The importance of radiation for semi-empirical water-use efficiency models

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Abstract

Water-use efficiency (WUE) is a fundamental property for the coupling of carbon and water cycles in plants and ecosystems. Existing model formulations predicting this variable differ in the type of response of WUE to the atmospheric vapor pressure deficit of water (VPD). We tested a representative WUE model on ecosystem scale at 110 eddy-covariance sites of the

10 FLUXNET initiative by predicting evapotranspiration (ET) based on gross primary productivity (GPP) and VPD. We found that introducing an intercept term in the formulation increases model performance considerably, indicating that an additional factor needs to be considered. We demonstrate that this intercept term varies seasonally and we subsequently associate it with radiation. Replacing the constant intercept term with a linear function of global radiation was found to further improve model predictions of ET. Our new semi-empirical ecosystem WUE formulation indicates that, averaged over all sites, this

15 radiation term accounts for up to half (40–49 %) of transpiration. These empirical findings challenge the current understanding of water-use efficiency on ecosystem-scale.

1   Introduction

Understanding the coupling of carbon and water cycles is as a central question of Global Change research, as changes in one

20 of the cycles could directly propagate to the other (Churkina et al., 1999; Gerten et al., 2004; Ito & Inatomi, 2012). Carbon assimilation through photosynthesis (*A*) and transpiration (*T*) constitute major fluxes in these two cycles and the Earth system (Jasechko et al., 2013; Ciais et al., 2014). On the leaf-scale, *water-use efficiency* (WUE) is defined as WUE = A/T, quantifying the ability of a plant to assimilate atmospheric carbon dioxide per water loss by transpiration. An understanding of this quantity can hence translate into the ability to predict one of the two fluxes from the other.

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Both fluxes are limited by the stomatal conductance (g_s) of plant leaves (Cowan and Farquhar, 1977), allowing for the definition of *intrinsic water-use efficiency*, $WUE_i = A/g_s$. This quantity is less contingent on the vapor pressure deficit of atmospheric water vapor (VPD) affecting both fluxes differently. At the ecosystem scale, neither carbon assimilation nor transpiration can be observed directly. However, the eddy-covariance (EC) method (Baldocchi et al., 2001) can be used to

obtain data of the gross-primary productivity (GPP) and the evapotranspiration (ET). On ecosystem scale, water-use efficiency is then defined as WUE = GPP/ET, while the intrinsic water-use-efficiency is accordingly formulated as WUE_i = GPP/G_s, where G_s denotes the surface conductance of the ecosystem.

5 Analytical models that predict WUE on the leaf-scale (Katul et al., 2010; Medlyn et al., 2011) were derived from theoretical optimality considerations. Corresponding variants were evaluated with ecosystem-scale flux measurements gathered by the FLUXNET in empirical studies (Beer et al., 2009; Zhou et al., 2014; Zhou et al., 2015). The central difference between the existing models is the response of g_s or G_s to VPD, resulting in different dependencies of WUE on VPD. The concept by Beer et al. (2009) assumed an inverse dependency between WUE and VPD due to an increasing diffusion of water vapor 10 with higher values of VPD. On the other hand, physiological models (e.g. Katul et al., 2010), imply stomatal contraction with increasing VPD, as plants aim to minimize water loss. This was found to be an important factor on ecosystem scale as shown by Zhou et al. (2014) for half-hourly and by Zhou et al. (2015) for daily observations. In both studies, the response of WUE could be approximated to be proportional to VPD$^{-0.5}$. Despite their discrepancy, both the models of Beer et al. and Zhou et al. imply that, at ecosystem-scale, WUE is strictly an inverse function of VPD or VPD$^{0.5}$, respectively.

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By contrast, physiological WUE models that were derived on plant scale include an additional conductance term g_0 that is invariable to changing levels of photosynthesis (Ball et al., 1987; Medlyn et al., 2011). Any transpiration resulting from this part of stomatal conductance should be expected to be proportional to the gradient of the partial pressure of water vapor, quantified by the atmospheric VPD observations. This presents a process that current ecosystem-scale WUE models do not 20 accommodate.

Incoming solar radiation is a driving factor for both photosynthesis and transpiration, yet in the existing WUE model formulations, radiation is not explicitly considered. The models implicitly assume that, at ecosystem-scale, GPP and ET respond equally to changes in radiation and that, therefore, the ratio of both is constant with regard to this factor. However, 25 photosynthesis saturates at high radiation levels (Farquhar et al., 1980), even under well-watered conditions. Models of Potential Evapotranspiration (PET), by contrast, do not include a similar limiting behavior (Leuning et al., 2008). Mechanistically, the process of equilibrium transpiration (Jarvis and McNaughton, 1986) implies that sizeable transpiration can occur even when the leaf is fully decoupled from the atmosphere, i.e. when VPD is very low. This is a second process that current ecosystem WUE models cannot accommodate.

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In this study, we address these unresolved inconsistencies regarding the importance of additional model terms for predictions of ecosystem-scale transpiration. We do this empirically on ecosystem scale by optimizing and assessing different WUE models with FLUXNET observations from 110 globally distributed towers. In our approach, ET is selected as target variable, while the different WUE models utilize GPP as one of multiple explanatory variables. The substantial degree of

correlation between GPP and ET is thus harnessed for the predictions of ET. In a first step, we identify existing biases in ecosystem-scale WUE models. In the next step, these biases are tested for their dependency on VPD and radiation. Lastly, we infer a tentative partitioning of transpiration according to its association with radiation and discuss the substantial magnitude of this metric.

