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Authors: Anne Klosterhalfen, Alexander Graf, Nicolas Brüggemann, Clemens Drüe, Odilia Esser, María Pat González Dugo, Günther Heinemann, Cor M.J. Jacobs, Matthias Mauder, Arnold F. Moene, Patrizia Ney, Thomas Pütz, Corinna Rebmann, Mario Ramos Rodríguez, Todd M. Scanlon, Marius Schmidt, Rainer Steinbrecher, Christoph K. Thomas, Veronika Valler, Matthias J. Zeeman, Harry Vereecken,

Title: Source Partitioning of H_2O and CO_2 Fluxes Based on High Frequency Eddy Covariance Data: a Comparison between Study Sites.

Response Letter

Dear Trevor Keenan, Dear Reviewers

Thank you very much for your review of the abovementioned manuscript. We have carefully inspected and replied to all reviewer comments and implemented the suggestions as documented in the following response letter. As primarily suggested by Reviewer #2, we revised our writing thoroughly for a better communication of our findings. We also improved most figures as suggested by both Reviewers (comments 1.4.11, 2.2). The page and line numbers in the following reply refer to the revised manuscript version. Below, we included a version of the manuscript where all changes with respect to the previous version have been marked.

We hope that you will find the result satisfying.

Sincerely,

Anne Klosterhalfen, Alexander Graf, Nicolas Brüggemann, Clemens Drüe, Odilia Esser, María Pat González Dugo, Günther Heinemann, Cor M.J. Jacobs, Matthias Mauder, Arnold F. Moene, Patrizia Ney, Thomas Pütz, Corinna Rebmann, Mario Ramos Rodríguez, Todd M. Scanlon, Marius Schmidt, Rainer Steinbrecher, Christoph K. Thomas, Veronika Valler, Matthias J. Zeeman, and Harry Vereecken

Referee # 1

This manuscript presents a comparison of two turbulence-based flux partitioning methods across multiple sites representing a range of vegetation types (forest, grassland, and crop) and geographic zones. These emerging flux partitioning methods represent an effort to develop partitioning strategies that do not require assumptions about functional relationships, and this comparison between two methods across sites is a highly valuable contribution to the continuing development of new flux partitioning strategies. I have not seen a comprehensive comparison of two turbulence-based partitioning methods like this, and I think it represents an important step forward in understanding the performance of these methods. The comparison of multiple variations of each method and the analysis of specific site factors such as LAI and canopy height and how they affect the methods are especially valuable contributions to development of these partitioning strategies. I thought the manuscript was clear, easy to follow, and well written overall. I only have a few comments for areas where the manuscript could be improved:
Thank you very much for this positive feedback.

1.1
1. The manuscript refers several times to a manuscript by the same first author that is still in review in another journal. Until that manuscript is available to readers of this manuscript, I don't think it's useful to cite it. In particular, methodological details that have a bearing on this manuscript should be included in the supplemental material or main text, and not only cited to another manuscript that is not available at this time.
The cited paper was accepted just recently and is now available online. We updated the reference in this manuscript.

1.2
2. Tables 2 and 3 and A1 highlight the highest and lowest values of the metrics that they show. This makes it easy to ignore cases where there are multiple high values. It would be better to color code all the cells in the table based on their values, so readers could tell at a glance how the values looked. In addition, I think the correlations in Tables 2 and 3 should show whether they were statistically significant using bold text or asterisks.
Our original versions of Tables 2, 3, and A1 were in color. But as far as we know (after contacting the Journal's Typesetting Department) tables in color are not possible.
In Tables 2 and 3 (pages 29, 30), we also added asterisks for statistically significant correlations. Because the sample sizes were small and the data was often not normally distributed, the results have to be handled with care. For Forest_LA we received an estimate for LAI, which was missing before. Therefore, some results of the correlation analysis (Tab. 2, 3) differ from the previous manuscript version, but the main findings did not change.

1.3
3. The analysis used the ratio of LAI to canopy height as one of the predictors because "LAI can correlate with hc of a study site" (page 11, line 1). But LAI does not appear to be strongly correlated with hc for the sites in this study. Unless there is a strong relationship, this ratio seems difficult to interpret and I'm not sure I would include it in the analysis unless there is a clear interpretation.
The ratio of LAI to canopy height (h_c) was used because it corresponds to plant area density. Considering only the study sites of one ecosystem type (forest, cropland, or grassland), correlations between LAI and h_c can be found (see Fig. R1 below). For forests, the correlation was low because of Forest_LA, where a dense spruce forest is regrowing after windthrow and the ratio between LAI and h_c is similar to the ration in croplands. For croplands, the correlation was weak, because for maize and sugar beet h_c increased and LAI decreased with increasing maturity. Also, in this subset of sites in this particular study the maize crop in Dijkgraaf

(Maize_DI_07 and Maize_DI_08) was a special case regarding its large (and expected) h_c. The correlation for grasslands was negative because of the very small sample size and different management strategies (dates of cutting) for each grassland, which influence both, LAI and h_c.
For clarification, we rephrased the following section: "For the chosen study sites, LAI correlated with h_c when considering a specific ecosystem type (forest, cropland, or grassland). Thus, LAI h_c^{-1} was also considered to distinguish between their impacts on partitioning performance" (page 11, line 24).
We also think that this LAI-h_c-ratio may be useful for comparison to additional study sites. Thus, we would like to further include it in our analysis.

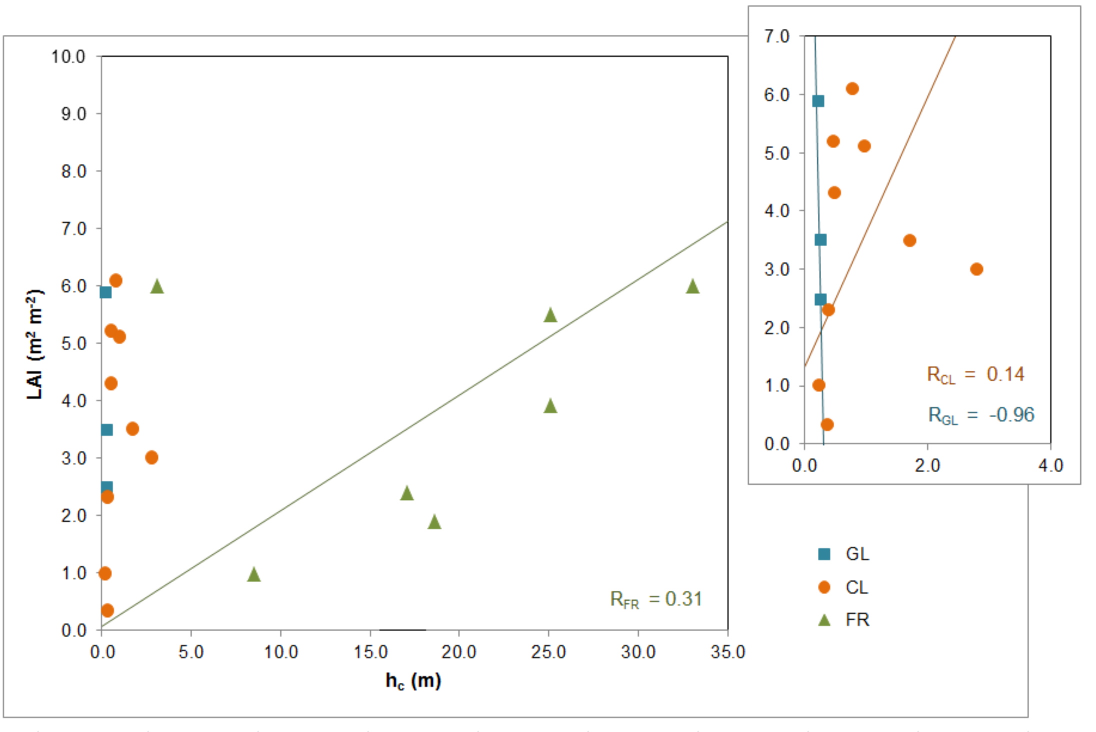

Fig. R1: Correlation between canopy height (h_c) and leaf area index (LAI) for each ecosystem type (FR: forest; CL: cropland; GL: grassland; R: Pearson product-moment correlation coefficient). Lines show reduced major axis regressions (after Webster 1997, European Journal of Soil Science 48:557).

1.4
Technical comments:

1.4.1
Page 7, line 5: Does "two models" refer to the two partitioning methods? They are not referred to as models elsewhere in the manuscript
Yes. For clarification, we rephrased the sentence to: "Within this evaluation step two source partitioning approaches (approach after Reichstein et al., 2005 versus SK10 or TH08) were examined and compared including their different assumptions and uncertainties,…" (page 7, line 10).

1.4.2

Page 7, line 21: What distribution were the random numbers sampled from? Normal? If so, what were the mean and standard distribution?

Yes. For clarification, we modified the sentence to: "To each generated data point of w', q' *and* c' *a random number, sampled from a standard normal distribution and rescaled to a standard deviation of 5% of the magnitude of the variable, was added to simulate additional sources of variance not related to the degree of mixing" (page 7, line 28).*

1.4.3

Page 8, lines 7-8: This should include a brief explanation of why that site and those methods were chosen for the examples. Presumably because those methods had the best performance?

Done. We included following explanation: "In the following, figures are shown for some selected sites, which were deemed most representative for all study sites, and/or for some selected method versions of SK10 and TH08, which usually exhibited the best partitioning performance" (page 8, line 10).

1.4.4

Page 8, line 21: It should be "fewer data points"

Done (page 10, line 33).

1.4.5

Page 8, line 28: "TH08_REA_H performed best" needs more explanation. Based on what metric? Did it perform best for all sites and metrics, or a subset?

Done. We included following explanation: "Regarding the error metrics in Fig. 6, TH08 REA H, among all TH08 method versions, yielded the best result for the largest number of sites and error metrics" (page 11, line 7).

1.4.6

Page 9, line 3: The title of this section suggests that the following text will focus on comparing partitioning results to published analyses, but only a couple of the sites compare directly to publications. It might be more accurate to describe this as a detailed description of results for each site.

Due to rewriting and restructuring this section '3.1 Evaluation of Source Partitioning Results' (as suggested in comment 2.1 by Reviewer #2), we evaluate the partitioning results on the one hand based on their flux magnitudes and in reference to former publications ('3.1.1 Flux Components Magnitudes'), and on the other hand based on error metrics in reference to chamber measurements, estimates of soil evaporation and the approach after Reichstein et al. (2005) ('3.1.2 Error Metrics') (pages 8-11).

1.4.7

I think this paragraph should include a reference to Figure 5, since the bar plots are a helpful summary for many of the results described here.

Done (e.g., page 8, line 31).

1.4.8

I think this paragraph would be easier to follow if the supplementary figures were in the same order that they were referred to in the text.

We organized the figures in the supplementary material as the study sites are listed in Tab. 1 (organized by first canopy type and second latitude). Based on your comment, we reorganized the description and evaluation of the study sites in the text after the same scheme (page 9, line 4).

1.4.9

Page 10, line 13-14: "both methods converged": It's not clear how they converged, or how that is shown in Fig. 6c and d.

For clarification, we rephrased the sentence as follows: "When using the gap-filling model after Reichstein et al. (2005) as a reference, high HiR GPP were relatively frequent for TH08, with a minimum of 66.7% for SugarBeet_SE_06, while HiR GPP for SK10 were considerably lower (Fig. 6c). For HiR TER, such a clear difference in performance could not be observed (Fig. 6d)" (page 10, line 17).

1.4.10

Page 11, line 29: It's not clear how this was contradictory. Contradictory relative to what?

We rephrased the sentence as follows: "Also, the correlation between partitioning performance by TH08 and LAI h_c^{-1} *at forest sites contradicted our assumption that a higher plant density would have a strong negative effect" (page 12, line 23).*

1.4.11

Figure 5: It is difficult to compare the two partitioning methods to each other across panels b and c. I suggest putting the two partitioning methods in the same panel so they can be directly compared, given the importance of these comparisons to the results. Perhaps panel b could show C fluxes and panel c could show LE, with bars for the two partitioning methods side-by-side in each panel.

Done (page 25). We changed Fig. 5 as suggested in comment 1.4.11 and 2.2.4 by Reviewer #2.

1.4.12

Table 1: The abbreviations in the site column need to be defined (NL, ST, DE, PNL,: : :). Some of these are countries, some are regions, and some I didn't understand at all.

We adjusted Tab. 1 mentioning only the countries (page 28). For a more fluent reading, we changed the acronyms of the study sites as suggested in comment 2.1 by Reviewer #2.

1.4.13

Page 29, line 3: The blue and red lettering is not in the table. As I said above, I think color coding would be a good idea but it would be better to reflect the actual values rather than just where the highest/lowest value is.

Thank you for noticing this mistake (page 31). The reference to the blue and red lettering in the table's caption was the description of the original colored table and was forgotten to be removed while changing the table format (cf. comment 1.2). As far as we know, tables in color cannot be included in this journal.

Thank you very much for your very constructive comments and your time!

Referee # 2

This study evaluates two approaches for partitioning eddy covariance fluxes into principle components (NPP and Soil respiration for carbon, and Transpiration and soil respiration for water). Both of the approaches (SK10 and TH08) rely on information contained in the raw, high frequency flux data, interpreted with assumptions about how the deviations in wind and gas concentrations should be correlated/coordinated for air parcels emerging from the canopy versus subcanopy. The developers of these approaches (Scanlon, Thomas) appear as co-authors on the paper, and the literature describing the approaches has been described elsewhere. Thus, while neither SK10 or TH08 is a perfect partitioning approach, I will focus my comments specifically on this effort to compare them (as opposed to comments about the underlying assumptions of each).

I applaud the authors for this ambitious undertaking; it is not easy to handle raw data from so many flux sites. Methodologically (with one exception I'll address later), the work is sound. While it's may be a bit disappointing that the results weren't in better agreement, I think the paper contains information that will be of interest and useful to the flux community.

However, in its present form, I'm not certain that information is being successfully conveyed. Following are some comments on presentation, analysis, and methodology that may help to make the more accessible to others in the community who are seeking ways to better partition their tower-derived fluxes.

Thank you very much for this constructive feedback.

2.1

First, the paper is hard to read at times. This is due to many factors, including:

2.1.1

1. heavy reliance on acronyms,

For a more fluent reading, we changed the acronyms of the study sites (e.g., HH_FR to Forest_HH). Thus, Tab. 1 and A1, and Fig. 4, 5 and 6 had to be adjusted (pages 24-26, 28, 31-32). We have also refrained from using acronyms for the terms "foliage temperature" (page 4, lines 19-23).

2.1.2

2. very detailed explanation of methodology (i.e. the description of the 'GMM' approach on page 5),

We tried to shorten the indicated paragraph (page 5, lines 9-22). It describes a new conditional sampling technique and the subsequent flux calculation, so we try to explain our procedure completely and comprehensibly. Thus, we would not shorten the paragraph further.

2.1.3

3. Very nuanced description of some results that isn't organized around clear themes or patterns, (for example, the site-by-site analysis of performance in section 3.1.1),

We reorganized the description and evaluation of the partitioning results by first canopy type and second latitude (cf. comment 1.4.8 by Reviewer #1; page 9, line 4).

2.1.4

4. some issues with grammar, and

We reviewed our writing thoroughly and hope that all grammar mistakes etc. have been corrected.

2.1.5

5) a few very long paragraphs (i.e. page 9), and a few very short and choppy ones (page 13).
Based on your comment, we restructured most paragraphs.

2.1.6
I urge the authors to carefully edit the writing with an eye towards: 1) moving information that is tangential to understanding the results to the SI (e.g. the GMM method description), 2) organizing results around clear patterns, and reducing words spent on detailed description of the site-by-site, or method-by-method results, and 3) carefully reviewing the text for language.
We reviewed our writing thoroughly considering the above mentioned points and hope the result is satisfying.

2.2
Second, the figures are also difficult to interpret, often because there are too many panels. Some ideas for clearer presentation include:

2.2.1
Figure 2: Could the authors include fewer days of data, and perhaps consider omitting some of the different methods from the panel (for example, show TH08_REA_Q1 or TH08_REA_H, but not both). They seem quite similar.
Done (page 22). Fig. 2 shows now only 4 days of the considered time period in Loobos and following methods: SK10 with WUE_{meanT}*,* WUE_{MOST}*, and* WUE_{OLR}*, and TH08 CV Q1, REA H, and CV GMM (cf. comment 1.4.3 by Reviewer #1).*
We added a figure for Loobos with results of all days and for every method version to the supplementary material.

2.2.2
Figure 3: Again, is it necessary to show each method's results?
Done (page 23). Fig. 3 shows now only following methods: SK10 with WUE_{meanT}*,* WUE_{MOST}*, and* WUE_{OLR}*, and TH08 CV Q1, REA H, and CV GMM.*

2.2.3
Figure 4: Since you've already shown some of the diurnal dynamics, perhaps this figure could present daily-averages?
With Fig. 4 we wanted to show at least once results of all study sites next to each other in the manuscript (page 24). Otherwise, we only show selected sites in the manuscript. We assume that daily averages would give a similar picture as Fig. 5.

2.2.4
Figure 5: This figure is nice! It might be helpful (in a separate figure) to also show the estimated ratio of E:T, as this is often reported in the literature (see, for example, Good et al. 2015, Li et al. 2019).
Thank you for this suggestion. Done (page 25). We changed Fig. 5 as suggested in comments 1.4.11 by Reviewer #1 and 2.2.4, also showing the partitioning factor E/ET. Also, we included the suggested literature in our discussions comparing our partitioning factors (page 8, line 31).

