothing windows, the SMA leads to a systematic misfit when sudden changes take place (see, for instance, the orange line with a 31 min smoothing window). The SG smoother, on the other hand, has a slight tendency to overshoot. This illustrates that the smoothing algorithm and width of the smoothing window are interrelated. Using the smoothed line as a reconstruction of the true signal, any over-smoothing will lead to an underestimation of P and ET, whereas insufficient smoothing will lead to the opposite.

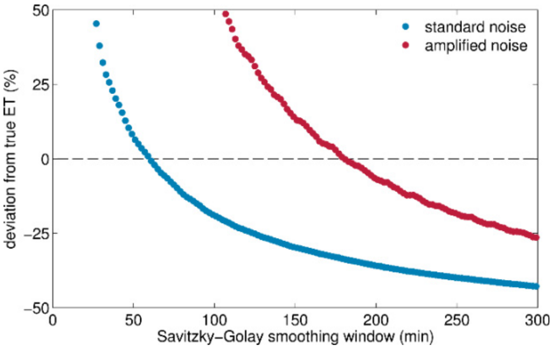

Fig. 5. Effect of width of smoothing window on the water balance calculated from the smoothed data by Eq. (1). Underlying data are taken from a virtual reality (with known truth), which approximate real measured data from a SoilCan lysimeter at Bad Lauchstädt, Germany. Blue: with standard noise. Red: with amplified noise.

Finding an appropriate smoothing technique and defining moving window lengths for different lysimeter systems in different environmental conditions poses a considerable challenge. We illustrate the problem with Fig.5, which shows the effect of changing the selected window of the SG smoother on the data reconstruction. The key message here is the enormous sensitivity of the calculated fluxes on the width of the smoothing window. For data with a small noise (blue), smoothing with a time window of 1 hour would lead to correct results; any wider time window underestimates ET, and any narrower window greatly overestimates ET. For the same underlying data affected by a larger noise, the ideal smoothing window would be around 3 hours. To date we have not found a clear and simple relationship between the magnitude of the noise, which can be characterized by the magnitude of the residuals between raw and smoothed data, and the proper size of the smoothing window, and we doubt that there is such a relationship.

To overcome the smoothing problem, we follow a strategy proposed by Fank [15] and add a further step in the data analysis, by separating significant from insignificant weight changes. This is achieved by defining a threshold δ [kg] for the (smoothed) lysimeter weight differences between two measurements, which must be exceeded to count as significant flux across the SPA boundary. The value of δ can be either set constant, or variable, depending on the pattern and intensity of the noise. Figure 6 illustrates this approach with synthetic data, based on true measurements of a SoilCan lysimeter at Bad Lauchstädt.

3.3. Validation

Figure 7 shows exemplarily the reconstruction of a summerly 8 week period at Wagna, which is based on real data from July to August 2010. Cumulative ET of the synthetic true data in this period was 151 mm, cumulative P was 187 mm, and net infiltration into the lysimeter was 35 mm. The reconstruction of the daily values of P and ET, using a constant threshold of $\delta = 0.01$ kg and an SG smoothing window of 31 min, yields promising results. The accurate reconstruction of P and ET on a daily basis (and also on an hourly basis, not shown) shows the great potential of lysimeter measurements to determine true P and ET fluxes. Further efforts are currently under way to find optimal selection criteria for suitable smoothing window widths and δ values, and also for estimating the uncertainty of the method, but results are not available yet. We therefore cannot say at this time whether it will be possible to derive an automatic, datadriven approach for the choice of appropriate smoothing parameters and the threshold value. Future work will show whether this goal can be accomplished or not.