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2   Data & methods

2.1   Data

The daily day-time integrals of gross primary productivity (GPP) and evapotranspiration (ET) were taken from the La Thuile

10   FLUXNET (open and fair use data policy sites) collection (Baldocchi et al., 2001). The aggregation to day-time values was based on values of potential radiation larger than 10 W m^{-2}. Additionally, we used global radiation (Rg) and the day-time vapor pressure deficit (VPD) measured at the same eddy-covariance (EC) sites. For some analyses we further used long-term data of precipitation (P) and potential evapotranspiration (PET) based on a bias-corrected ERA-Interim reanalysis.[1]

15   The EC data were processed according to the standard methods (Papale et al., 2006; Reichstein et al., 2005) to assure consistent quality of the observations. Eddy-covariance GPP results were based on the flux partitioning method of Reichstein (2005). We used only data with GPP > 0.1 gC d^{-1} m^{-2}, ET > 0.05 mm d^{-1} and VPD > 0.001 kPa) to reduce the relatively large impact of random measurement errors under low flux conditions. Following the procedure of Beer et al. (2009) we further used only data after three consecutive rain free days. This reduces contributions by evaporation to the measured

20   evapotranspiration as physical evaporation typically declines rapidly after rain events due to the depletion of water stored in the topmost soil layer (Wythers et al., 1999). That assumption similarly applies to precipitation that is intercepted on leaf-surfaces and other plant parts in the canopy. As Miralles et al. (2010) summarize, the interception storage for forest ecosystems reported in different studies amounted to a mean of 1.2 mm (± 0.4 mm). With the mean interception evaporation rates reported as 0.3 mm h^{-1} (± 0.1 mm h^{-1}), this storage can be concluded to be typically depleted within the first days after a

25   precipitation event. Therefore, the measured evapotranspiration after three consecutive rain free days is expected to approximate transpiration, and we additionally verified that our results are robust when considering longer rain free periods (see below). For the main analysis, we included sites with at least 25 data-points fulfilling the requirements noted above. A list of these 110 sites used for the parameter estimation can be found in the Supplement (S2).

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[1] Harmonized site-observation/ERA-Interim data set derived with the gap-filling tool of Antje Moffat and Olaf Menzler (http://www.bgc-jena.mpg.de/~MDIwork/meteo/)

The presented analyses presume that the observed evapotranspiration is dominated by transpiration after three consecutive rain-free days. To test the robustness of our findings against this assumption, we varied the number of consecutive rain free days from 0 to 14. For each considered step, the data were filtered accordingly and parameters of the WUE models were estimated for each site. We then calculated the mean of the parameter estimates over all sites and the associated uncertainty

5   (95% confidence interval) of the mean via bootstrapping. We excluded some humid sites from this sensitivity analysis for which too few data points were available when filtering for longer rain free periods. This procedure can thus ensure that

When analyzing the collinearity of parameters, we tested to what degree our results were affected by water limitation. The criterion used to classify sites into *arid* and *non-arid* was a cumulative difference between PET and P of more than 300 mm

10   annually.

2.2   Concepts & models

For our analysis, we started out with the WUE model of Zhou et al. (2015), which we converted for an inversion against ET

15   data:

$$\mathrm{ET} \; = \; \frac{\mathrm{GPP} \cdot \mathrm{VPD}^{0.5}}{\mathrm{uWUE}} \qquad\qquad (1)$$

The introduced WUE model states that no transpiration occurs independently from $\mathrm{GPP} \cdot \mathrm{VPD}^{0.5}$. To test this hypothesis, we

20   introduced an intercept term ($\mathrm{ET_{res}}$) in the generic WUE model, which we call $+\mathrm{ET_{res}}$ model:

$$\mathrm{ET} \; = \; \frac{\mathrm{GPP} \cdot \mathrm{VPD}^{0.5}}{\mathrm{uWUE}} + \mathrm{ET_{res}} \; . \qquad\qquad (2)$$

Hence, any significant intercept would indicate transpiration that cannot be explained by $\mathrm{GPP} \cdot \mathrm{VPD}^{0.5}$. The relative

25   contribution of $\mathrm{ET_{res}}$ to the mean predicted flux, C_{ETres}, was calculated as:

$$C_{\mathrm{ETres}} \; = \; \frac{\mathrm{ET_{res}}}{\frac{\mathrm{GPP} \cdot \mathrm{VPD}^{0.5}}{\mathrm{uWUE}} + \mathrm{ET_{res}}} \; , \qquad\qquad (3)$$

where the denominator contains the mean predicted daily ET of the model.