2.2.5
Figure 6: Averaging across sites (or at least across plant functional types) would make it easier to understand the performance of the different partitioning methods.

We agree that Fig. 6 is quite crowded (page 26), but averaging a performance metric / error quantity is not straightforward. It would probably require different strategies for the different error quantities and involve some arbitrary decisions. We see a high risk that the figure would be condensed at the cost of a much more difficult documentation of the methodology behind the figure. We would therefore prefer to keep it as it is.

2.3

Third, the authors focus most of their analysis on understanding differences in the magnitude of the partitioned fluxes (across a day, across sites). In my view, the magnitude of tower-derived fluxes will always be uncertainty, but as long as the sources of biases don't change too much in time, we can be more confident in using tower data to understand trends. How do these different partitioning methods agree in key functional relationships (for example, NPP versus PAR, Surface Conductance versus VPD)? Are the recovered trends as expected?

Thank you for this nice idea. We had a closer look at such key functional relationships.

As an example, Fig. R2 (below) shows the relationship between the averaged partitioning factor E/ET and LAI for each study site and method version, where the E/ET derived by SK10 seems to be dependent on LAI. Fig. R3 (below) shows relationships between global radiation and hourly NPP, between air temperature and hourly R_{soil}, between vapor pressure deficit (VPD) and hourly T, and between VPD and estimated hourly, leaf-level WUE for the deforested area in Wüstebach (Grass_WU) for various method versions. The relationship between global radiation and estimated NPP showed a clear pattern for all method versions. For the other relationships (and for most of the study sites), no clear dependencies could be found in the hourly data because of too narrow data ranges in the considered time periods (e.g., VPD only between 600 and 1200 Pa in Grass_WU) and many additional and confounding factors (e.g., the relationship between global radiation and NPP is also dependent on vegetation water status).

If desired, we can include these exemplary figures very gladly to the manuscript or Supplementary material (after some additional formatting) and discuss them in the manuscript.

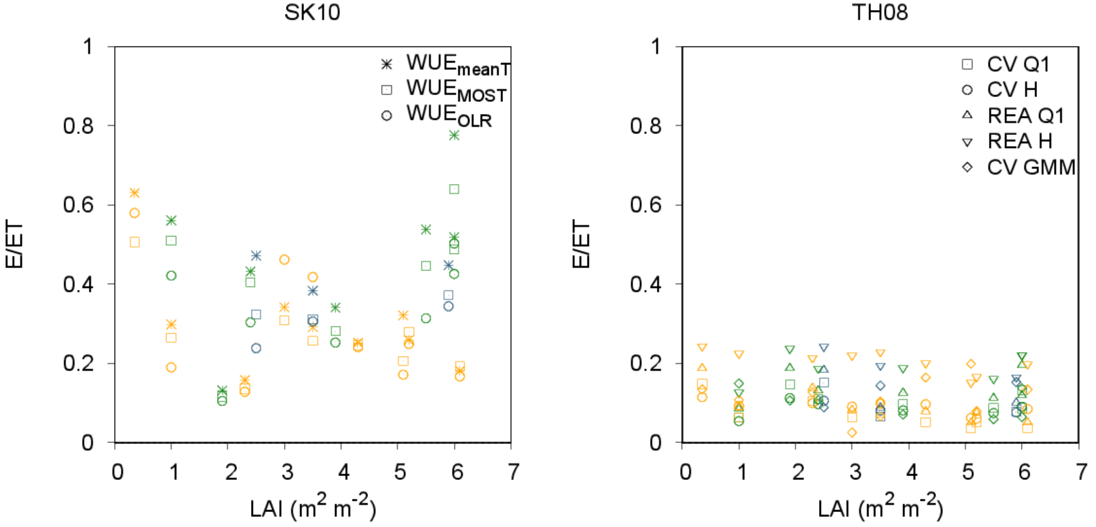

Fig. R2: Relationship between averaged partitioning factor E/ET (fraction of evaporation in evapotranspiration) and leaf area index LAI. Left diagram shows partitioning results of the method versions after Scanlon and Kustas (2010, SK10), and the right diagram of the method versions after Thomas et al. (2008, TH08). Green markers indicate forest sites, blue grassland sites, and yellow cropland sites.

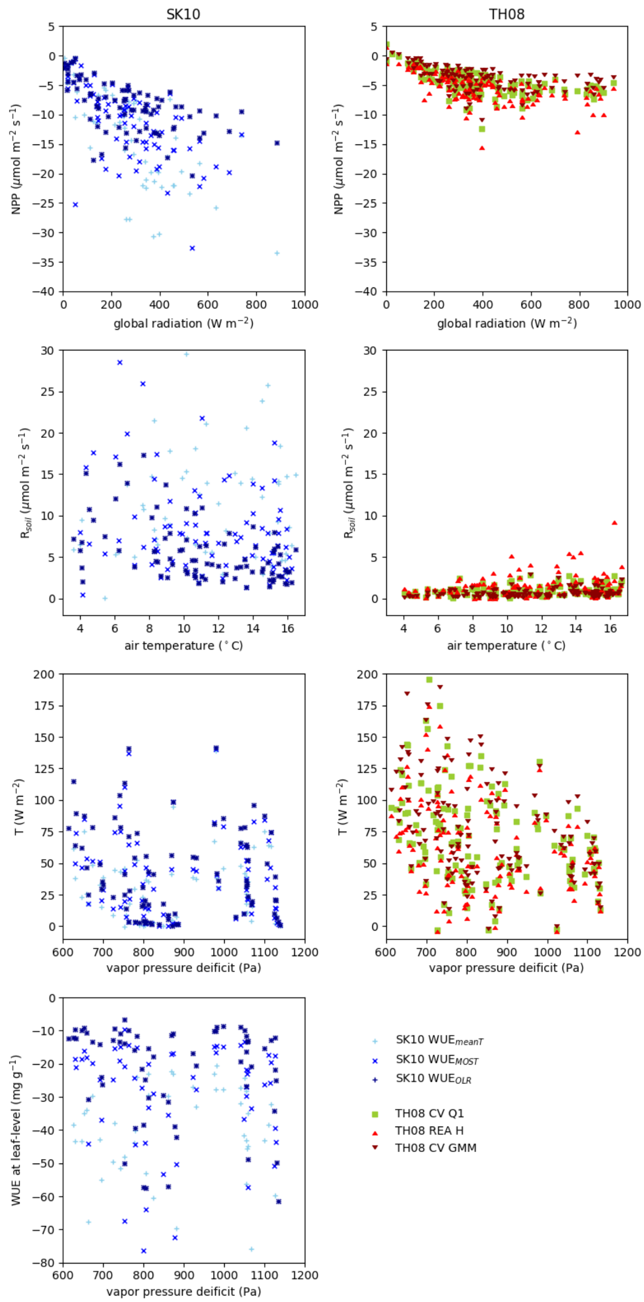

Fig. R3: Relationships between global radiation and hourly net primary production (NPP), between air temperature and hourly soil respiration (R_{soil}), between vapor pressure deficit and hourly transpiration (T), and between vapor pressure deficit and estimated hourly, leaf-level water use efficiency (WUE) for the deforested area in Wüstebach (Grass_WU) for various method versions. Left column shows partitioning results of the method versions after Scanlon and Kustas (2010, SK10), and the right column of the method versions after Thomas et al. (2008, TH08).

2.4

Fourth, I was confused by the HiP GPP and TER metric…it seems like the authors are filtering the data to consider only periods when the partitioned fluxes are similar in magnitude to those expected from conventional partitioning approaches (which are highly uncertain), and then using those filtered data to evaluated the partitioned fluxes? This seems like an approach that may obscure problems in one or the other partitioned fluxes…I would suggest a more straightforward comparison between the NPP and GPP (without the HiP) filtering.

We are sorry if the first manuscript version gave rise to a misunderstanding. The "Hit in Range" (HiR) criterion was solely used as one of three evaluation criteria (partitioning results in reference to R_{soil} chamber measurements, HiR with respect to the approach after Reichstein et al. (2005), E_{soil} estimation according to Beer's law). It was NOT used to filter the data before any of the other analyses presented in the paper. We are aware that all of the abovementioned reference methods have their issues, which is why we used multiple of them and discuss them carefully.

2.5

Finally, are there any independent estimates of WUE (for example, from gas exchange data) in these sites, or similar biomes, that could provide a reality check on the towerderived WUE estimates?

We conducted a more thorough literature search concerning estimates of WUE at the leaf level and included references in our discussion (page 11, line 14). Unfortunately, no direct measurements of WUE were conducted at any study site.

Work cited: Li et al. 2019. A simple and objective method to partition evapotranspiration into transpiration and evaporation at eddy-covariance sites. Agricultural and Forest Meteorology. https://www.sciencedirect.com/science/article/pii/S016819231830371X?via%3Dihub

Good et al. 2015. Hydrologic connectivity constrains partitioning of global terrestrial water fluxes. Science. http://science.sciencemag.org/content/349/6244/175

Thank you very much for your comments and your time!

Source Partitioning of H_2O and CO_2 Fluxes Based on High Frequency Eddy Covariance Data: a Comparison between Study Sites

Anne Klosterhalfen[1], Alexander Graf[1], Nicolas Brüggemann[1], Clemens Drüe[2], Odilia Esser[1], María Pat González Dugo[3], Günther Heinemann[2], Cor M.J. Jacobs[4], Matthias Mauder[5], Arnold F. Moene[6], Patrizia Ney[1], Thomas Pütz[1], Corinna Rebmann[7], Mario Ramos Rodríguez[3], Todd M. Scanlon[8], Marius Schmidt[1], Rainer Steinbrecher[5], Christoph K. Thomas[9], Veronika Valler[1], Matthias J. Zeeman[5], Harry Vereecken[1]

[1]Agrosphere Institute, IBG-3, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
[2]Department of Environmental Meteorology, University of Trier, 54296 Trier, Germany
[3]IFAPA - Consejería de Agricultura, Pesca y Desarrollo Rural, Centro Alameda del Obispo, 14080 Córdoba, Spain
[4]Wageningen Environmental Research, Wageningen University and Research, 6708 PB Wageningen, the Netherlands
[5]Institute of Meteorology and Climate Research, IMK-IFU, Karlsruhe Institute of Technology (KIT), 82467 Garmisch-Partenkirchen, Germany
[6]Meteorology and Air Quality Group, Wageningen University and Research, 6708 PB Wageningen, the Netherlands
[7]Department Computational Hydrosystems, Helmholtz Centre for Environmental Research (UFZ), 04318 Leipzig, Germany
[8]Department of Environmental Sciences, University of Virginia, Charlottesville, VA 22904, United States
[9]Micrometeorology Group, University of Bayreuth, 95447 Bayreuth, Germany

Correspondence to: Anne Klosterhalfen (a.klosterhalfen@fz-juelich.de)

Abstract. For an assessment of the roles of soil and vegetation in the climate system, a further understanding of the flux components of H_2O and CO_2 (e.g., transpiration, soil respiration) and their interaction with physical conditions and physiological functioning of plants and ecosystems is necessary. To obtain magnitudes of these flux components, we applied the source partitioning approaches after Scanlon and Kustas (2010; SK10) and after Thomas et al. (2008; TH08) to high frequency eddy covariance measurements of twelve study sites covering including various different ecosystems (croplands, grasslands, and forests) in differenta number of countries climatic regions. Both partitioning methods are based on higher-order statistics of the H_2O and CO_2 fluctuations, but proceed differently to estimate transpiration, evaporation, net primary production, and soil respiration. We compared and evaluated the partitioning results obtained with SK10 and TH08 including slight modifications of both approaches. Further, we analyzed the interrelations between the performance of the partitioning methods, turbulence characteristics, and site characteristics (such as plant cover type, canopy height, canopy density, and measurement height), and performance of the partitioning methods. We were able tocould identify characteristics of a data set that areas prerequisite for adequate a sufficient performance of the partitioning methods.

SK10 had the tendency to overestimate and TH08 to underestimate soil flux components. For both methods, the partitioning of CO_2 fluxes was more irregularless robust than of H_2O fluxes. Results derived with SK10 showed relatively large dependencies on estimated water use efficiency (WUE) at the leaf - level, which is a requiredneeded as an input. Measurements of outgoing longwave radiation used for the estimation of foliage temperature (used in and WUE) could

slightly increase the quality of the partitioning results. A modification of the TH08 approach, by applying a cluster analysis for the conditional sampling of respiration/evaporation events, performed satisfactorily, but did not result in significant advantages compared to the original other method versions (developed by Thomas et al., (2008). The performance of each partitioning approach was dependent on meteorological conditions, plant development, canopy height, canopy density, and measurement height. Foremost, the performance of SK10 correlated negatively with the ratio between measurement height and canopy height. The performance of TH08 was more dependent on canopy height and leaf area index. In general,It was found, that all site characteristics which increase dissimilarities between scalars appeared to enhance partitioning performance for SK10 and TH08.

1 Introduction

The eddy covariance (EC) method is a micrometeorological technique commonly used to measure the energy, water vapor, and carbon dioxide exchange between biosphere and atmosphere across a large range of scales in time and space (Baldocchi et al., 2001; Reichstein et al., 2012). The measurements help to understand the temporal and spatial variations of these fluxes at the land-atmosphere interface. However, the EC method quantifies only net fluxes of water vapor, i.e., evapotranspiration (ET), and the net ecosystem exchange of CO_2 (NEE). Thus, for a better assessment of the role of soil and vegetation in the climate system, a further understanding of the flux components of H_2O and CO_2 and their interaction with physical conditions and physiological functioning of plants and ecosystems is necessary (Baldocchi et al., 2001). To obtain magnitudes of transpiration (T), evaporation (E), photosynthesis, and respiration by soil and vegetation, certain measurements with additional instrumentation independent of the EC technique can be conducted. Alternatively or additionally, so-called source partitioning approaches can be applied to the net fluxes obtained with the EC method. For instance, with the notion that during night no CO_2 is assimilated by plants (and hence, observed NEE equals respiration), respiratory fluxes are often estimated based on semi-empirical models describing the relationship between a physical driver (e.g., temperature) and respiration (Lloyd and Taylor, 1994; Reichstein et al., 2005, 2012). To estimate soil surface fluxes of both H_2O and CO_2 directly from high frequency EC data without assumptions on such drivers, two new distinct partitioning approaches were developed by Scanlon and coauthors (Scanlon and Sahu, 2008; Scanlon and Kustas, 2010), and Thomas et al. (2008). Both approaches rely on the assumption that the presence of multiple sources and sinks in and below the canopy will lead to decorrelation of the high frequency scalar concentrations measured by the EC method available in the framework of EC measurements above the canopy. This decorrelation contains information about the strength of these sinks and sources, which can be quantified by applying the flux-variance similarity theory or conditional sampling strategies. The scalar-scalar-correlations of H_2O and CO_2 are however not only influenced by the sink-source distribution, but also by height (atmospheric surface layer, roughness sublayer), surface heterogeneity (Williams et al., 2007), canopy density, and coherent structures (Edburg et al., 2012; Huang et al., 2013).

The source partitioning approach after Scanlon and Sahu (2008) and Scanlon and Kustas (2010) has already been applied to data acquired aboveof a corn field (eastern USA; Scanlon and Kustas, 2012), has been compared to an isotopic H_2O flux partitioning method (Good et al., 2014) and to the Noah Land Surface Model (Wang et al., 2016) both for grasslands, and has been evaluated on a forest site on a decadal time scale (Sulman et al., 2016). Zeeman et al. (2013) further investigated the partitioning approach after Thomas et al. (2008) in association with coherent structures. To better assess these two approaches and their theoretical background, an intercomparison at a variety of study sites is necessary (Anderson et al., 2018).

The objective of this study is to compare and evaluate the source partitioning approaches after Scanlon and Kustas (2010) and after Thomas et al. (2008) by applying them to high frequency scalar measurements of various study sites in different ecosystems. In additionNext to testing slight modifications of both partitioning methods, conditions and characteristics of study sites are identified under which the methods perform best. Based on findings of the above-mentioned authors and a large eddy simulation (LES) study (Klosterhalfen et al., 2019in review), we hypothesize that the methods' performance is dependent on the canopy height (h_c), which should represent the vertical separation of sinks and sources of H_2O and CO_2 between canopy top and soil surface, on the canopy density (leaf area index LAI, or expressed as the ratio LAI h_c^{-1}), and on the ratio between measurement height (z) and h_c, respectively. All these factors affect the degree of mixing of the scalars detected bywhen they reach the EC sensors. With a high and sparse canopy and a low z h_c^{-1}, we hypothesizeassume a larger dissimilarity between scalar fluctuations and a more precise partitioning result of both source partitioning approaches. To summarize, goals of this study are:

- The comparison and evaluation of the partitioning results obtained with the approaches after Scanlon and Kustas (2010) and after Thomas et al. (2008) for various ecosystems, and testing slight modifications of the approaches
- An analysis of the two approaches with respect to their dependence on their underlying assumptions
- The description of the interrelations between performance of the partitioning methods, turbulence characteristics, and site characteristics (such as canopy type, h_c, z h_c^{-1}, LAI, and LAI h_c^{-1}), and performance of the partitioning methods
- The identification of characteristics of a data set (i.e. of study site and period properties), which lead to a satisfactory performance of the partitioning methods, if such characteristics exist.