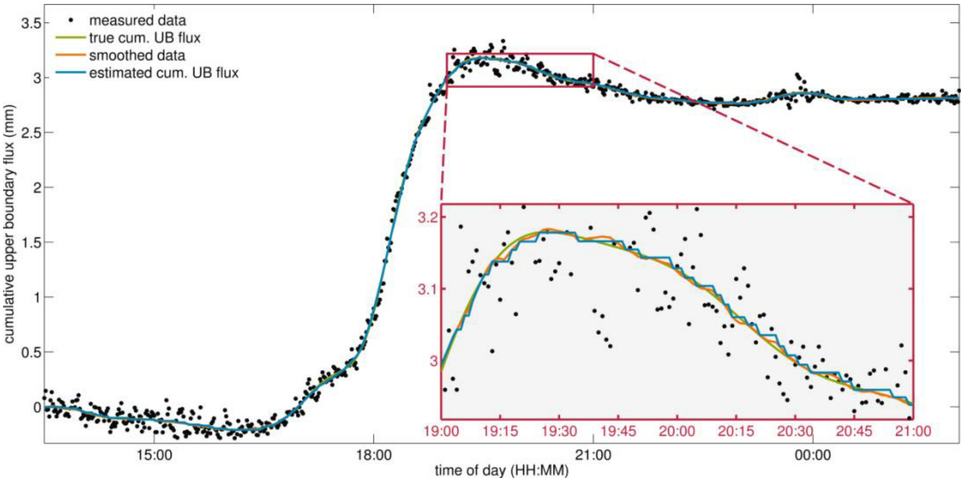

Fig. 6. Strong precipitation event and onset of interception/evapotranspiration in late afternoon of 9 June 2011 at a SoilCan lysimeter in Bad Lauchstädt. Measurements are shown as black dots, recorded in minute resolution. The underlying "true" flux is shown by the drawn green line, the smoothed SG interpolation with a one-hour window as an orange line, and the reconstructed upper boundary condition, which is used for P and ET calculation, by a blue line. Afternoon ET is overridden at 17:30 by a convective rain event that delivers 3.36 mm precipitation. In this magnification, the lines representing true, smoothed and reconstructed cumulative fluxes at the upper boundary are virtually indistinguishable. Insert shows magnification of the end of the rain event and illustrates the meaning of the threshold value δ, which must be exceeded to count a change as "significant".

4. Summary and Conclusions

We presented ongoing research towards the development of a standard procedure for evaluating weight and drainage data from precision lysimeters, in order to calculate P and ET in high temporal resolution. The data quality of precision lysimeters allows studying water fluxes at the soil-plant-atmosphere interface in hitherto unprecedented detail. Examples are the accumulation of dew or rime during night hours, the reaction of plants on transpiration demand, or the calculation of interception and the dynamics of interception loss. From our analysis, we conclude that it is possible to accurately calculate P and ET with automated procedures, but the calculation involves parameters such as the width of a smoothing window or the magnitude of a threshold value. To date, it is not clear whether it will possible to find universal scaling laws for these parameters that allow automated and reliable data evaluation, without subjective intervention and without consultation of data from external measurements, such as independent rain data. As such, our paper reflects an intermediate state of a work in progress, and hints in a direction where further research is needed. The proposed validation strategy that will help to answer some of these questions, and contribute to developing lysimeters to indispensable tools for obtaining a better understanding of the controlling factors for fluxes of water at the soil-plant-atmosphere interface.

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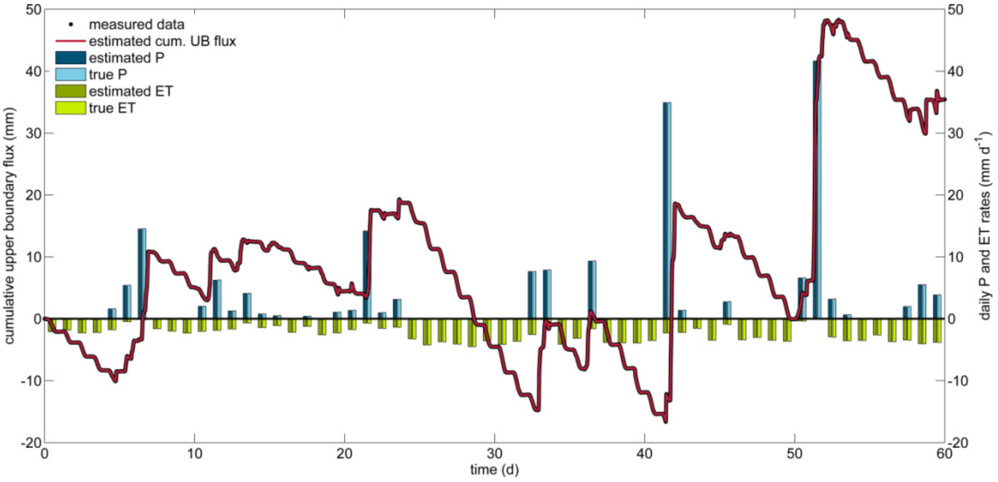

Fig. 7. Daily estimates of P and ET during a summerly 8 week period at Wagna, July - August 2010. Dark red line is related to left axis and indicates the calculated net flux between lysimeter and atmosphere. Bars are related to right axis and show daily sums of P and ET. Bright colors indicate true values, dark colors estimated values.

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