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To further test whether ET_{res} relates to atmospheric variables, we postulated three different alternative models. The residual transpiration could be driven by an additional VPD term that is independent from photosynthesis, as some stomatal conductance models (Medlyn et al., 2011) already include a residual conductance term g_0, in which case the WUE model could take the form:

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$$\mathrm{ET} = \frac{\mathrm{GPP} \cdot \mathrm{VPD}^{0.5}}{\mathrm{uWUE}} + g_0 \cdot \mathrm{VPD} \, . \tag{4}$$

We also considered the possibility that ET_{res} is related to global radiation (Rg):

10 $$\mathrm{ET} = \frac{\mathrm{GPP} \cdot \mathrm{VPD}^{0.5}}{\mathrm{uWUE}} + r \cdot \mathrm{Rg}. \tag{5}$$

To test for possible interactions between the two additional variables, we considered a third alternative where ET_{res} was modelled by included both Rg and VPD as independent factors:

15 $$\mathrm{ET} = \frac{\mathrm{GPP} \cdot \mathrm{VPD}^{0.5}}{\mathrm{uWUE}} + g_0 \cdot \mathrm{VPD} + r \cdot \mathrm{Rg}. \tag{6}$$

In the following, we refer to the reference WUE definition (Eq. 1) as "Zhou". We abbreviate models with additional covariates by omitting the reference to the GPP-VPD-term ($\frac{\mathrm{GPP} \cdot \mathrm{VPD}^{0.5}}{\mathrm{uWUE}}$) of Zhou, which is always used unless denoted otherwise. The model with an additional VPD term, for example, is thus designated "+VPD".

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2.3   Parameter estimation & statistics

In the following, we refer to Eq. 1, 2, 4, 5, 6 as models, as we optimize their fit to the EC data by estimating free parameters.
25 The estimation was conducted with the Levenberg-Marquardt technique, minimizing the sum of squares of the model residuals. The residuals were calculated as the difference between observed and predicted ET. We used the nlsLM package in R (Elzhov *et al.*, 2015). The uncertainties and correlations of the parameters were calculated with the variance-covariance matrix returned by the fitting function (Omlin & Reichert, 1999).

30 The model performance was assessed for each site with the Nash-Sutcliffe model efficiency (MEF):

$$\text{MEF} = 1 - \frac{\sum(Y_{\text{prd}} - Y_{\text{obs}})^2}{\sum(Y_{\text{obs}} - \overline{Y_{\text{obs}}})^2}, \tag{7}$$

where Y_{obs} are observations and Y_{prd} are predictions by a model.

5   A MEF of 1 implies a perfect fit of the model to the data. A MEF below 0 implies that the mean of the observations outperforms the fit of the model. All MEFs were calculated in a *leave-one-out* cross-validation to account for the problem of over-fitting. Thus, the cross-validated MEFs can be used to compare models with differing numbers of free parameters.

2.4   Partitioning of linear models

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To assess the contribution of driving variables to the predicted fluxes, we performed an analysis of attribution to the individual model terms. Consider a simple multiple linear regression model,

$$Y = a_1 \cdot X_1 + a_2 \cdot X_2, \tag{8}$$

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where Y is the dependent variable, X_1 and X_2 are independent variables and a_1 and a_2 denote the model parameters. Due to the additive character of the model, the contribution of one variable (e.g. X_1) to the total flux is given by its product with the slope ($a \cdot X_1$). In our analysis, we tested the contribution of the linear radiation term (Eq. 5) to the total modelled evapotranspiration. Thus we defined the fraction of evapotranspiration that was attributed to the radiation term as:

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$$\text{ET}_{\text{frac}} = \frac{\sum r \cdot \text{Rg}}{\sum \frac{\text{GPP} \cdot \sqrt{\text{VPD}}}{\text{uWUE}} + r \cdot \text{Rg}} \tag{9}$$

We considered two variants to estimate this metric: *parallel* and *hierarchical*. In the first case, both parameters, uWUE and r were estimated in a standard parameter estimation, i.e. concurrently. In the second case, uWUE was first estimated in the

25    $+\text{ET}_{\text{res}}$ model. We then defined a term M as:

$$M = \text{ET}_{\text{res}} + \varepsilon, \tag{10}$$

where ε denotes the residuals and ET_{res} denotes the intercept parameter of the $+\text{ET}_{\text{res}}$ model. The parameter r was then

30   estimated in a linear regression of the form:

$$M = r \cdot Rg + c,\qquad\qquad(11)$$

where c denotes a constant intercept. By giving precedence to the uWUE parameter in this approach, we expect to get an estimate of a reasonable lower bound for ET_{frac}. All parameters were constrained to positive values.

To further assess uncertainties due to problems of parameter identifiability among uWUE and r in the *parallel* variant, we sampled 200 parameter vectors from the posterior parameter uncertainty distribution for each site (See Supplement S1 for a full description of the applied procedure).

3   Results

In our analysis we tested different water-use efficiency (WUE) models that predicted evapotranspiration (ET) using the product of gross-primary productivity (GPP) and the water vapor pressure deficit, $GPP \cdot VPD^{0.5}$ as predictor variable. When plotting ET as a function of STO, we observed significant intercepts, e.g. for the Mediterranean FLUXNET site IT-BCi (Fig. 1a). In these cases, significant ET was observed when the driving force of the established models, the GPP-VPD-term, was small or zero. When we explicitly included this term in the model (+ETres), the cross-validated MEF increased notably (Fig. 1b). As Table 1 shows, the +ETres variant outperformed the Zhou model at 91% of the sites. The respective mean difference in MEF between the two variants was 0.08 (Table 2).