2 Material and Methods

2.1 Source Partitioning after Scanlon and Kustas (2010) - SK10

To estimate the contributions of transpiration (T)T, Eevaporation (E), photosynthesis as net primary production (NPP), and soil respiration ($R_{soil,}$ autotrophic and heterotrophic sources) to the measured net fluxes, Scanlon and Sahu (2008) and Scanlon and Kustas (2010) proposed a source partitioning method using high frequency time series from a typical EC station. This method (SK10 in the following) is based on the spatial separation and relative strength of sinks and sources of water vapor and CO_2 below the canopy (source of both water vapor and CO_2), in the canopy (source of water vapor and

~~during daylight~~ sink of CO_2 during daylight), and the atmosphere. Assuming that air from those sinks and sources is not yet perfectly mixed before reaching the EC sensors, partitioning is estimated based on the separate application of the flux-variance similarity theory to the stomatal and non-stomatal components of the ~~regarded~~ scalars, as well as an estimation of canopy ~~on additional assumptions on stomatal~~ water use efficiency (WUE). The slope of the relationship between water vapor fluctuations (*q'*) and CO_2 fluctuations (*c'*) originating from stomatal and non-stomatal processes usually differs from the WUE at the leaf level~~T~~ and the correlation between the two scalars ($\rho_{q'c'}$) usually deviates from -1 during daytime. This ~~reduction of correlation and its~~ deviation of the slope of the *q'* versus *c'* relationship from WUE at leaf-level and the reduction of correlation are~~is~~ used to estimate the composition of the measured fluxes (Scanlon and Kustas, 2010; Scanlon and Sahu, 2008). For a detailed analytical description of SK10 see Scanlon and Albertson (2001), Scanlon and Sahu (2008), Scanlon and Kustas (2010, 2012), and Palatella et al. (2014). Furthermore, Skaggs et al. (2018) implemented SK10 in the open source Python 3 module Fluxpart. In the present study, SK10 was applied to high frequency EC data and the flux components were estimated using the implementation of SK10 as described by Klosterhalfen et al. (~~in review~~2019).

As mentioned before, the WUE at the leaf ~~-~~level has to be estimated for the application of SK10. WUE at the leaf ~~-~~level describes the relation between the amount of CO_2 uptake through stomata (photosynthesis) and the corresponding amount of H_2O loss (T). One way to derive WUE (without additional measurements at leaf-level) is to relate the difference in mean CO_2 concentration between air outside and inside the leaf to the difference in mean water vapor concentration between air outside and inside the leaf including a factor that accounts for the difference in diffusion rate between H_2O and CO_2 through the stomatal aperture (Campbell and Norman, 1998; Scanlon and Sahu, 2008). The mean H_2O and CO_2 concentrations just outside the leaf can be inferred from EC measurements by considering logarithmic mean concentration profiles implementing the Monin-Obukhov similarity theory (MOST; Scanlon and Kustas, 2010, 2012; Scanlon and Sahu, 2008). For the internal CO_2 concentration, a constant value of 270 or 130 ppm was presumed, typical for C_3 or C_4 plants, respectively (Campbell and Norman, 1998; Špunda et al., 2005; Williams et al., 1996; Xue et al., 2004). Values for the internal water vapor concentration were estimated based on 100% relative humidity at foliage temperature ~~(T_f)~~. Measurements of foliage temperature~~T_f~~ were not available at the study sites, so for the source partitioning foliage temperature~~T_f~~ was set equal to measured air temperature (WUE_{meanT}; Scanlon and Sahu, 2008). Additionally, to investigate the sensitivity of WUE, foliage temperature~~T_f~~ was also derived by means of measured outgoing longwave radiation (WUE_{OLR}; with a surface emissivity of 0.98), or calculated similar to the external concentrations by considering a mean profile based on MOST (WUE_{MOST}). Thus, three different approaches of~~to~~ SK10 with differing inputs for WUE were applied to all study sites.

2.2 Source Partitioning after Thomas et al. (2008) - TH08

Thomas et al. (2008) presented a new method (TH08 in the following) to estimate daytime sub-canopy respiration of forests directly from EC raw data by conditional sampling. ~~At the same time~~In an analogous way, evaporation can be quantified by exchanging *c'* with *q'* in the equations given by Thomas et al. (2008, equations 1-11, pages 1212-1215). The method assumes that occasionally air parcels moving upward (vertical wind fluctuations $w' > 0$) carry unaltered H_2O/CO_2

concentration combinations of the sub-canopy. Looking at the fluctuations q' and c', both normalized with the corresponding standard deviation, respiration/evaporation signals should occur within the part of the joint probability distribution where w', q' and c' are positive, i.e. in the first quadrant in the q'-c' plane (where $q' > 0$ and $c' > 0$). Additionally, Thomas et al. (2008) introduced a hyperbolic threshold criterion within quadrant 1, in order to only sample ~~thus sampling~~ all data points above this hyperbola. Thomas et al. (2008) found realistic respiration estimates with a hyperbolic threshold of 0.25, which was also applied here. Subsequently, daytime evaporation and respiration can be determined ~~estimated~~ from the conditionally sampled w', q', and c' time series within quadrant 1 (Q1) or using the hyperbola threshold criterion (H). F~~urthermore,~~or the determination of the turbulent H_2O and CO_2 fluxes either ~~can be calculated by~~ the covariance between w' and the corresponding scalar (CV) can be used, or ~~represented by~~ the relaxed eddy accumulation (REA) technique (Businger and Oncley, 1990) using the coefficient β as described in equation 4, page 1213 and statements on page 1215 in Thomas et al. (2008). ~~Therefore~~Hence, Thomas et al. (2008) applied four different approaches to quantify the respiration/evaporation events, combining the two conditional sampling criteri a~~ons~~ (Q1 or H) and the two calculation strategies (CV or REA technique).

For some averaging periods in our data, a potential respiration/evaporation 'cloud' was evident but did not occur (completely) within quadrant 1 (Fig. 1). As a modification of the conditional sampling strategy and a more tolerant detection of respiration/evaporation events, a distribution-based cluster analysis was conducted (fifth approach, GMM). With the Gaussian Mixture Model (Canty, 2010) using the Expectation-Maximization Algorithm, two clusters ~~or components, respectively,~~ were defined for each averaging period: the respiration/evaporation 'cloud' and all further points associated with T and photosynthesis independent of the sign of w'. ~~The GMM method is based on taking random samples from each component and fitting a certain number of Gaussian distributions to the samples, optimizing their parameters iteratively to model the data (Canty, 2010).~~ Soil surface fluxes were calculated by CV from data in the respiration/evaporation 'cloud', where the deviations from the averages of all sampled cluster data points (instead of all data points) were used for q' and c' (w' kept unchanged). Because the sampled respiration/evaporation 'cloud' by GMM would not always lie within quadrant 1 (often in quadrant 1 and 4, or in 1 and 2), and q' and/or c' of the defined 'cloud' could correlate negatively with w', the corresponding surface flux would often be negative (Fig. 1). If this was the case for H_2O and/or CO_2 soil fluxes, the corresponding flux was recalculated considering the deviations from the averages of all data points for w', q', and c', and only including data points within quadrant 1 of the original q'-c' plane and with $w' > 0$. This recalculated flux represented only a minimal fraction of the corresponding flux component in the considered averaging period. Also, as a result of this procedure the number of data points could differ between H_2O and CO_2 for TH08 CV GMM depending on the ~~used~~ calculation step used.

2.3 Study Sites and Data Processing

For the application and evaluation of the source partitioning methods, various study sites in a number of countries with differing cover types, canopy densities (represented by~~regarding~~ LAI), and measurement heights were chosen (Table 1).

Almost all study sites are part of the FLUXNET network (Baldocchi et al., 2001). Detailed site and measurement descriptions can be found in the listed references. Besides~~Next to~~ coniferous and deciduous forests with closed canopy cover, grasslands, and croplands, some sites represent special canopy types: in Forest_SC~~_FR~~ (for site abbreviations see Table 1) EC measurements have been conducted above a~~n~~ Mediterranean oak savanna (dehesa; Andreu et al., 2018); in Wüstebach an area of about 9 ha was deforested in 2013 and so measurements were obtained above the still present spruce forest (Forest_WU~~_FR~~) and the deforested area (Grass_WU~~_GL~~) (Graf et al., 2014; Wiekenkamp et al., 2016), where grass, shrubs, and young deciduous trees have been regrowing swiftly; and in Forest_LA~~_FR~~ a coniferous forest has been regrowing gradually after a non-cleared windthrow in 2007 (Matiu et al., 2017). These three study sites represent the most heterogeneous landcover types in this study.

For each study site, measurements from days with a high-productive state of the vegetation and fair-weather conditions were selected to exclude factors interfering with the performance of the partitioning method. Time periods with precipitation events were excluded. Furthermore, the quality assessment scheme after Mauder et al. (2013) was applied to each data set and source partitioning was only conducted for time periods with the highest or intermediate quality flag levels assigned by this scheme. We only considered partitioning results of daytime data, because both methods require the presence of photosynthesis. Here, daytime was determined by calculating sunrise and sunset times by means of local time. Additionally, the TH08 method was only applied to time periods with a negative $\rho_{q'c'}$, and if less than 1% of the total data points in one half-hour time period were sampled as the respiration/evaporation 'event', the partitioning result was disregarded.

The high frequency H_2O and CO_2 time series of all study sites were pre-processed and prepared for the application of the source partitioning approaches as described by Klosterhalfen et al. (~~in review~~2019). For each study site, physically impossible values and spikes were excluded in the high frequency EC data of vertical wind, total H_2O and CO_2 concentrations. T~~, t~~he time delay was corrected, missing raw data within a half-hour period were gap-filled by linear interpolation, and a planar-fit rotation was conducted, where the rotation matrix was calculated for only a maximum time period of two weeks. Further, the EC data was corrected for density fluctuations after Detto and Katul (2007). Then, the source partitioning approaches were applied to half-hourly time series of these pre-processed high frequency data, partitioning fractions~~factors~~ (E/ET or R_{soil}/NEE, respectively) were calculated, and applied to the post-processed half-hourly EC data.

2.4 Evaluation of Source Partitioning Results

The evaluation of the source partitioning performance was conducted in multiple ways for the various study sites depending on data-availability~~ (Fig. 6)~~. At some study sites, R_{soil} was measured additionally with closed-chamber measurements independently of the EC measurements. In Grass_RO~~_GL~~ and the cropland in Selhausen (Wheat_SE, Barley_SE, Intercrop_SE, SugarBeet_SE~~SE_CL~~), continuous measurements of multiple longterm-chambers were available for the considered time periods (half-hourly at Selhausen~~SE_CL~~ and hourly interpolated to half-hourly at Grass_RO~~_GL~~). In Maize_DI~~_CL~~, Forest_WU~~_FR~~, and Grass_WU~~_GL~~, R_{soil} was measured with survey-chambers at several measurement points on one day during the considered time periods, so spatial and temporal averages for the hours in question could be calculated. For all study sites (except for LA_FR), soil evaporation (E_{soil}) was estimated as a fraction of measured ET based on Beer's law depending on LAI (E_{soil} = ET exp(-0.6 LAI); Campbell and Norman, 1998; Denmead et al., 1996). Thus, the root mean square error (RMSE) and the bias could be calculated between the partitioning results for E or R_{soil} and the estimated E_{soil} or chamber measurements, respectively. RMSE was sensitive to bias and outliers, and the distribution of errors was skewed. The positive outliers/errors (overestimations) were larger than negative errors (underestimations). An overestimation of the flux component magnitude may result in method overestimating the magnitude of a flux component may earn a larger RMSE than an underestimationing one. Therefore, we also calculated a version of the RMSE based on log-transformed data ($RMSE_{ln}$; data transformed with ln(x +1)) before computing differences between estimated and reference E or R_{soil}. Furthermore, one has to keep in mind that the measurements of R_{soil} and LAI can also contain errors and that E_{soil} is only a rough model approximation and can only give an order of magnitude to expect.

In addition, partitioned CO_2 fluxes were compared evaluated in reference to results of the established partitioning approach after Reichstein et al. (2005), if available; even though this approach targets other flux components (total ecosystem respiration TER and gross primary production GPP). For Forest_MMP and Forest_WA, results of this partitioning approach were not available, thus, we chose for these sites maximal margins for GPP and TER based on partitioning results of previous years and experience. For all sitesHere,, the estimated NPP and R_{soil} for every time step were classified as reasonable if their magnitudes were smaller than the calculated determined GPP or TER, respectively. Since all data sets were from the main growing season and for weather conditions favorable to high respiration, we assumed that R_{soil} should additionally be larger than 1 μmol m^{-2} s^{-1}. In the following, NPP and R_{soil} estimates meeting these criteria ("hits in range") will be counted as HiR GPP (magnitude of NPP smaller than magnitude of GPP) and HiR TER (R_{soil} smaller than TER and larger than 1 μmol m^{-2} s^{-1}). We calculated the percentrelative fraction of HiR GPP and HiR TER in relation to the count of time steps with valid partitioning solutions. WAgain, within this evaluation step two source partitioning approaches (approach after Reichstein et al., 2005 versus SK10 or TH08)models were examined and compared including their different assumptions and uncertainties were examined and compared, and the results have to be handled with care. An evaluation of the estimated flux magnitudes was also possible for some study sites by means of prior former publications.

2.5 Analysis of Source Partitioning Approaches

To compare the strengths and limitations of SK10 and TH08 and to gain a better insight in their functionality and dependencies on turbulence and site characteristics, a correlation analysis was conducted between HiR GPP or HiR TER and the variables z, h_c, z h_c^{-1}, LAI, or LAI h_c^{-1}. Here, we have chosen HiR GPP and HiR TER as the criteria of partitioning performance, because thesey could be calculated for all considered study sites, unnot like the error quantitiesmetrics (RMSE, bias, etc.) regarding R_{soil}. Different subsets of sites were considered for the calculation of to calculate the correlations: all study sites, only forest sites, or only cropland and grassland sites.

SK10 was already thoroughly analyzed by means of synthetic high frequency data derived by LES (Klosterhalfen et al., 2019). To obtain a better understanding of the strengths and limitations of TH08, we constructeddeveloped a conceptual model to generate simple, synthetic data sets of *w'*, *q'*, and *c'* (with sample sizes of N = 100) with different degrees of mixing between scalar sinks and sources from the soil, canopy, and boundary layer (Fig. 7, *upper panels*). We considered no mixing, complete mixing, and partial mixing between scalars originating from soil and canopy (with positive *w'*). For , all three sets, excluding mixing with scalars originating from the boundary layer (with negative *w'*) was excluded. Averages of fluctuations were all specified as zero, and each scalar sink/source strength was determined such that the net H_2O flux equalsequates to 1 mmol m^{-2} s^{-1} and the net CO_2 flux to -1 µmol m^{-2} s^{-1}. To each generated data point of *w'*, *q'* and *c'* a random number, sampled from a standard normal distribution and rescaled to a standard deviation of 5% of the magnitude of the variable, was added to simulate additional sources of variance not related to the degree of mixing. TH08 was applied to these synthetic data sets and could be validated with the true known partitioning fractionsactors, while SK10 was already thoroughly analyzed by means of the synthetic high frequency data derived by LES (Klosterhalfen et al., in review).

3 Results and Discussion

For each study site, the number of half-hourly time steps during daylight per considered time period is shown in Table A1 in the Appendix. Also, the relative fraction of daylight time steps of high-quality (HQ) data which were used in the application of SK10 and TH08 are shown, where for SK10 only a good or intermediate quality flag (after Mauder et al., 2013) and no precipitation were required, and for TH08 additionally a negative $\rho_{q'c'}$ had to be given. Furthermore, the relative fraction of these HQ-time steps, for which partitioning solutions were found, is shown for each method version. Thus, from the original data, only a part remained for the partitioning, and for only a part of theis remaining data a partitioning result could be obtained.

3.1 Evaluation of Source Partitioning Results

3.1.1 Flux Components Magnitudes

In the following, figures are shown for some selected sites, which were deemed most representative for all study sites, and/or for some selected method versions of SK10 and TH08, which usually exhibited the best partitioning performance. In Fig. 2 the source partitioning results for H_2O and CO_2 fluxes for Forest_LO_FR are shown in half-hourly time steps as an example. The partitioning results for all sites and all method versions are shown in the Supplementary material, including E_{soil} estimations based on Beer's law, R_{soil} chamber measurements of R_{soil}, and/or partitioning results after Reichstein et al. (2005), depending on data-availability. Figures 3 and 4 show the mean diurnal variation of H_2O and CO_2 fluxes and their components. Figure 3 shows data from one site (Forest_WA) and all method versions, whereas Fig. 4 shows results for all study sites and just two method versionsThe diurnal dynamics of H_2O and CO_2 fluxes, their components, and WUE and all method versions are shown in Fig. 3 for WA_FR. An overview of the partitioning results for all study sites is given in Fig. 4

~~using just two methods~~: SK10 with WUE_{OLR} and TH08 with REA H. In Fig. 5 the total averages of the flux components over the available time periods are shown. ~~on the one hand comparing~~The top panel compares all method versions for a single site (Forest_MMP~~_FR~~) ~~(*top panel*), and on the other hand~~ whereas the lower two panels compare~~ing~~ all sites for two~~one~~ method versions (SK10 with WUE_{OLR} and TH08 with REA H~~; *lower two panels*~~). For the calculation of these mean diurnal variations as well as the total ~~dynamics and total~~ averages, large spikes in the estimated flux components (deviation from the mean by more than ten times of the standard deviation) were excluded. Figure 6 shows the error quantities, $RMSE_{ln}$ and bias relative to R_{soil} chamber measurements, HiR GPP, HiR TER, and E_{soil} estimation, for each site and method version. In all figures, timestamps ~~Timestamps in all following figures~~ are in local time.

In general, the partitioned CO_2 fluxes showed a higher variability and more spikes than the partitioned H_2O fluxes for all sites (e.g., at Forest_HH, Fig. S2 in Supplementary material). Furthermore, ~~In general,~~ SK10 and TH08 gave differing results for each study site and performed disparately between method versions. In Fig. 2-5, it is apparent that TH08 mostly resulted in lower magnitudes of the flux components originating from the soil surface or sub-canopy~~,~~ than SK10. The source partitioning results of Forest_LO~~_FR~~ (Fig. 2, 4, 5) were an exception to this rule. For this study site, the partitioning fractions of SK10 and TH08 were very similar and thus suggest a ~~very~~ low uncertainty of the results. For the other study sites, larger discrepancies were observed between SK10 and TH08. Furthermore, the partitioning fractions E/ET and NPP/NEE varied much less between sites for TH08 than for SK10 (Fig. 5). Good et al. (2015) determined a global estimate for T/ET of 0.65 and Schlesinger and Jasechko (2014) an estimate of 0.61. Li et al. (2019) deduced mean annual partitioning fractions of 0.75, 0.62, and 0.56 for evergreen coniferous forests, croplands, and grasslands, respectively. Our derived partitioning fractions had approximately the same magnitudes or assigned a larger fraction to transpiration, most likely due to the seasons chosen. We could not observe a clear difference in partitioning fractions between ecosystem types as Li et al. (2019).

For a number of our sites, information on component fluxes is available from literature. For Forest_LO in 1997, Dolman et al. (2002) reported a peak respiration measurement of 12 $\mu mol\ m^{-2}\ s^{-1}$, Falge et al. (2002) a seasonal maximum GPP of -24 $\mu mol\ m^{-2}\ s^{-1}$ and seasonal maximum TER of 5.3 $\mu mol\ m^{-2}\ s^{-1}$, and chamber measurements in June 2003 revealed a maximum soil respiration rate of 17.3 $\mu mol\ m^{-2}\ s^{-1}$. Our partitioning results for Forest_LO based on SK10, TH08, and the approach after Reichstein et al. (2005) laid within the range of these reported flux magnitudes (Fig. 2, S1 in Supplementary material). For Forest_WA, SK10-derived partitioning fractions, with T/ET > 0.5 and NPP/NEE > 2, were relatively large. On 8 July 2016, however, the CO_2 flux components were smaller, with NPP/NEE < 1.4 and R_{soil} < 10 $\mu mol\ m^{-2}\ s^{-1}$ (Fig. S4 in Supplementary material). On this day no significant differences in weather conditions or scalar statistics were apparent in contrast to the other days. For Forest_MMP, Thomas et al. (2009) derived a T/ET ratio of 50% from sap flow measurements, which agrees well with the partitioning results obtained with the SK10 approach (Fig. 5, Fig. S6 in Supplementary material). Results of the TH08 approach and estimated E_{soil} imply a relatively larger fraction of T. At Forest_SC, the results of the different source partitioning methods were impacted by water stress. For a very dry period in August 2016, both partitioning approaches were not applicable, because transpiration and photosynthesis almost ceased due to water stress, and the correlations between H_2O and CO_2 fluxes were almost always positive (not shown). In April 2017, partitioning results were obtained showing an increase in R_{soil} estimated with SK10 and a decrease in estimated E (Fig. S7 in Supplementary material). Spring 2017 was considered as relatively dry in this region, and the last precipitation event was five days before the respective time period, so that it can be assumed that water stress increased steadily in April 2017. No respiration/evaporation events were apparent in the *q'-c'* planes, which could be caused by the sub-canopy in the oak savanna, thus, TH08 probably underestimated soil fluxes substantially.

In Grass_RO the continuous chamber measurements of R_{soil} and TER estimated with the approach after Reichstein et al. (2005) did not agree well. TER decreased steadily over the seven days (this could also be observed for Grass_FE) and was mostly lower than measured R_{soil} (Fig. S8 in Supplementary material). In comparison to measured R_{soil}, SK10 still overestimated and TH08 underestimated R_{soil} fluxes. For Forest_WU and Grass_WU, TH08 yielded results matching comparatively well with the modeled estimate E_{soil} and the gap-filling approach after Reichstein et al. (2005) (Fig. S3, S9 in Supplementary material). As mentioned before, Grass_WU is a very heterogeneous site with regrowing vegetation of grasses, shrubs, and trees on dry and wet areas. Thus, the measured signals might display fluxes originating from different sinks and sources distributed horizontally rather than vertically. The present variety of plant types increased the uncertainty in the estimation of WUE. Usage of WUE_{OLR} improved the partitioning by SK10 significantly, but could not avoid overestimation of R_{soil} (in reference to chamber measurements and TER). For Forest_LA, we observed a behavior similar to Grass_WU (Fig. S5 in Supplementary material). Here, the forest is also regrowing, but spruce trees are already more abundant and larger.

For Maize_DI in 2007, Jans et al. (2010) reported a mean R_{soil} flux of 3.16 µmol m^{-2} s^{-1} and a peak R_{soil} of 23 µmol m^{-2} s^{-1}. R_{soil} estimates by SK10 were often as large as this peak, but the maximum observed by Jans et al. (2010) was triggered by precipitation, which does not apply in our case (Fig. S11 in Supplementary material). The partitioning results for the cropland in Selhausen (Wheat_SE, Barley_SE, Intercrop_SE, SugarBeet_SE) showed large differences between crops and were more robust for H_2O fluxes than CO_2 fluxes.

~~For TH08, the calculation of the fluxes via REA yielded larger fluxes than via CV. Because averaging in the flux calculation is performed differently for CV and REA (i.e. equations 1, page 1212 and equation 8, page 1214 in Thomas et al., 2008), and less data points are sampled with the hyperbolic threshold than using data from the entire Q1, the largest magnitudes were obtained by using REA with the hyperbolic threshold (REA H). In some time steps, no respiration/evaporation 'cloud' was apparent in the *q'-c'* plane, thus, the applied conditional sampling strategies could not be as effective as intended and an assessment of a correct sampling was not possible. Compared to the magnitude of GPP and TER estimated by the gap-filling model after Reichstein et al. (2005), components estimated by TH08 almost always were within this prescribed range (magnitude of NPP smaller than magnitude of GPP, and R_{soil} smaller than TER) because of their small resulting fluxes, whereby R_{soil} was often below the assumed minimal threshold of 1 µmol m^{-2} s^{-1} and thus underestimated (Fig. 6, S1-S12 in Supplementary material). Regarding the error quantities in Fig. 6, TH08 REA H performed best. Partitioning results obtained~~

by TH08 CV GMM were not systematically different from the other method versions but showed no extreme spikes in the soil flux components.

The SK10 approach had the tendency to produce very high magnitudes of the soil flux components. Considering the diurnal dynamics and averages (Fig. 3-5), results of SK10 were satisfactory, but of course still relatively large. For most of the study sites, the magnitudes and variability in the half-hourly results of the soil flux components were decreased by using WUE_{MOST} or WUE_{OLR} instead of WUE_{meanT}. The differing WUE inputs had a larger effect on the CO_2 flux components than on H_2O. Considering the error quantities in Fig. 6, SK10 with WUE_{OLR} very often gave the best results.

3.1.1 Evaluation by Means of Publications

The partitioned CO_2 fluxes generally showed a higher variability and more spikes than the partitioned H_2O fluxes for all sites. Jans et al. (2010) reported a mean R_{soil} measurement of 3.16 µmol m^{-2} s^{-1} and a peak event of 23 µmol m^{-2} s^{-1} for DI_CL_MA in 2007. R_{soil} estimates by SK10 were often as large as this peak, but the maximum observed by Jans et al. (2010) was triggered by precipitation, which does not apply for our considered time periods (Fig. S10 in Supplementary material). For LO_FR in 1997, Dolman et al. (2002) reported a peak respiration measurement of 12 µmol m^{-2} s^{-1}, Falge et al. (2002) a seasonal maximum GPP of −24 µmol m^{-2} s^{-1} and seasonal maximum TER of 5.3 µmol m^{-2} s^{-1}, and chamber measurements from June 2003 had a magnitude of 17.3 µmol m^{-2} s^{-1}. All these quantities support our partitioning results for LO_FR based on SK10, TH08, and the approach after Reichstein et al. (2005) (Fig. 2). For MMP_FR, Thomas et al. (2009) derived a T/ET ratio of 50% from sap flux measurements, which agrees well with the partitioning results by SK10 (Fig. S5 in Supplementary material). Results by TH08 and estimated E_{soil} imply a larger fraction of T. For WU_GL, TH08 yielded results matching comparatively well to the modeled estimate E_{soil} and the gap-filling approach after Reichstein et al. (2005) (Fig. S8 in Supplementary material). As mentioned before, WU_GL is a very heterogeneous site with regrowing vegetation of grasses, shrubs, and trees on dry and wet areas. Thus, the measured signals could display fluxes coming from different sinks and sources distributed horizontally rather than vertically. The present variety of plant types increased the uncertainty in the estimation of WUE, where the usage of WUE_{OLR} improved the partitioning by SK10 significantly, but the overestimation of R_{soil} (compared to chamber measurements and TER) was not be avoided. For LA_FR we observed a behavior similar to WU_GL. Here too, the forest is regrowing, but trees are already more abundant and larger. At SC_FR the impact of water stress on the application of source partitioning methods could be observed. For a very dry period in August 2016, both partitioning approaches were not applicable, because transpiration and photosynthesis almost ceased due to water stress and the correlations between H_2O and CO_2 fluxes were almost always positive (not shown). For a period in April 2017, partitioning results could be obtained, where an increase in R_{soil} estimated with SK10 and a decrease in estimated E was evident during the respective time period (Fig. S6 in Supplementary material). Spring 2017 was considered as relatively dry in this region, and the last precipitation event was five days before the respective time period, so that it can be assumed that water stress increased steadily in April 2017. TH08 underestimated soil fluxes substantially, because no respiration/evaporation events were apparent, which could be caused by the sub-canopy in the oak savanna. For WA_FR, SK10-derived E and R_{soil} were generally relatively large, only on 8 July 2016, the CO_2 flux components were smaller

~~(Fig. S3 in Supplementary material). On this day no significant differences in weather conditions or scalar statistics were apparent in contrast to the other days. In RO_GL the continuous R_{soil} chamber measurements and TER estimated with the approach after Reichstein et al. (2005) did not agree well, where the latter decreased steadily over the seven days (this could also be observed for FE_GL) and was mostly lower than measured R_{soil}. Compared to TER and measured R_{soil}, SK10 still overestimated and TH08 underestimated R_{soil} fluxes.~~

3.1.2 ~~Evaluation by Means of~~ Error Metrics~~Quantities~~

Figure 6 shows the error metrics $RMSE_{ln}$ and bias relative to chamber measurements of R_{soil}, HiR GPP, HiR TER, and $RMSE_{ln}$ and bias relative to E_{soil} estimation, for each site and method version. A clear pattern in the performance of the source partitioning depending on method version or on study site characteristics could not be identified in the error metrics ~~quantities~~ (Fig. 6). However, ~~T~~the following general statements can be made:

1) The RMSE in R_{soil} was usually larger for SK10 than for TH08 (not shown). Considering $RMSE_{ln}$ in R_{soil}, SK10 performed better at forest sites than TH08, and slightly worse at crop- and grasslands (Fig. 6a). The bias in R_{soil} was always positive for SK10 (except for Forest_WU~~_FR~~) and often negative for TH08 (except for TH08 REA H; Fig. 6b); ~~. Therefore,~~ SK10 has the tendency to overestimate and TH08 to underestimate R_{soil} compared to respiration chamber measurements. The lowest RMSE, $RMSE_{ln}$, and bias were found for the SK10 method versions in Forest_WU~~_FR~~ and for TH08 in Forest_WU~~_FR~~, Grass_WU~~_GL~~, and SugarBeet_SE~~_CL_SB~~_09.

2) ~~In comparison~~When using ~~to~~ the gap-filling model after Reichstein et al. (2005) as a reference, high HiR GPP were relatively frequent for TH08, with a minimum of 66.7% for SugarBeet_SE~~_CL_SB~~_06, while HiR GPP for SK10 were ~~usually less frequent~~considerably lower (Fig. 6c). For HiR TER, such a clear difference in performance could not be observed ~~both methods converged~~ (Fig. 6~~c,~~ d). While SK10 mostly overestimated TER, TH08 often estimated soil fluxes smaller than the minimum~~al~~ R_{soil} threshold of 1 µmol m^{-2} s^{-1}. TH08 REA H usually gave ~~usually~~ the best results for HiR TER and the worst for HiR GPP within the method versions of TH08. Also, the performance of SK10 improved for CO_2 in Maize_DI~~_CL_MA~~ with increasing crop height and lower LAI (Fig. 4, 6).

3) The RMSE (not shown), $RMSE_{ln}$, and bias of E (in reference to E_{soil} estimated using ~~compared to the modeled estimate E_{soil} after~~ Beer's law) were mostly similar or slightly larger for SK10 than for TH08 except for the low crop canopies, Forest_LO~~_FR~~, Forest_MMP~~_FR~~, and Forest_SC~~_FR~~ (Fig. 6e, f). These sites also had a relatively low LAI. The error metrics~~quantities~~ were low in Forest_WU~~_FR~~ and Grass_WU~~_GL~~ for SK10 and TH08. The worst performance regarding E could be found in Forest_HH~~_FR~~ for SK10, and in Forest_SC~~_FR~~, Maize_DI~~_CL_MA~~_06, and Intercrop_SE~~_CL_IC~~ for TH08. The bias indicated that SK10 underestimated E for all canopies with a LAI lower than 2.3 (Forest_LO~~_FR~~, Forest_SC~~_FR~~, Maize_DI~~_CL_MA~~_06, SugarBeet_SE_~~CL_SB_~~06, Intercrop_SE~~_CL_IC~~, the latter three have relatively short canopies). This could also be explained by the larger E_{soil} estimates based on Beer's law due to the smaller LAIs, thus preventing an overestimation by SK10.

To summarize, for TH08 the calculation of the fluxes via REA yielded larger fluxes than via CV (Fig. 2, 3, 5). Because averaging in the flux calculation is performed differently for CV and REA (i.e. equations 1, page 1212 and equation 8, page 1214 in Thomas et al., 2008), and fewer data points are sampled with the hyperbolic threshold than using data from the entire Q1, the largest magnitudes were obtained by using REA with the hyperbolic threshold (REA H). In some time steps, no respiration/evaporation 'cloud' was apparent in the *q'-c'* plane, thus, the applied conditional sampling strategies were not as effective as intended, and an assessment of a correct sampling was not possible. Using GPP and TER estimated with the gap-filling model after Reichstein et al. (2005) as reference, components estimated by TH08 almost always were within this prescribed range (i.e. magnitude of NPP smaller than magnitude of GPP, and R_{soil} smaller than TER) because of their small resulting fluxes, whereby R_{soil} was often below the assumed minimum threshold of 1 µmol m^{-2} s^{-1}; thus, we assume these values to be underestimated (Fig. 6, S1-S13 in Supplementary material). Regarding the error metrics in Fig. 6, TH08 REA H, among all TH08 method versions, yielded the best result for the largest number of sites and error metrics. Partitioning results obtained by TH08 CV GMM were not systematically different from the other method versions, but showed no extreme spikes in the soil flux components.

The SK10 approach had the tendency to produce very high values of the soil flux components. Considering the diurnal dynamics and averages (Fig. 3-5), results of SK10 were satisfactory, but still relatively large. For most of the study sites, the magnitudes and variability in the half-hourly results of the soil flux components were decreased by using WUE_{MOST} or WUE_{OLR} instead of WUE_{meanT}. The differing WUE inputs had a larger effect on the CO_2 flux components than on H_2O. The magnitudes of the estimated leaf-level WUEs agreed well with magnitudes stated by Good et al. (2014), Linderson et al. (2012), and Sulman et al. (2016). Considering the error metrics in Fig. 6, SK10 with WUE_{OLR} very often gave the best results.

3.2 Analysis of Source Partitioning Approaches

3.2.1 Analysis by Means of Correlation Analysis

We studied the interrelations between partitioning performance (expressed in HiR GPP and HiR TER) and site characteristics such as canopy height h_c, LAI, canopy density (using LAI h_c^{-1} as proxy), measurement height z, and the position of the measurements relative to the roughness sublayer (using z h_c^{-1} as a proxy) by means of a correlation analysis (Tables 2, 3). Here, h_c represents the vertical separation of sinks and sources of passive scalars between canopy top and soil surface. For the chosen study sites, LAI correlated with h_c when considering a specific ecosystem type (forest, cropland, or grassland). Thus, ~~As LAI can correlate with h_c of a study site,~~ LAI h_c^{-1} was also considered to distinguish between their impacts on partitioning performance. The ecosystem type "cropland" included only two different sites, Maize_DI and Selhausen (Wheat_SE, Barley_SE, Intercrop_SE, SugarBeet_SE), and thus only two different measurement heights z, but a total of nine data sets resulting from the considered time periods and various crops (Table 1). Therefore, ~~measurement height z was constant for each cropland, DI_CL_MA or SE_CL, for all considered time periods, thus~~ the correlation coefficients with z including this ecosystem type have to be handled with care. All these ~~geometric~~ site characteristics contain~~represent~~ some information about~~on~~ the characteristics of the observed turbulence and also affect the degree of mixing of the scalars when they reach the EC sensor. Furthermore, we assume that with increasing LAI, LAI h_c^{-1} and z h_c^{-1}, and with decreasing h_c the dissimilarity between *q'* and *c'* decreases and EC measurements contain less information for the partitioning approaches (Edburg et al., 2012; Huang et al., 2013; Williams et al., 2007). Results of Klosterhalfen et al. (~~in review~~2019) suggest a decreasing performance of SK10 with increasing z h_c^{-1}.