Table 1. Fraction of sites at which the model of the respective row was superior to the model of the respective column according to MEF_{diff}.

|	Zhou	+ETres	+VPD	+Rg	+VPD+Rg
Zhou	-	0.09	0.14	0.03	0.02
+ETres	0.91	-	0.42	0.05	0.02
+VPD	0.86	0.58	-	0.11	0.05
+Rg	0.97	0.95	0.89	-	0.38
+VPD+Rg	0.98	0.98	0.95	0.62	-

Table 2. Mean MEF$_{diff}$ comparison for different model variants. Entries indicate the median of the comparison MEF(row) − MEF(column).

	Zhou	+ETres	+VPD	+Rg	+VPD+Rg
Zhou	-	-0.08	-0.10	-0.17	-0.18
+ETres	0.08	-	-0.02	-0.09	-0.10
+VPD	0.10	0.02	-	-0.07	-0.08
+Rg	0.17	0.09	0.07	-	-0.01
+VPD+Rg	0.18	0.10	0.08	0.01	-

(a) (b)
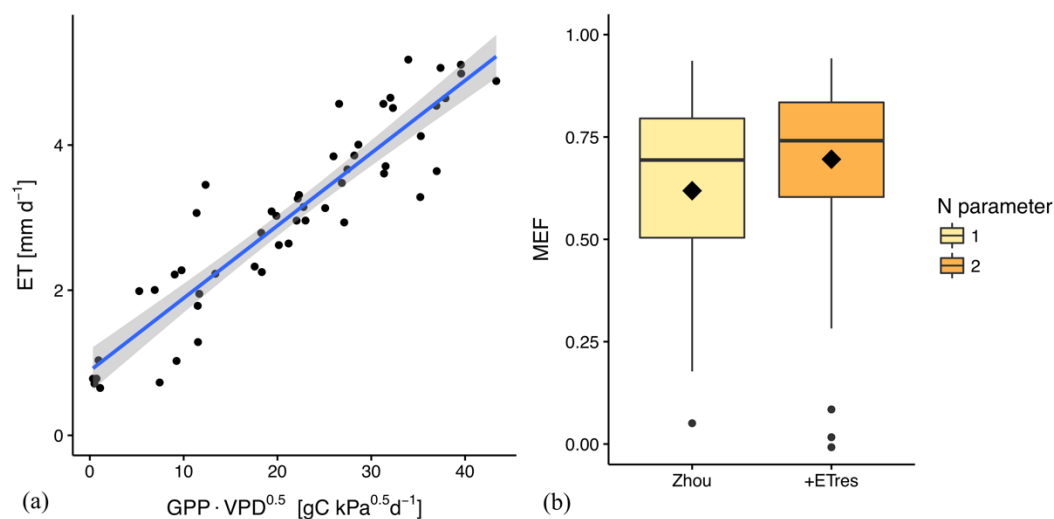
5 **Figure 1. Linear regression between the product of GPP and VPD$^{0.5}$ and the daily ET; the shaded area indicates the 95% confidence interval of the predictions (a). Model performance of the Zhou model compared to the +ET$_{res}$ variant (b). The thick horizontal lines of the boxplots denote the median, the diamonds denote the mean of the MEF of all sites.**
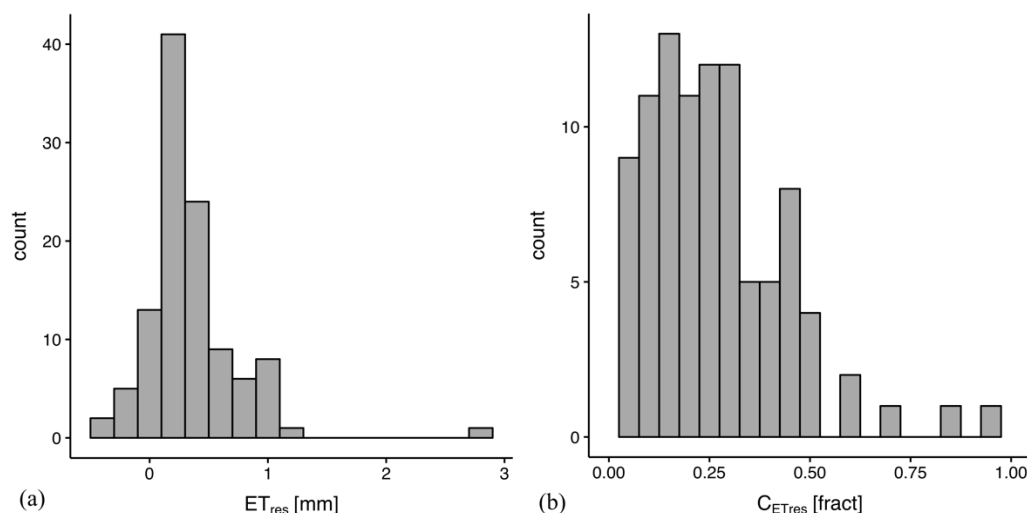
Figure 2. Distribution of the estimated intercepts. The majority of sites had values between 0–1.2 mm for the absolute intercept (a). The relative contribution of ET$_{res}$ to the daily mean evapotranspiration as quantified by C_{ETres} reached up to 0.94 (negative values excluded) (b).