Correlation coefficients between partitioning performance and site characteristics were calculated for all sites together, for forests only, or for crop- and grasslands only, respectively (Tables 2, 3). For the SK10 method versions, the correlation coefficients showed similar relations between variables and partitioning results for both HiR GPP and HiR TER, because SK10 had the tendency to overestimate both NPP and R_{soil}. For the TH08 method versions, relations slightly differ between HiR GPP and HiR TER, because TH08 had the tendency to underestimate R_{soil} fluxes (< 1 µmol m^{-2} s^{-1}), thus HiR TER were smaller than HiR GPP. For the~~Only considering~~ forest sites, the correlations were relatively high between variables and partitioning performance, even though mostly not significantly different from zero.

The performance of all SK10 method versions correlated negatively with LAI h_c^{-1} and z h_c^{-1}, and positively with h_c and z, where the correlation with z h_c^{-1} was often significant. The correlation coefficients regarding LAI, despite being also positive, were the smallest~~, where for the forest sites LAI was more important than for the remaining sites~~. Therefore, partitioning performance of SK10 was mostly enhanced with a sparse canopy and measurements obtained close to the canopy (close to or within roughness sublayer). ~~LAI h_c^{-1} correlated always negatively with performance of SK10 except for the forest sites, where the coefficients of LAI and LAI h_c^{-1} were similar.~~

For the TH08 method versions, LAI had larger effects on partitioning performance than for SK10 method versions, and h_c, z h_c^{-1}, and LAI h_c^{-1} had smaller effects~~ on partitioning performance than for SK10 method versions~~. ~~For HiR TER and only forests or only crop- and grasslands, h_c was more important again in TH08 method versions (especially while neglecting the correlation with z).~~ Correlation coefficients of LAI and LAI h_c^{-1} were mostly positive with a few exceptions (e.g., regarding HiR TER for crop- and grasslands). For the TH08 method versions, all site characteristics correlated positively with HiR GPP, except for z h_c^{-1} considering all study sites. The correlations between site characteristics and HiR TER were weak while considering all study sites. For forest sites~~ and~~, HiR TER correlated negatively with LAI h_c^{-1} and z h_c^{-1} and positively with h_c, LAI, and z. For crop- and grasslands, similar results were obtained, except the negative correlation between HiR TER and LAI. Also, the correlations with h_c and z increased in significance. ~~TH08, only positive correlations were evident except for the relationship between HiR TER and z h_c^{-1}. Also, the impacts of h_c and LAI h_c^{-1} were reversed between HiR GPP and HiR TER.~~ Apparently, a dense ~~forest~~ canopy yielded too low sub-canopy fluxes derived by TH08, but more reasonable canopy fluxes~~, and a high canopy less reasonable canopy fluxes~~.

The variable LAI mostly~~usually~~ correlated positively with partitioning performance for ~~SK10 and~~ TH08 method versions and very weak with partitioning performance for SK10 method versions, ~~and all canopies, making it the sole variable~~ which ~~clearly~~ contradicted our initial hypotheses. Also, the correlation between partitioning performance by TH08 and LAI h_c^{-1} at forest sites was contradictorycontradicted our assumption that a higher plant density would have a strong negative effect. Next to canopy density, LAI could also be connected to larger sinks and sources of canopy fluxes (T and photosynthesis) relative to soil surface fluxes due to larger biomass, and to the appearance and frequency of coherent structures. A dense canopy prevents frequent ejections of air parcels from the sub-canopy, but provokes higher scalar concentrations in such air parcels because of a longer accumulation under the canopy. Respiration/evaporation events could occur less frequently but be of higher magnitude. Also, small gaps in an otherwise dense canopy can play an important role regarding ejection events. Thus, how canopy density affects scalar-scalar-correlation measured above the canopy (and associated with that the partitioning performance), cannot be easily assessed. In this study, canopy density (LAI and LAI h_c^{-1}) and partitioning performance (especially regarding HiR TER) correlated negatively at crop- and grassland sites and mostly positively at the forest sites for TH08. Assuming gaps in the canopy can be more expected frequent in forests than in crop- or grasslands, these results support the above-mentioned aspects. Zeeman et al. (2013) found a clear connection between the appearance of coherent structures and the detection of respiration/evaporation events following the TH08 approach, where the best results were obtained for an open canopy (Forest_MMP). They found a temporal separation of 10-20 s between sub-, mid-, and above-canopy measurements. In order to assess to what extent these effects play a role in the current data setsFor further assessments, an estimate aboutof the (large-scale) heterogeneity and density of the vegetation at all study sites (gap fraction, canopy openness) has to be made and included in this analysiswould be necessary, which is beyond the scope of this paper.

3.2.2 Analysis by Means of a Conceptual Model

SK10 was already thoroughly analyzed by means of the synthetic high frequency data derived by LES (Klosterhalfen et al., in review2019). In the present study, TH08 was applied to various synthetic *w'*-, *q'*-, and *c'*-data sets including soil, canopy, and boundary layer scalar sink/sources derived by a simple conceptual model as described above (Fig. 7, *top panel*). Defined by the conditional sampling concept, we hypothesized that TH08 would work perfectly with no mixing of the scalars from the three different origins, would not obtain any partitioning fractionsfactors in case of the complete mixing, and would underestimate the soil fluxes in case of partial mixing.

TH08 behaved as hypothesizedassumed except for TH08 REA H (see below; Fig. 7, *bottom panel*). For the partial mixing, a small difference in TH08-derived partitioning fractionsfactors (especially for H_2O) was observed between the sampling in Q1 and with H, because one data point was not sampled with the hyperbolic threshold, but was locatedlaid within Q1. TH08 REA H did not yield any partitioning results in case of no or partial mixing. This is due to the different definitions of β in the application of REA with the sampling in Q1 or with H (Thomas et al., 2008, equation 4, page 1213 and statement on page 1215). β is an empirical constant and can be approximated by the ratio between the standard deviation of *w'* ($\sigma_{w'}$) and the difference between the mean vertical velocities in updrafts and downdrafts ($\overline{w_+}$- $\overline{w_-}$). For the conditional sampling approach within Q1, β is derived including all data points (disregarding the sign of *q'* or *c'*). For the approach including the hyperbolic threshold criterion, β is derived from *w'* data points which satisfy the hyperbolic threshold criterion for positive

q' and c'. In case of our conceptual model for the partial mixing, no data point with negative w' satisfied this criterion, so without $\overline{w}_{-}$, β and a partitioning fraction~~factor~~ could not be calculated. Figure 7 shows the partitioning fractions~~factors~~ for TH08 REA H while applying β as calculated in TH08 REA Q1 (*non-filled markers*). TH08 CV GMM performed similar to the other method versions: it sampled the correct respiration/evaporation 'cloud' in case of no mixing and no 'cloud' in case of complete mixing. However, in case of the partial mixing all data points with $q' > 0$ were sampled by TH08 CV GMM, thus, considering also the fraction originating from the canopy. For the latter, the covariances applying the averages of q or c of the sampled cluster, and considering only data points with $w' > 0$, were negative for H_2O and CO_2 (not shown). Thus, E and R_{soil} were recalculated with the covariance taking the deviations of the average of q or c considering all data points, and including only data points with $w' > 0$, within quadrant 1, and within the sampled cluster. This way of~~, thus,~~ correcting the sampling by GMM~~, which~~ resulted in a similar partitioning fraction as the other method versions.

4 Summary and Conclusions

For all sites and all applied method versions, the partitioned CO_2 fluxes generally showed a higher variability and more spikes than the partitioned H_2O fluxes. Mean diurnal cycles averaged over each site's specific time period yielded satisfactory results. The partitioning approaches after Scanlon and Kustas (2010; SK10) and after Thomas et al. (2008; TH08) gave differing results and performed disparately between method versions. TH08 mostly resulted in lower magnitudes of the flux components originating from the soil surface than SK10. In addition, TH08 ~~, and~~ had the tendency to underestimate these flux components ~~compared~~ in reference to soil respiration flux measurements and estimates of E_{soil} based on Beer's law. SK10 usually had the tendency to overestimate soil flux components and yielded larger error ~~quantities~~metrics (RMSE and bias). T~~, because t~~he RMSE depends~~ is depended~~ on the bias and the error distribution was asymmetric. The positive errors (overestimations) were larger than negative errors (underestimations). Decreasing the weight of outliers by log-transforming R_{soil} data from chamber observations and partitioning estimations revealed a lower $RMSE_{ln}$ for SK10 at forest sites than for TH08.

SK10 was used with a variety of estimates of WUE. Estimating input WUE using foliage temperature ~~estimated~~ derived from the observed outgoing longwave radiation often ~~enhanced~~ improved the partitioning performance. For TH08, various options w~~h~~ere tested regarding the conditional sampling and flux calculation. Applying a Gaussian Mixture Model for the conditional sampling approach in TH08 did not improve partitioning performance significantly, because ~~to~~ obtaining a positive and correct flux estimation was difficult for~~from~~ data points outside~~not within~~ quadrant 1 in the q'-c' plane. For TH08, conditional sampling including a hyperbolic threshold and calculating flux components based on the relaxed eddy accumulation technique yielded the best partitioning results.

~~The partitioned CO_2 fluxes generally showed a higher variability and more spikes than the partitioned H_2O fluxes for all sites and both methods. Also, mean diurnal cycles averaged over each site's regarded time period yielded satisfactory results for both approaches.~~

The dependencies of the partitioning performance on turbulence and site characteristics were analyzed based on a correlation analysis and the application of TH08 to synthetic, conceptual data sets of scalar fluctuations. Foremost, the performance of SK10 was improved for sparse canopies and especially with ~~correlated negatively with the~~a low ratio between measurement height and canopy height. The performance of TH08 was more dependent on canopy height and leaf area index. Partitioning performance of TH08 improved with increasing canopy density for forests, whereas the opposite was observed for grass and crops. ~~Canopy density and partitioning performance of both methods correlated negatively at crop- and grassland sites and positively at the forest sites. All~~ In general, site characteristics which increase dissimilarities between scalars (due to less mixing, large sink-source separation, coherent structures, ejections, etc.) appeared to enhance partitioning performance for SK10 and TH08.

For the forest site Loobos in The Netherlands, SK10 and TH08 obtained similar partitioning results and sufficient error ~~quantities~~ metrics suggesting a low uncertainty. At this site with a relatively low leaf area index~~LAI~~, high canopy, and low ratio between measurement and canopy height, conditions for both partitioning approaches seemed to be appropriate.

Appendix A

In Table A1 the number of half-hourly time steps during daylight per considered time period is shown for each study site. Also, the~~ relative~~ fraction of daylight time steps of high-quality (HQ) which were used in the application of SK10 and TH08 are shown, where for SK10 only a good or intermediate quality flag (after Mauder et al., 2013) and no precipitation were required, and for TH08 additionally a negative $\rho_{q'c'}$ ~~had to be given~~. Furthermore, the ~~relative~~ fraction of these HQ-time steps, for which partitioning solutions were found, is shown for each method version. With TH08 by sampling in the first quadrant (Q1) a partitioning result could be obtained for almost every time step (minimum of 98.2%). With the hyperbolic threshold criteri~~a~~on and with GMM fewer solutions could be found, because quite often the number of sampled data points was less than 1% of the total number in one half-hour time period. SK10 sometimes could not find a partitioning solution, when the measured and estimated $\rho_{q'c'}$ were not equal and removing large-scale processes by Wavelet-transform could not help either to solve the system of equations. The most solutions were found for Forest_MMP~~_FR (forest)~~ and the least for Grass_RO~~_GL (grassland)~~, suggesting a dependence on vegetation height. For crop sites Maize_DI~~_CL_MA~~ and SugarBeet_SE~~, CL_SB~~ the number of solutions with SK10 increased with development stage of the maize or sugar beet, respectively, while the ratio between measurement height and h_c decreased. At the same sites the number of solutions for TH08 with hyperbolic threshold and GMM decreased (the conditional sampling in Q1 was not affected). Generally, for the grasslands and the lower crop canopies more solutions were obtained with TH08 than SK10. An exception was the low intercrop in Selhausen (Intercrop_SE~~_CL_IC~~).

Supplement Link.

Competing interests. The authors declare that they have no conflict of interest.

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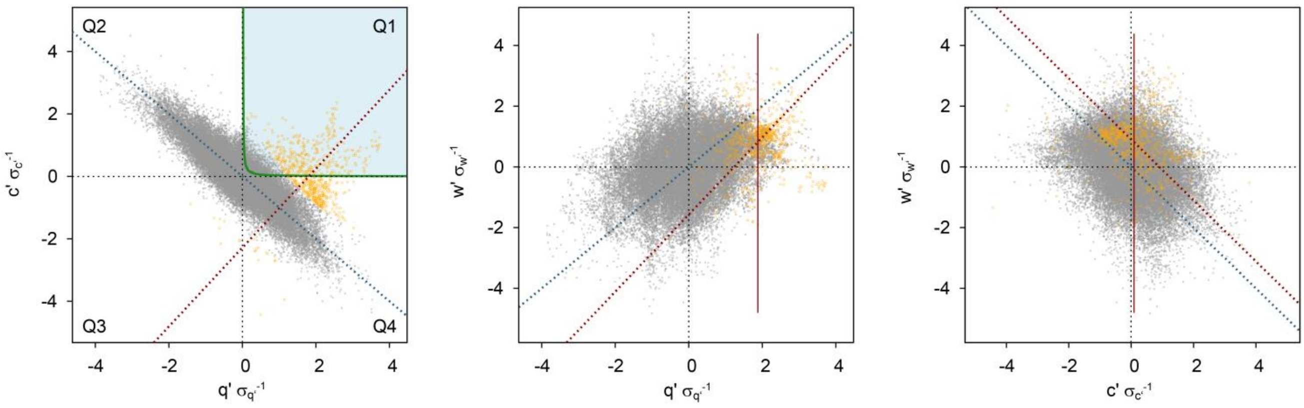
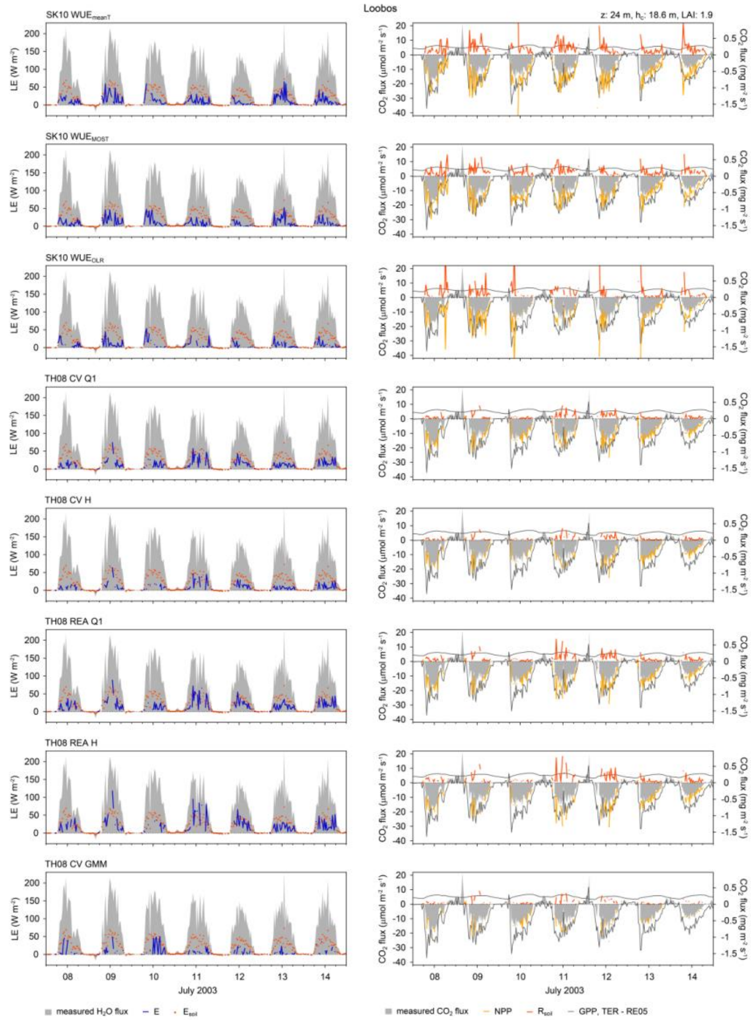


Figure 1: Exemplary scatterplots of *w'*, *q'*, and *c'* from the Wüstebach study site (forest)WU_FR, 18 May 2015, 12:00-12:30 p.m. including results of the cluster analysis by Gaussian Mixture Model (orange data points) for the conditional sampling. Also shown are the hyperbolic threshold (H = 0.25, green line) after Thomas et al. (2008), the averages of *q* and *c* only considering data points of the respiration/evaporation 'cloud' (red lines), and reduced major axis regression lines after Webster (1997) for all data points (blue dashed lines) and only 'cloud' data points (red dashed lines).
In this example, calculating the covariance for *w* and *c* considering the CO_2 average of the 'cloud' yielded a negative soil flux (negative correlation). Thus, only 'cloud' data points within quadrant 1 in the original *q'-c'* plane were considered for flux calculation using averages of all data points.