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The site specifically estimated intercept values range from -0.43 to 2.88 mm (1.25 mm when excluding the highest value) with a mean of 0.34mm (Fig. 2a). The mean relative intercept, C_{ETres}, was 0.25 when averaged over all sites, implying that a quarter of transpiration is was not attributed to GPP · VPD$^{0.5}$ in this model formulation (Fig. 2b). The importance of the intercept for the prediction of daily ET and its diverging values raise the question whether the intercept compensates for the

10 absence of a physical or biological process in the model or whether there is a problem with the observations.

Our first hypothesis was that the ET$_{res}$ intercept was due to remaining contributions of soil and interception evaporation to measured ET after three consecutive rain-free days. To test this, we estimated the parameter ET$_{res}$ for periods of successively longer consecutive rain free days. If our hypothesis was right, we would expect a trend of declining ET$_{res}$ with increasing

15 consecutive rain free days. However, no reduction of ET$_{res}$ beyond the exclusion of the three days after precipitation proposed by Beer et al. (dotted line) could be observed (Fig. 3a). We therefore concluded that potential contributions of soil and interception evaporation to ET cannot explain the existence of the intercept term in the WUE model.

We then hypothesized that a missing process representation in the model would be discernible as a temporal pattern in the

20 ET$_{res}$ estimates. For that, we estimated the intercept for each month and site separately. The monthly means of the intercept for all sites varied in a clear seasonal pattern (Fig. 3b).

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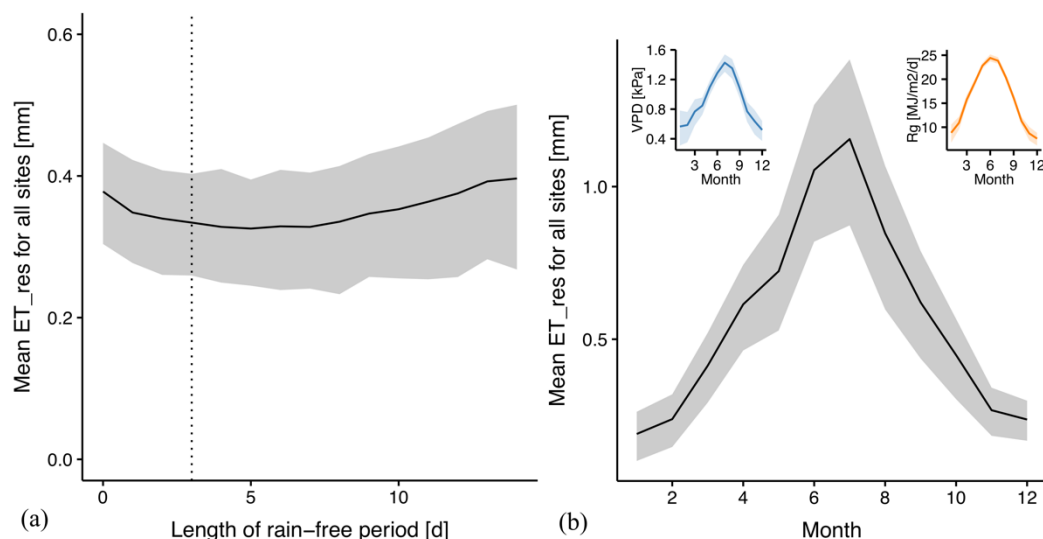
Figure 3. Sensitivity of ET$_{res}$ to varying length of filtering after precipitation events (a). The dotted, vertical line indicates the three-day period we adopted from Beer *et al*. Monthly estimation of the intercept parameter ET$_{res}$. The inset plots illustrate the mean seasonal variability of VPD and Rg for all sites on a monthly scale (b). In all plots, the solid line is the mean for all sites; the band denotes the 95% confidence interval of the mean derived by bootstrapping.

The seasonality of the parameter suggests a relationship to meteorological variables such as VPD or radiation that vary seasonally too. A relationship with VPD could represent the g_0 term of canopy conductance models (Ball et al., 1987). It was therefore introduced in an additional linear term (Eq. 4). A relationship with global radiation (Rg) (Eq. 5) could represent "equilibrium transpiration" (Jarvis and McNaughton, 1986), where the energy surplus of incoming radiation forces a transpirational flux independent from the vapor pressure gradient. We tested modeling the ETres intercept by including both variables separately (Eq. 4, 5) and jointly (Eq. 6).