Loobos
z: 24 m, h_c: 18.6 m, LAI: 1.9
SK10 WUE_{meanT}
SK10 WUE_{MOST}
SK10 WUE_{OLR}
TH08 CV Q1
TH08 CV H
TH08 REA Q1
TH08 REA H
TH08 CV GMM
LE (W m^{-2})
CO_2 flux (µmol m^{-2} s^{-1})
CO_2 flux (mg m^{-2} s^{-1})
08
09
10
11
12
13
14
July 2003
measured H_2O flux
E
E_{soil}
measured CO_2 flux
NPP
R_{soil}
GPP, TER - RE05

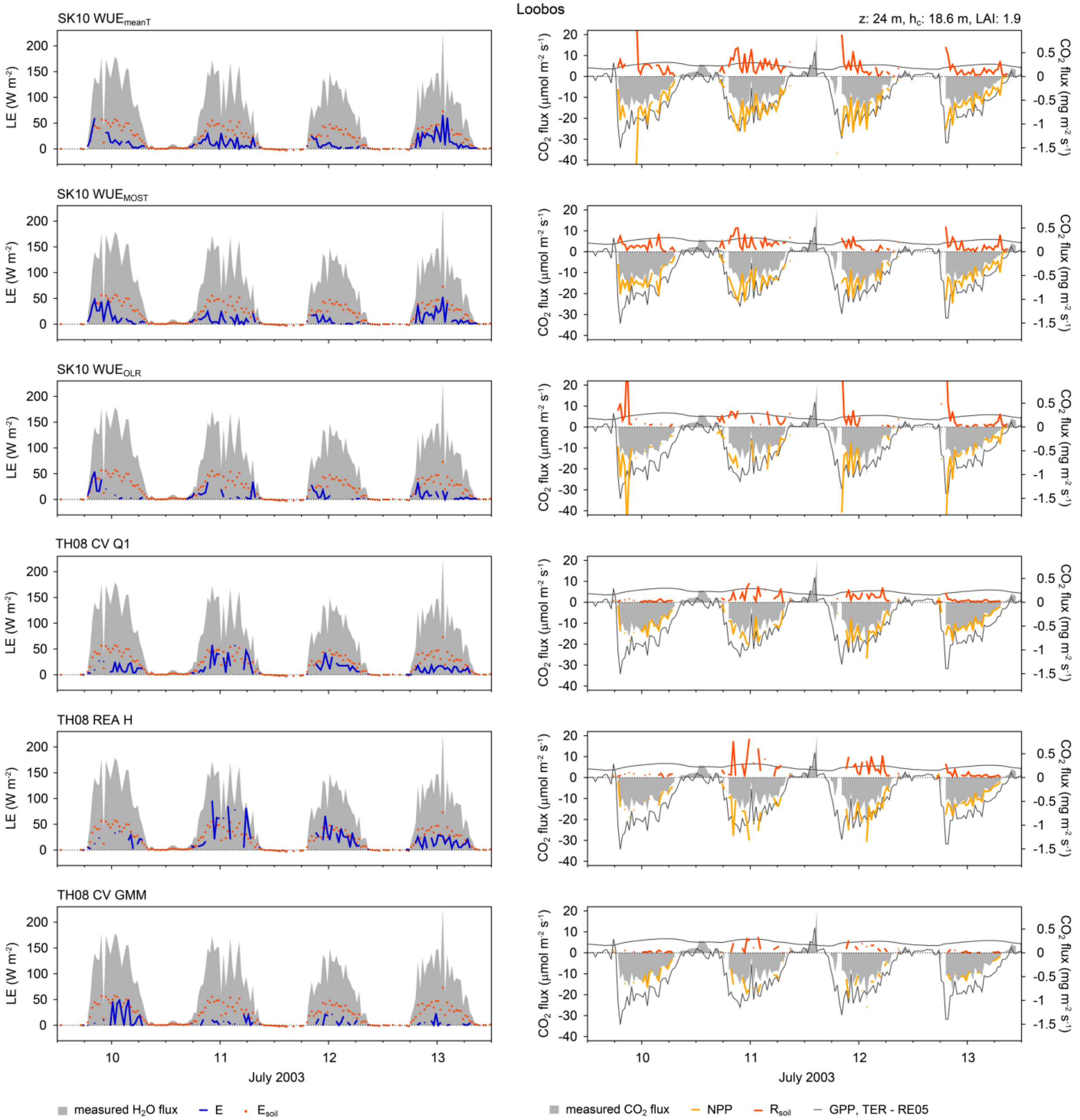
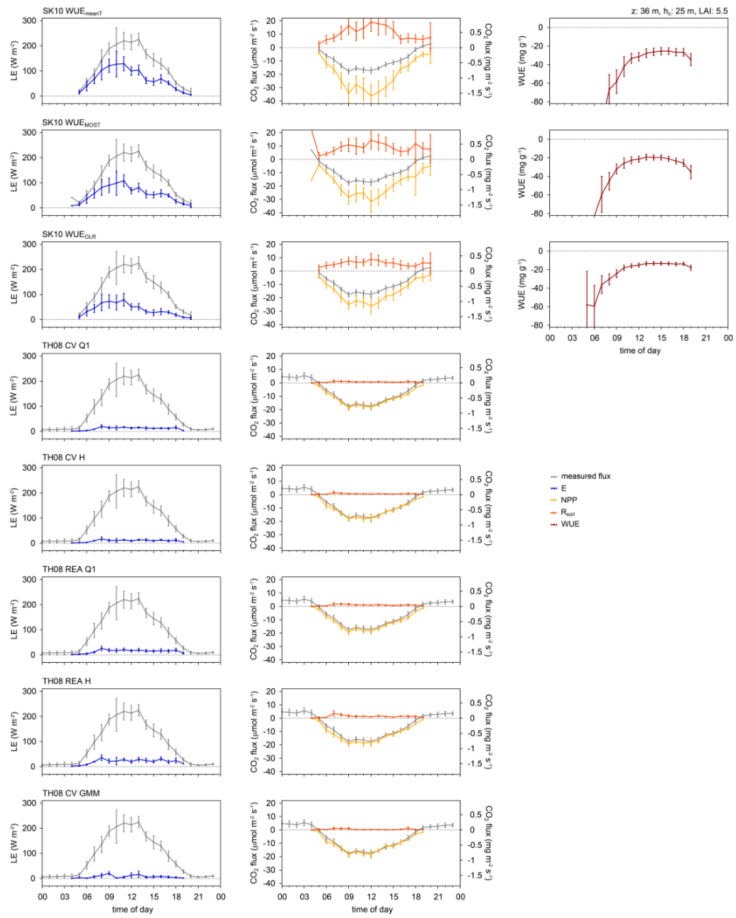


Figure 2: Source partitioning results of H_2O (left) and CO_2 (right) fluxes in half-hourly time steps for the Loobos study site (forest) in The Netherlands. The figure shows four days out of the considered time period and selected method versions (see text for description). Results of all days and for every method version are shown in the supplementary material. (see text for description). Grey areas show the measured water and CO_2 fluxes. Soil evaporation estimates derived based on Beer's law and CO_2 flux estimates by Reichstein et al. (2005; RE05) are also included (LE: latent heat flux; E: evaporation; E_{soil}: estimated soil evaporation; GPP: gross primary production; NPP: net primary production; TER: total ecosystem respiration; R_{soil}: soil respiration; z: measurement height; h_c: canopy height; LAI: leaf area index).


SK10 WUE$_{meanT}$
SK10 WUE$_{MOST}$
SK10 WUE$_{OLR}$
TH08 CV Q1
TH08 CV H
TH08 REA Q1
TH08 REA H
TH08 CV GMM
z: 36 m, h$_c$: 25 m, LAI: 5.5
LE (W m^{-2})
CO_2 flux (µmol m^{-2} s^{-1})
CO_2 flux (mg m^{-2} s^{-1})
WUE (mg g^{-1})
time of day
measured flux
E
NPP
R$_{soil}$
WUE

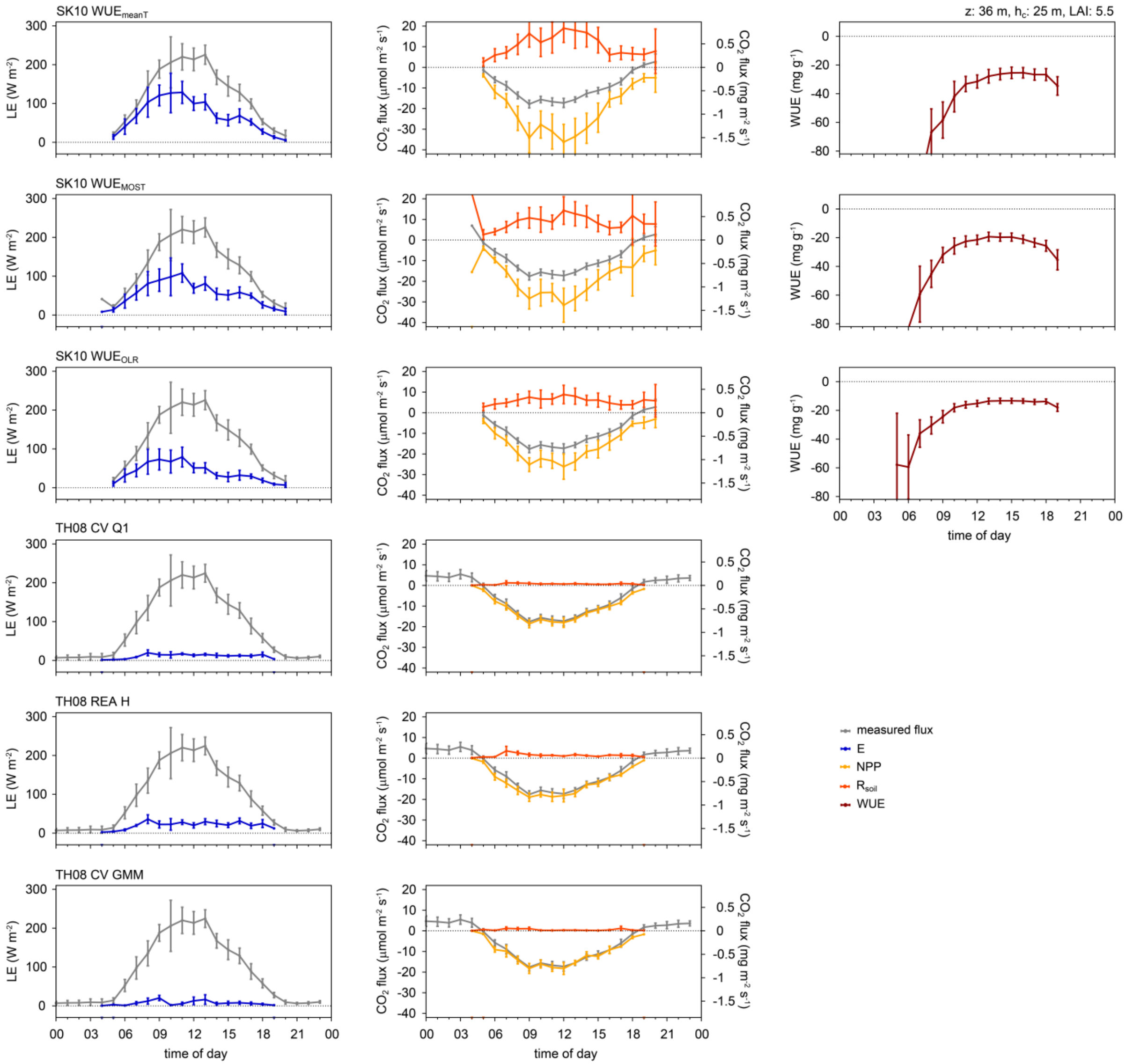
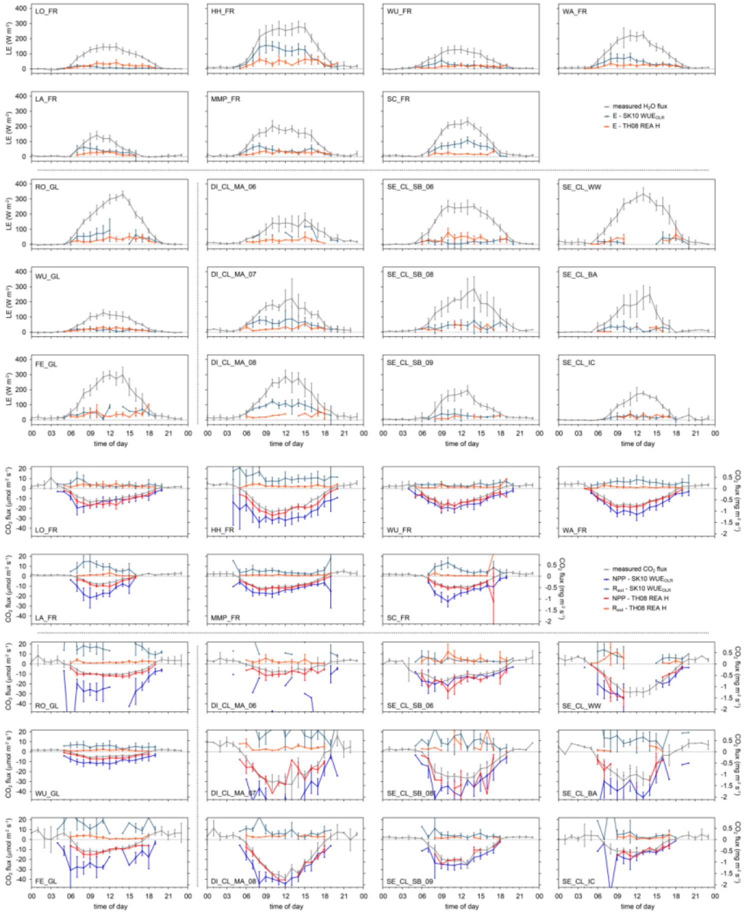


Figure 3: Diurnal dynamics of source partitioning results of H_2O (left) and CO_2 (middle) fluxes and water use efficiency (WUE, right) for the Waldstein study site (forest) in Germany for 4-10 July, 2016 and for ~~every~~selected method versions (see text for description; LE: latent heat flux; E: evaporation; NPP: net primary production; R_{soil}: soil respiration; z: measurement height; h_c: canopy height; LAI: leaf area index). Error bars indicate the 95% confidence intervals of the mean values.


LO_FR
HH_FR
WU_FR
WA_FR
LA_FR
MMP_FR
SC_FR
measured H2O flux
E - SK10 WUE_OLR
E - TH08 REA H
RO_GL
DI_CL_MA_06
SE_CL_SB_06
SE_CL_WW
WU_GL
DI_CL_MA_07
SE_CL_SB_08
SE_CL_BA
FE_GL
DI_CL_MA_08
SE_CL_SB_09
SE_CL_IC
LE (W m-2)
time of day
measured CO2 flux
NPP - SK10 WUE_OLR
R_soil - SK10 WUE_OLR
NPP - TH08 REA H
R_soil - TH08 REA H
CO2 flux (µmol m-2 s-1)
CO2 flux (mg m-2 s-1)

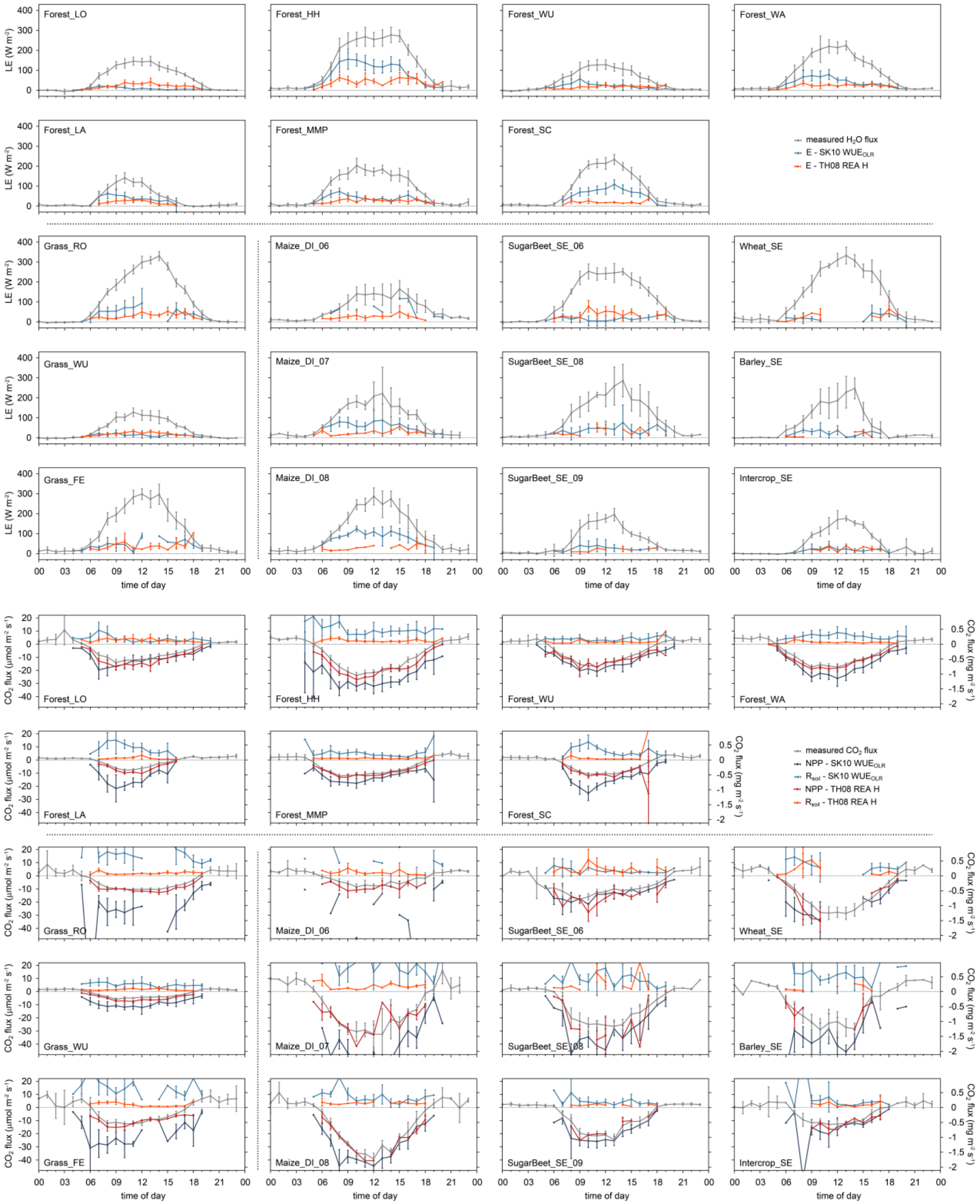
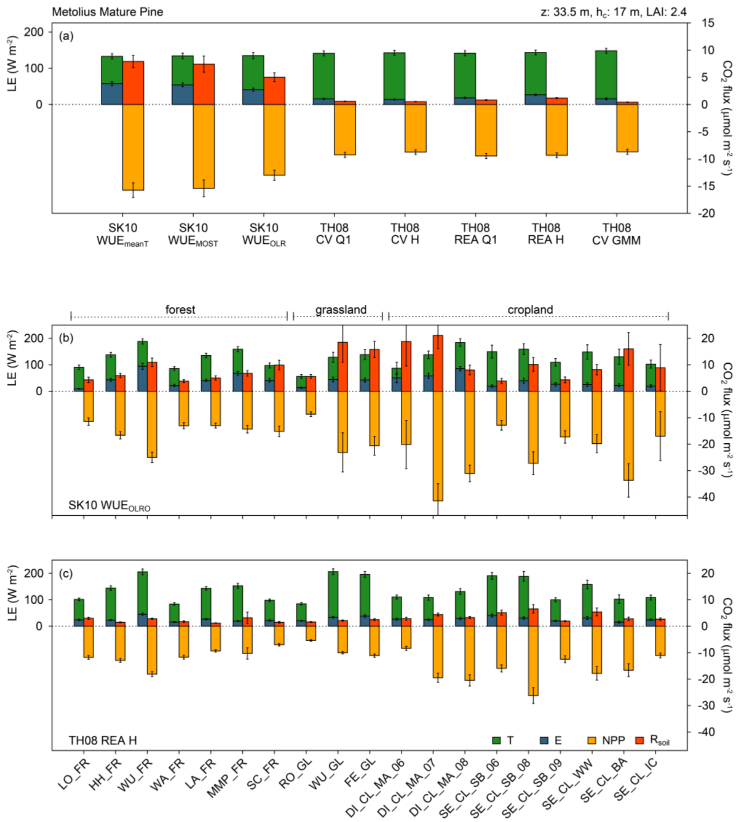


Figure 4: Diurnal dynamics of source partitioning results of H_2O (upper panels) and CO_2 (lower panels) fluxes for all study sites and for the approach after Scanlon and Kustas (2010; SK10) with WUE_{OLR} and after Thomas et al. (2008; TH08) with REA H (see text for description; LE: latent heat flux; E: evaporation; NPP: net primary production; R_{soil}: soil respiration). Error bars indicate the 95% confidence intervals of the mean values.



Metolius Mature Pine
z: 33.5 m, h_c: 17 m, LAI: 2.4
(a)
LE (W m^{-2})
CO_2 flux (µmol m^{-2} s^{-1})
SK10 WUE_{meanT}
SK10 WUE_{MOST}
SK10 WUE_{OLR}
TH08 CV Q1
TH08 CV H
TH08 REA Q1
TH08 REA H
TH08 CV GMM
forest
grassland
cropland
(b)
SK10 WUE_{OLRO}
(c)
TH08 REA H
T
E
NPP
R_{soil}
LO_FR
HH_FR
WU_FR
WA_FR
LA_FR
MMP_FR
SC_FR
RO_GL
WU_GL
FE_GL
DI_CL_MA_06
DI_CL_MA_07
DI_CL_MA_08
SE_CL_SB_06
SE_CL_SB_08
SE_CL_SB_09
SE_CL_WW
SE_CL_BA
SE_CL_IC

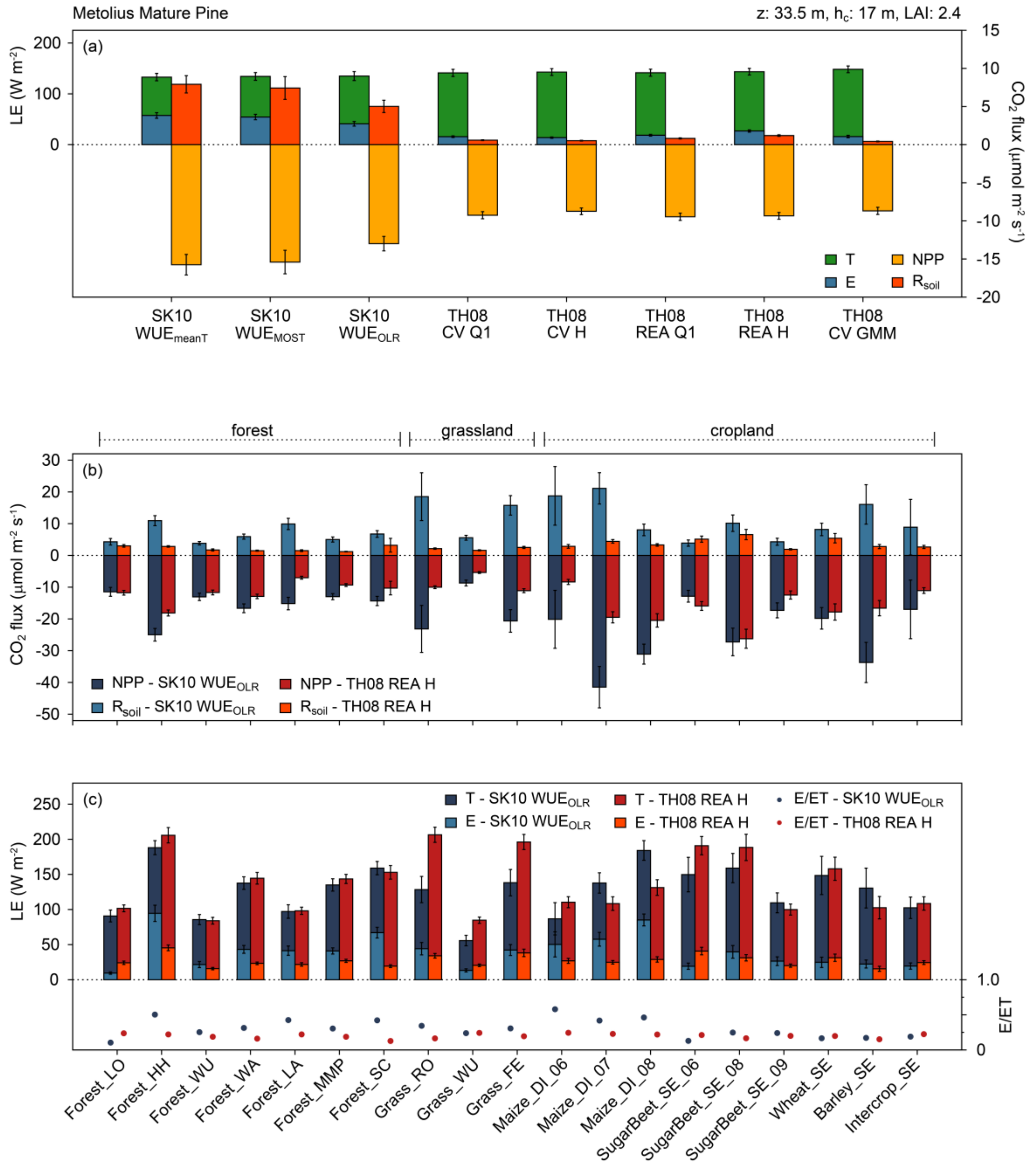
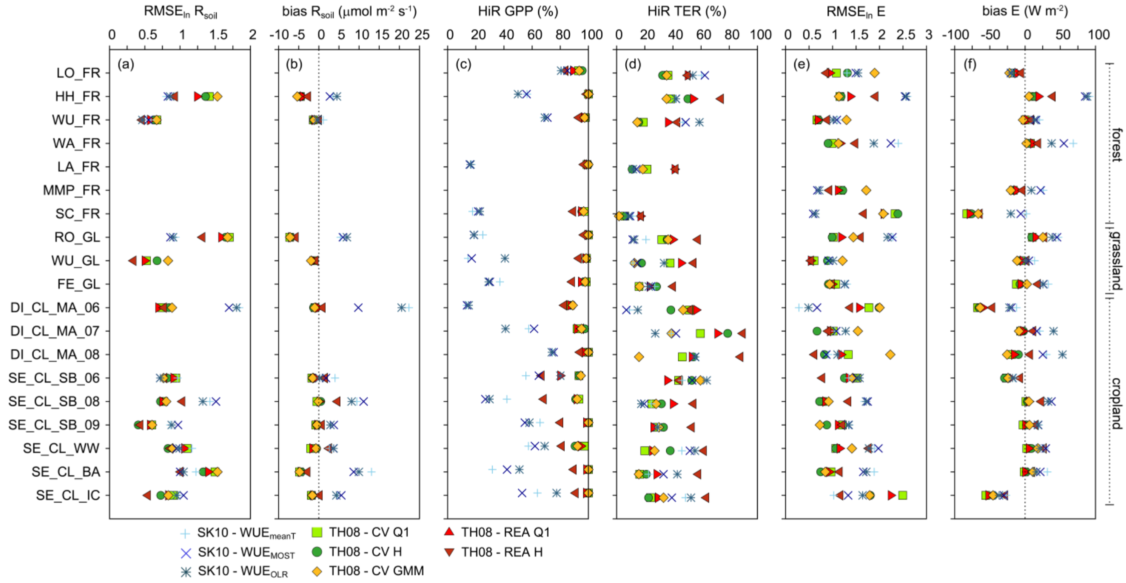


Figure 5: Averages of source partitioning results (a) of H_2O and CO_2 fluxes, (a) for the Metolius Mature Pine study site (forest) in US and for allevery method versions, (b) of CO_2 fluxes, for all study sites and for the approaches after Scanlon and Kustas (2010; SK10) with WUE_{OLR}, and (c) after Thomas et al. (2008; TH08) with REA H, and (c) of H_2O fluxes and the partitioning fraction E/ET, for all study sites and for the approaches SK10 WUE_{OLR} and TH08 REA H (see text for description; LE: latent heat flux; E: evaporation; NPP: net primary production; R_{soil}: soil respiration; z: measurement height; h_c: canopy height; LAI: leaf area index). Error bars indicate the 95% confidence intervals of the mean values. For each study site, net fluxes (evapotranspiration and net ecosystem exchange) differ between method versionsthe two lower panels, because each method version found a different number of partitioning solutions, thus, the averages were taken from different subsets of the original data.



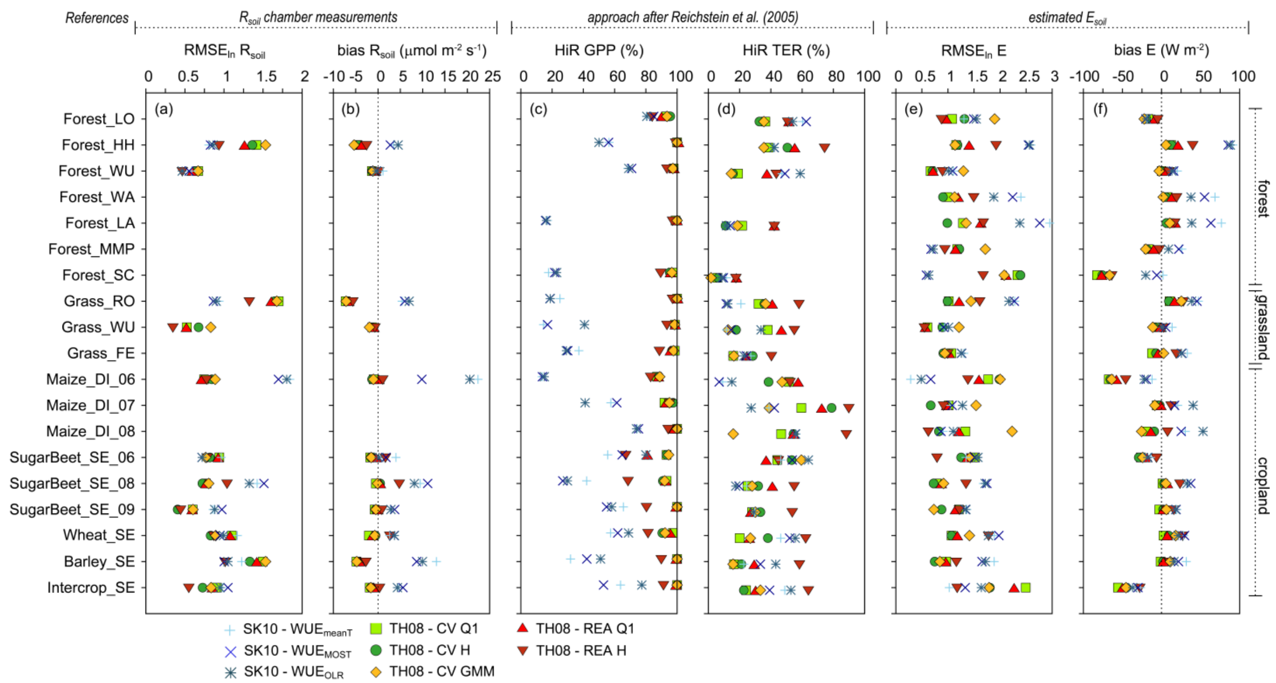


Figure 6: Error ~~quantities~~ metrics of source partitioning results for each study site and method version (see text for description). (a)-(b) Root mean square error in log-transformed data (RMSE$_{ln}$) and bias considering soil respiration (R_{soil}) chamber measurements, (c)-(d) percent~~relative~~ fraction of time steps with partitioning results in range (HiR) of estimated gross primary production (GPP) and total ecosystem respiration (TER) by the approach after Reichstein et al. (2005), (e)-(f) RMSE$_{ln}$ and bias considering soil evaporation (E_{soil}) estimated based on Beer's law.

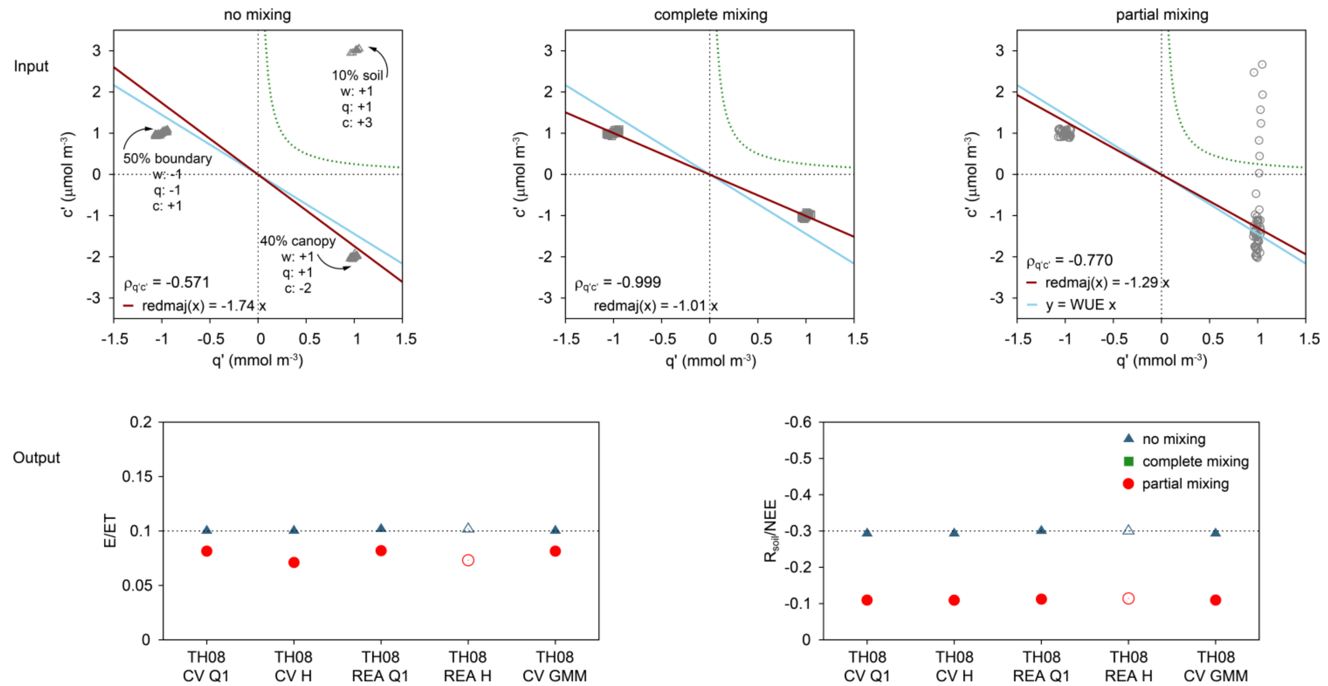


Figure 7: Top: Setup of conceptual model for synthetic fluctuations (*q'* and *c'*) originating from soil, canopy, or boundary layer with differing degrees of mixing (no, complete, or partial mixing between soil and canopy sink/source) including water use efficiency (WUE = -1.444 µmol mmol^{-1} = -3.53 mg g^{-1}; blue line), reduced major axis regression (red line) after Webster (1997), hyperbolic threshold criterion~~a~~ after Thomas et al. (2008; TH08) (H = 0.25; green dashed line) and correlation coefficient between *q'* and *c'* ($\rho_{q'c'}$). Bottom: True known partitioning ratios (dashed line) and source partitioning results of all TH08 method versions (see text for description) for each degree of mixing.