We found only a small performance increase of the VPD-variant with regard to the Zhou model with intercept term ("+ETres", Fig. 4a). In fact, the MEF$_{diff}$ suggested that the ET$_{res}$-model was still superior to the VPD-variant at 42% of the sites (Table 1). By comparison, the Rg-model showed a substantial increase in MEF; compared to the ET$_{res}$ –model. The increased model complexity (two free parameters) was justified at 81% of the sites. The model variant with both VPD and Rg terms ("+VPD+Rg") was only slightly better than considering only the Rg term: Superior at 62% of the sites (Table 1), but with a small mean MEF$_{diff}$ of 0.01 (Table 2).
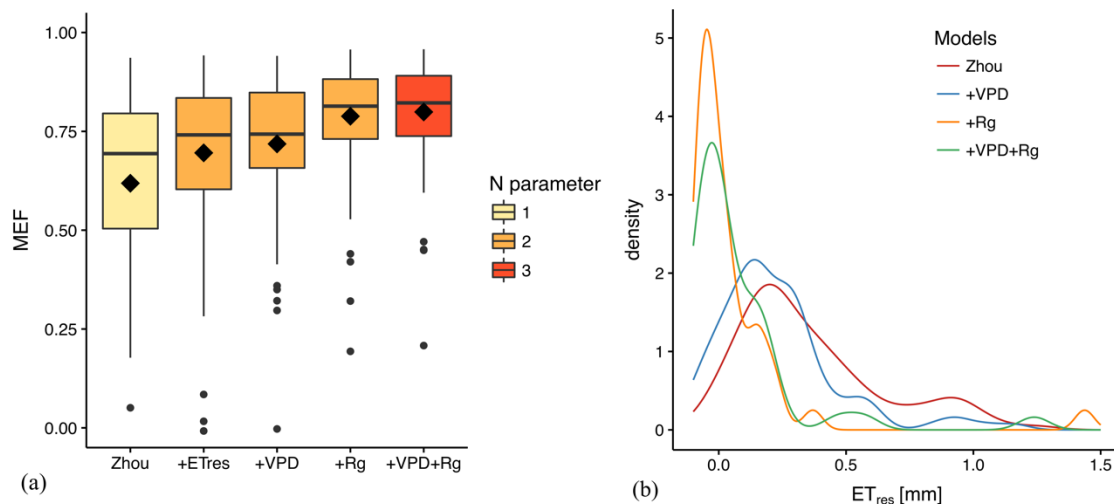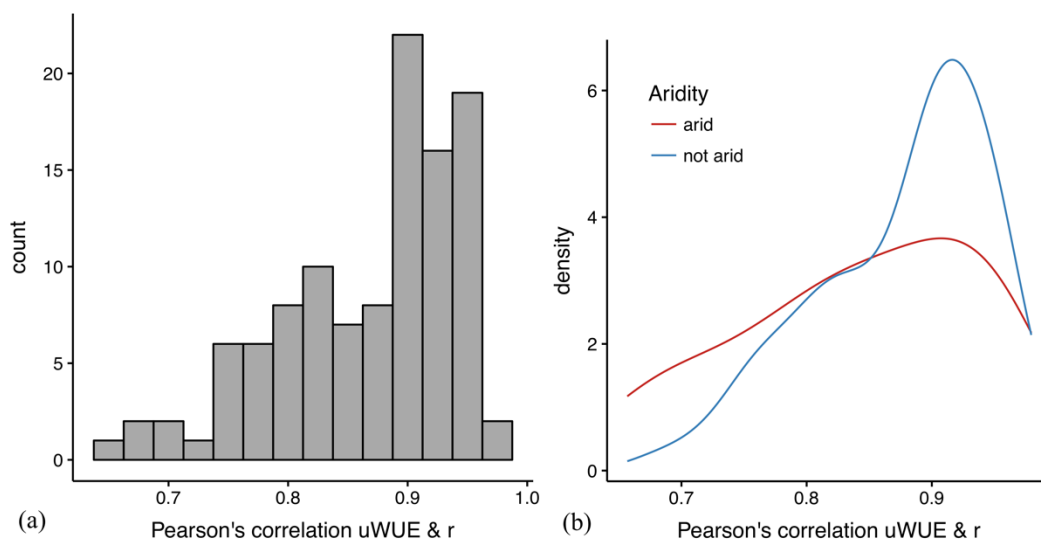
Figure 4. Cross-validated MEFs of the model variants with additional covariates (a). The Rg-variant lead to a further increase of model performance when comparing to the ET_{res}-variant. By contrast, the VPD-variant showed only a small increase of performance. Global distribution of the residual intercept for all model variants (b).

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Figure 5. Correlation of the parameter estimates for *r* and uWUE across sites (a). Distribution of the parameter correlations split according to aridity state of the site (b).

10   The difference between the +Rg- and +VPD-model is equally distinct, when the presence of a remaining model bias was tested. For this, the intercept was estimated with all four model variants (Zhou, +VPD, +Rg, +VPD+Rg). Only the models with an Rg-term had considerably reduced residual intercepts (Fig. 4b).

All models compared to the original definition Zhou had two or more parameters. Of those models with two parameters, the +Rg emerged as the best model after cross-validation, indicating that the additional model complexity was in fact justified. The presence of two parameters raised the question whether they could be identified independently. In fact, we found a high

5 degree of correlation between the parameters for all sites (Fig. 5a). It is likely that the correlation originates from the correlation between GPP and Rg. This is confirmed by noting that the correlation was lower at sites classified as arid (Fig. 5b), where the water limitation of GPP reduces correlations with radiation.

As transpiration of the +Rg model is a linear combination of stomatal and radiation-driven components, it is possible to

10 calculate the relative contribution of each component to daily ET fluxes. We compared two approaches to calculate this quantitiy: *Parallel* for estimating both parameters concurrently, *hierarchical* for estimating *r* only after uWUE has been calibrated (Eq. 10, 11). In both approaches, we observed that a sizeable fraction of mean daily ET could be attributed to the radiation term (Fig. 6). For the *hierarchical* approach, the mean global ET_{frac} was 24% (95% confidence interval 21...28%); for the *parallel* approach, the mean global ET_{frac} was 45% (95% confidence interval 40...49%).

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Notably, ET_{frac} estimated with the *parallel* approach varied widely between the sites (Fig. 7a). We assessed to which degree this variability can be interpreted as between-site variability of the expected value of ET_{frac} or whether it is due to poorly constrained and correlated parameters (Fig. 5a). The 'within-site' uncertainty of ET_{frac} caused by parameter uncertainty was quantified as the range between the 97.5 and the 2.5 percentiles (95% confidence interval, CI) of ET_{frac} estimates from 200

20 parameter vectors sampled from their respective posterior distributions. The majority of sites had an CI lower than 0.3 (Fig. 7b). This suggests that the large variability of ET_{frac} was not a result of parameter uncertainties. The conducted ANOVA (see Supplement S1) supported this conclusion, as it revealed that 95% of the global ET_{frac} variability could be attributed to the variability between sites.
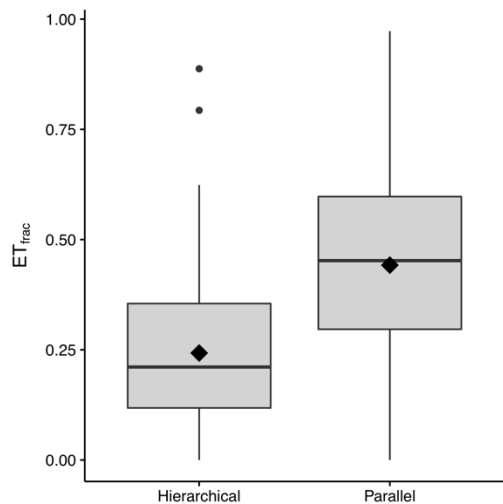
Figure 6. Distributions of ET_{frac} estimates for all sites. The diamonds indicate the mean, the bold horizontal lines indicate the median. The hierarchical approach yielded substantially lower values and can be interpreted as a conservative estimate of the quantity.

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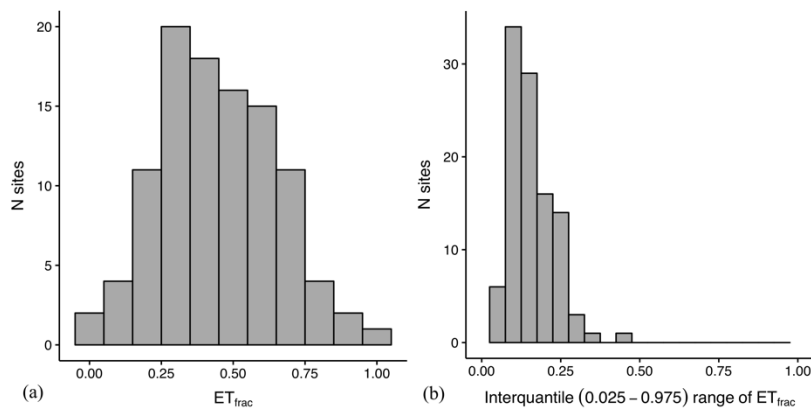
Figure 7ab. Distribution of the fraction of mean daily transpiration (ET_{frac}) attributed to the radiation term for all sites, calculated with the *parallel* approach (a). Distribution of the within-site variability of ET_{frac}, calculated as the difference between the 97.5 and 2.5 percentiles of the ET_{frac} estimates derived by sampling from the posterior parameter densities, parallel approach (b).
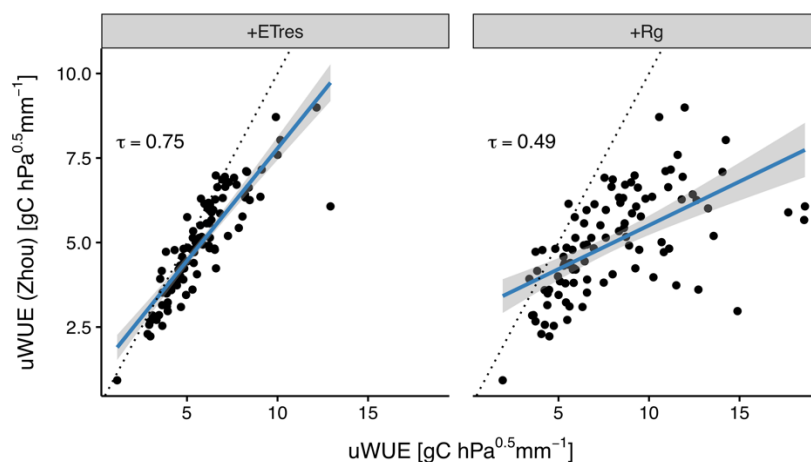
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Figure 8. Effect of different model variants on global uWUE estimates. The 1:1 line is dotted. A linear dependency would indicate that uWUE estimates are commensurable across sites, even if only after a linear scaling. When comparing with the estimates of the original Zhou model, the correlation is notably weaker for +Rg than for +ET$_{res}$. Sites with negative parameter estimates or high parameter uncertainties were removed for all models.