Table 1: Study sites and their characteristics (organized by first canopy type and second latitude; FR: forest; GL: grassland; CL: cropland).

abbrevi-ation	site	Latitude Longitude	elevation (m a.s.l.)	canopy type	period	LAI (m^2 m^{-2})	canopy height (m)	EC meas height (m)	mean annual Temp (°C)	mean annual P sum (mm a^{-1})	prevail-ing wind direction	references
Forest_LO_FR	**Loobos**	52.1666581	25	**FR** (pine)	08.-14. July 2003	1.9	18.6	24.0	10.0	966	W-SW	Dolman et al., 2002
	NetherGelderlands, NL	5.74366556										Elbers et al., 2011
Forest_HH_FR	**Hohes Holz**	52.085306	210	**FR** (deciduous broadleaf)	03.-09. July 2016	6.0	33.0	49.0	9.8	516	SW	Wollschläger et al., 2017
	GermanyST, DE	11.222233										
Forest_WU_FR	**Wüstebach (forest)**	50.504907	610	**FR** (spruce)	18.-24. May 2015	3.9	25.0	38.0	7.5	1220	SSW	Ney et al., in review
	GermanyNRW, DE	6.331019										Graf et al., 2014
Forest_WA_FR	**Waldstein**	50.14194	775	**FR** (spruce)	04.-10. July 2016	5.5	25.0	36.0	5.8	885	SSW	Babel et al., 2017
	GermanyBY, DE	11.86694										Foken et al., 2017
Forest_LA_FR	**Lackenberg**	49.0996177	1308	**FR** (spruce/grass)	24.-30. September 2017	6.0*-	3.0	9.0	3.7	1480	SSW	Lindauer et al., 2014
	GermanyBY, DE	13.3047667										Matiu et al., 2017
Forest_MMP_FR	**Metolius Mature Pine**	44.4523	1253	**FR** (pine)	06.-12. June 2014	2.4	17.0	33.5	6.3	523	SSW	Thomas et al., 2009
	OregonPNW, USA	-121.5574										Vickers et al., 2012
Forest_SC_FR	**Sta. Clotilde**	38.210142	736	**FR** (oak savanna)	01.-07. April 2017	1.0	8.5	18.0	15.3	720	SW	Andreu et al., 2018
	SpainAndalusia, ES	-4.2875495										
Grass_RO_GL	**Rollesbroich**	50.621914	515	**GL**	15.-21. July 2013	5.9	0.19	2.6	7.7	1033	SSW	Borchard et al., 2015
	GermanyNRW, DE	6.304126										Gebler et al., 2015
Grass_WU_GL	**Wüstebach (clear cut)**	50.503046	610	**GL** (deforested area)	18.-24. May 2015	< 2.5	0.25	2.5	7.5	1220	SSW	Ney et al., in review
	GermanyNRW, DE	6.335946										Wiekenkamp et al., 2016
Grass_FE_GL	**Fendt**	47.8329	595	**GL**	11.-17. July 2015	3.5	0.25	3.5	8.4	1081	SW	Zeeman et al., 2017
	GermanyBY, DE	11.0607										
Maize_DI_CL_MA_06	**Dijkgraaf**	51.9921061	9	**CL** (maize)	14.-16. June 2007	0.35	0.35	4.0	10.5	803	S-SW	Jans et al., 2010
Maize_DI_CL_MA_07	NetherlGelderlands, NL	5.645944			14.-16. July 2007	3.5	1.70					
Maize_DI_CL_MA_08					04.-06. August 2007	3.0	2.80					
Wheat_SE_CL_WW	**Selhausen**	50.8658339	103	**CL** (winter wheat)	03.-05. June 2015	6.1	0.79	2.4	9.9	698	WSW	Eder et al., 2015
Barley_SE_CL_BA	GermanyNRW, DE	6.44743888		(barley)	27.-29. May 2016	5.1	0.95					Ney and Graf, 2018

Intercrop_SE_CL_IC	(intercrop)	23.-25. September 2016	1.0	0.22
SugarBeet_SE_CL_SB_06	(sugar beet)	20.-22. June 2017	2.3	0.37
SugarBeet_SE_CL_SB_08		02.-04. August 2017	5.2	0.46
SugarBeet_SE_CL_SB_09		04.-06. September 2017	4.3	0.50

LAI: leaf area index; EC: eddy covariance; meas: measurement; T: temperature; P: precipitation

* LAI estimated based on remotely sensed plant phenology index (PPI; Matiu et al., 2017) and approach after Jin and Eklundh (2014)

Table 2: Correlation coefficients between partitioning performance of each method version regarding HiR GPP (see text for description) and study site characteristics (h_c: canopy height; LAI: leaf area index; z: measurement height) considering different sets of sites: all, only forest, or only crop- and grassland sites. Bold lettering indicates highest positive and highest negative correlation. U~~, and u~~nderlined ~~(italic)~~ lettering indicates highest ~~(lowest)~~ magnitude of correlation and italic lettering lowest magnitude of correlation. Also, the statistical significance of the correlations is indicated with one asterisk for $p \leq 0.1$ and two asterisks for $p \leq 0.05$.

variable	SK10 WUE_{meanT}	SK10 WUE_{MOST}	SK10 WUE_{OLR}	TH08 CV Q1	TH08 CV H	TH08 REA Q1	TH08 REA H	TH08 CV GMM
all								
h_c	0.52 **	0.56 **	0.44 *	0.21	0.27	0.28	0.45 *	0.23
LAI	0.04~~0.15~~	0.01~~0.12~~	0.08~~-0.02~~	0.44~~0.43~~ *	0.25~~0.21~~	0.45~~0.43~~ *	0.17~~0.12~~	0.30~~0.26~~
z	0.48 **	0.52 **	0.40 *	0.23	0.27	0.31	0.48 **	0.25
z h_c^{-1}	-0.51 **	-0.60 **	-0.45 *	-0.11	-0.15	-0.13	-0.15	-0.10
LAI h_c^{-1}	-0.38~~-0.44~~	-0.47~~-0.53~~ **	-0.41~~-0.47~~ *	0.18~~0.19~~	0.03~~0.05~~	0.09~~0.11~~	-0.13~~-0.11~~	0.09~~0.12~~
forests								
h_c	0.64	0.63	0.56	0.20	0.21	0.21	0.27	0.11
LAI	0.03~~-0.35~~	0.07~~-0.32~~	0.10~~-0.26~~	0.61	0.77~~0.74~~ **	0.68 *	0.69~~0.70~~ *	0.69~~0.65~~ *
z	0.62	0.60	0.55	0.37	0.31	0.36	0.41	0.27
z h_c^{-1}	-0.74 *	-0.75 *	-0.68 *	0.27	0.25	0.28	0.20	0.37
LAI h_c^{-1}	0.59~~-0.35~~	0.61~~-0.33~~	0.59~~-0.34~~	0.19~~0.77~~	0.38~~0.78~~	0.26~~0.81~~	0.22~~0.83~~	0.36~~0.79~~
croplands, grasslands								
h_c	0.54 *	0.64 **	0.33	0.07	0.23	0.12	0.31	0.16
LAI	0.07	0.05	-0.10	0.40	0.10	0.37	-0.03	0.15
z	0.02	0.07	-0.29	-0.44	-0.11	-0.17	0.37	-0.23
z h_c^{-1}	-0.58 **	-0.71 **	-0.51 *	-0.01	-0.01	0.03	0.17	0.03
LAI h_c^{-1}	-0.37	-0.49	-0.46	0.37	0.21	0.32	0.16	0.28

Table 3: Correlation coefficients between partitioning performance of each method version regarding HiR TER (see text for description) and study site characteristics (h_c: canopy height; LAI: leaf area index; z: measurement height) considering different sets of sites: all, only forest, or only crop- and grassland sites. Bold lettering indicates highest positive and highest negative ~~correlatio~~correlation. U~~n, and u~~nderlined ~~(italic)~~ lettering indicates highest ~~(lowest)~~ magnitude of correlation and italic lettering lowest magnitude of correlation. Also, the statistical significance of the correlations is indicated with one asterisk for $p \leq 0.1$ and two asterisks for $p \leq 0.05$.

variable	SK10 WUE_{meanT}	SK10 WUE_{MOST}	SK10 WUE_{OLR}	TH08 CV Q1	TH08 CV H	TH08 REA Q1	TH08 REA H	TH08 CV GMM
all								
h_c	**0.52** **	**0.52** **	**0.47** **	-0.12	-0.18	**0.17**	*0.01*	-0.23
LAI	*0.01~~0.11~~*	*0.06~~0.16~~*	*-0.03~~0.07~~*	**-0.20~~-0.17~~**	0.04~~0.13~~	*-0.01~~-0.02~~*	**0.24~~0.33~~**	*-0.12~~-0.09~~*
z	0.48 **	0.47 **	0.44 *	-0.17	**-0.24**	0.12	-0.06	**-0.27**
z h_c^{-1}	**-0.47** **	**-0.57** **	**-0.42** *	**0.08**	*-0.01*	-0.14	**-0.15**	**0.30**
LAI h_c^{-1}	~~-0.42~~-0.37	~~-0.50~~-0.44 *	~~-0.47~~-0.41 *	*~~-0.08~~-0.06*	**~~0.03~~0.06**	**-0.21**	~~-0.06~~-0.04	~~0.17~~0.18
forests								
h_c	**0.63**	**0.63**	0.63	**0.59**	**0.68** *	0.56	**0.76** **	**0.43**
LAI	*~~0.34~~-0.02*	*~~0.38~~0.02*	*~~0.41~~0.05*	~~0.53~~0.43	~~0.51~~0.31	**~~0.65~~0.61**	~~0.82~~0.65	~~0.31~~0.28
z	0.60	0.59	**0.64**	0.46	0.60	0.41	0.72 *	0.30
z h_c^{-1}	**-0.72** *	**-0.73** *	**-0.66**	**-0.48**	**-0.52**	**-0.39**	**-0.47**	**-0.35**
LAI h_c^{-1}	~~0.32~~-0.56	~~0.36~~-0.54	~~0.46~~-0.53	*~~0.19~~-0.07*	*~~0.10~~-0.26*	*~~0.33~~0.09*	*~~0.61~~-0.13*	*-~~0.11~~0.01*
croplands, grasslands								
h_c	**0.54** *	**0.59** **	**0.34**	0.42	**0.61** **	0.50 *	**0.85** **	-0.25
LAI	*0.01*	0.06	*-0.13*	**-0.49**	*-0.04*	**-0.33**	*0.03*	**-0.32**
z	0.04	*0.01*	-0.23	**0.64** **	0.59 **	**0.70** **	0.48	*-0.03*
z h_c^{-1}	**-0.48**	**-0.66** **	-0.47	*-0.16*	**-0.45**	*-0.20*	**-0.59** **	**0.12**
LAI h_c^{-1}	-0.34	-0.47	**-0.47**	-0.36	-0.30	-0.31	-0.37	-0.06

Table A1: Count of half-hourly time steps during daylight (CoD) per considered time period for each study site, corresponding ~~relative~~ percent fractions of CoD of high-quality (HQ) and percent~~relative~~ fractions of these HQ-time steps with a found partitioning solution for each method version. ~~Blue (red) lettering indicates the highest (lowest) fraction of solutions for each site.~~ Bold (italic) lettering indicates the highest (lowest) fraction of solutions for each site. P~~Superscript asterisk~~lus (minus) indicates the highest (lowest) fraction for each method version.

method	site / time period	CoD	rel CoD used (HQ)	rel HQ with partitioning solution	site / time period	CoD	rel CoD used (HQ)	rel HQ with partitioning solution
SK10 WUE_{meanT}				84.4				26.2
SK10 WUE_{MOST}			91.8	82.1			84.8	34.5
SK10 WUE_{OLR}	**Forest_LO~~_FR~~**	231		65.6	**Maize_DI_~~CL_MA_~~06**	99		*23.8* -
TH08 CV Q1, REA Q1	08.-14.07.2003			**99.4**	14.-16.06.2007			**98.4**
TH08 CV H, REA H			68.0	86.0			63.6	82.5
TH08 CV GMM				*59.2*				57.1
SK10 WUE_{meanT}				75.7				90.4
SK10 WUE_{MOST}			89.2	76.2			97.9	88.3
SK10 WUE_{OLR}	**Forest_HH~~_FR~~**	231		74.8	**Maize_DI_~~CL_MA_~~07**	96		77.7
TH08 CV Q1, REA Q1	03.-09.07.2016			**100.0** +	14.-16.07.2007			**98.7**
TH08 CV H, REA H			59.7	55.8			78.1	*50.7*
TH08 CV GMM				*51.4*				52.0
SK10 WUE_{meanT}				80.6				95.3 +
SK10 WUE_{MOST}			78.0	78.8			94.5	94.2
SK10 WUE_{OLR}	**Forest_WU~~_FR~~**	218		70.6	**Maize_DI_~~CL_MA~~_08**	91		89.5
TH08 CV Q1, REA Q1	18.-24.05.2015			**100.0** +	04.-06.08.2007			**100.0** +
TH08 CV H, REA H			55.5	74.4			80.2	*45.2*
TH08 CV GMM				*51.2*				57.5
SK10 WUE_{meanT}				88.3				57.3
SK10 WUE_{MOST}			92.8	91.7			92.7	57.3
SK10 WUE_{OLR}	**Forest_WA~~_FR~~**	222		89.3	**SugarBeet_SE~~_CL_SB~~_06**	96		52.8
TH08 CV Q1, REA Q1	04.-10.07.2016			**100.0** +	20.-22.06.2017			**98.6**
TH08 CV H, REA H			75.2	65.9			76.0	58.9
TH08 CV GMM				*50.3*				*47.9*
SK10 WUE_{meanT}				*33.3*				72.9
SK10 WUE_{MOST}			84.1	38.4			77.8	71.4
SK10 WUE_{OLR}	**Forest_LA~~_FR~~**	164		56.5	**SugarBeet_SE_~~CL_SB_~~08**	90		72.9
TH08 CV Q1, REA Q1	24.-30.09.2017			**100.0** +	02.-04.08.2017			**100.0** +
TH08 CV H, REA H			54.9	93.3 +			62.2	*37.5*
TH08 CV GMM				58.9				41.1
SK10 WUE_{meanT}				95.0				80.6
SK10 WUE_{MOST}			84.8	95.0 +			92.3	81.9
SK10 WUE_{OLR}	**Forest_MMP~~_FR~~**	211		93.3 +	**SugarBeet_SE~~_CL_SB~~_09**	78		81.9
TH08 CV Q1, REA Q1	06.-12.06.2014			**100.0** +	04.-06.09.2017			**98.3**
TH08 CV H, REA H			73.0	70.8			76.9	25.0 -
TH08 CV GMM				*60.4*				*16.7* -
SK10 WUE_{meanT}		175	87.4	73.9		96	93.8	56.7
SK10 WUE_{MOST}				75.2				52.2

method	site / time period	CoD	rel CoD used (HQ)	rel HQ with part-itioning solution	site / time period	CoD	rel CoD used (HQ)	rel HQ with part-itioning solution
SK10 WUE_{OLR}	**Forest_SC~~_FR~~**			77.1	**Wheat_SE~~_CL_WW~~**			46.7
TH08 CV Q1, REA Q1	01.-07.04.2017			**99.3**	03.-05.06.2015			**98.6**
TH08 CV H, REA H			77.7	47.1			77.1	*25.7*
TH08 CV GMM				*40.4*				32.4

(continued)

Table A1 continued:

method	site / time period	CoD	rel CoD used (HQ)	rel HQ with part-itioning solution	site / time period	CoD	rel CoD used (HQ)	rel HQ with part-itioning solution
SK10 WUE_{meanT}				*21.1* -				50.6
SK10 WUE_{MOST}			91.7	32.7 -			82.3	51.9
SK10 WUE_{OLR}	**Grass_RO~~_GR~~**	217		28.6	**Barley_SE~~_CL_BA~~**	96		58.2
TH08 CV Q1, REA Q1	15.-21.07.2013			**100.0** +	27.-29.05.2016			**98.5**
TH08 CV H, REA H			73.3	53.5			67.7	*26.2*
TH08 CV GMM				53.5				27.7
SK10 WUE_{meanT}				*31.3*				64.6
SK10 WUE_{MOST}			82.1	38.0			91.5	70.8
SK10 WUE_{OLR}	**Grass_WU~~_GR~~**	218		40.8	**Intercrop_SE~~_CL_IC~~**	71		73.8
TH08 CV Q1, REA Q1	18.-24.05.2015			**100.0** +	23.-25.09.2016			**98.2** -
TH08 CV H, REA H			58.7	90.6			80.3	35.1
TH08 CV GMM				88.3 +				*28.1*
SK10 WUE_{meanT}				*34.8*				
SK10 WUE_{MOST}			82.0	36.0				
SK10 WUE_{OLR}	**Grass_FE~~_GR~~**	217		39.9				
TH08 CV Q1, REA Q1	11.-17.07.2015			**100.0** +				
TH08 CV H, REA H			58.5	46.5				
TH08 CV GMM				65.4				