Finally, we assessed the impact of ET$_{res}$ and Rg as additional covariates on the global variability of uWUE estimates (Fig. 8). We calculated Kendall's τ rank correlation coefficient (Kendall, 1938) between the site-level estimates of uWUEs derived from the Zhou model and two different variants: +ET$_{res}$ and +Rg. The degree of correlation of the uWUE estimates quantifies whether changes in the model structure permutes the ordering of the estimates between sites. The extent to which parameter estimates are affected by the model structure is crucial because any explanation or prediction of parameter values between sites would be highly desirable. While a moderate correlation between the uWUE estimates of the Zhou model with the +ET$_{res}$-variant can be seen (τ = 0.75), the correlation of the uWUE estimates of the Zhou model with the respective values of the +Rg-variant is low (τ = 0.49). The between-site variability of uWUE explained by the estimates of the Zhou variant was 77% for the +ET$_{res}$-variant and 34% for the +Rg-variant, as quantified by the R^2.

4   Discussion

4.1   Findings and mechanisms

In this study, we identified radiation as an important variable for ecosystem-scale transpiration and water-use efficiency. Depending on the approach used, we attributed between a quarter and half of mean daily transpiration of all included

FLUXNET sites to a linear radiation term. These findings raise the question which biophysical or ecophysiological processes can account for the estimated magnitudes of this attributed fraction.

The influence of radiation on stomatal conductance has been noted and discussed in the literature (Whitehead et al., 1981;
5   Jarvis and McNaughton, 1986) and is also reflected in existing transpiration models (Leuning et al., 2008). By contrast, we detected a substantial transpiration component that was statistically independent from the product of GPP and $VPD^{0.5}$, tentatively suggesting an insensitivity to stomatal conductance. Our results suggest that this additional flux could not be associated with a g_0 conductance term, as this would imply the dependency of the additional ET on a linear VPD term (Ball et al., 1987). By contrast, the intercept was shown to be more consistent with radiation. Consequently, models that integrated
10   radiation-driven transpiration with such an additive linear response had a superior predictive performance across flux towers.

The observed effect of radiation indicates that equilibrium transpiration could play an important role in ecosystem-scale transpiration. Equilibrium transpiration (or equilibrium evaporation rate) is the transpiration occurring if the leaf is completely decoupled from the atmosphere (Jarvis and McNaughton, 1986). Therefore, equilibrium transpiration is
15   independent from stomatal conductance and driven solely by the dissipation of energy, provided by incoming solar radiation. This can be contrasted with a competing explanation that the radiation dependency of transpiration does not reflect an additional process but rather a systematic problem of the VPD observations. VPD is measured together with the fluxes above the canopy. While the recorded water and carbon fluxes do in fact represent the net fluxes of the tower footprint, the same cannot be said for VPD. Its measurement above the canopy may differ substantially from the relevant magnitude of the
20   variable at the leaf-scale. However, leaf temperature and thus the VPD of the leaf boundary layer is dependent on solar radiation (Tenhunen et al., 1990). Adding solar radiation to the equation could therefore be seen as compensating for the lack of the aforementioned leaf-scale VPD observations.

One limitation stems from the selection of rain-free periods for the parameter estimation. As previously described, this is a
25   necessary step to justifiably assume that the observed latent heat fluxes constitute mostly a transpiration flux, rather than evaporation from bare-soil and leaf surfaces in addition to transpiration. It also makes our work comparable with the study of Beer et al. (2009) that used this method to derive their estimates. For the observed residual evapotranspiration ET_{res} we could show that it is not an artefact of insufficient exclusion of days after precipitation events. However, the environmental conditions during and after rain events generally represent some of these specific conditions: Low VPD due to the moisture
30   available for evaporation, a higher share of diffuse radiation and a more or less sudden increase in soil moisture among others. All mentioned variables could plausibly be assumed to have an influence on the stomatal opening of plants. Therefore, the presented WUE model must not necessarily predict flux relationships during or immediately after precipitation events due to the underrepresentation of similar conditions in the sample of observations used for parameter estimation.

The effect of atmospheric CO2 concentrations on WUE (Morison, 1985; Conley et al., 2001) was not considered in this analysis. One could suspect that the seasonal variability of ET_{res} is affected by seasonal CO2 variability if both were in phase. However, ET_{res} showed a global maximum during June–July, while northern hemisphere CO2 concentrations are at its minimum in September–October (Keeling et al., 1976), implying that CO2 concentrations are unlikely to cause the seasonal variation of ET_{res}.

The model structures we tested in this study were evaluated according to their global empirical adequacy. Thus, despite the possible identification of probable mechanisms responsible for the observed patterns, the model structure selected in the end likely does not reflect the exact physical mechanisms by which the ecosystem operates. Furthermore, this limitation can be specifically important in the case of water limitation. As the Rg-term is completely independent from any variable reflecting vegetation activity, our model would predict transpiration scaling with radiation during periods of severe drought. By principle, the same problem could affect periods of low temperatures before leaf flushing, although these periods are generally also associated with low radiation levels and hence may not be as problematic.

4.2   Implications

Our empirical analysis suggests that ecosystem-scale transpiration depends to a sizeable degree on variables other, which seem to be linked to radiation. This implies that photosynthesis and transpiration might be less strongly coupled on ecosystem scale than commonly assumed. We speculate that the additional effect of radiation could be due to "equilibrium transpiration" where radiation drives transpiration even when the canopy is fully decoupled from the atmosphere. However, we cannot disentangle direct physiological effects of radiation on transpiration from other radiation effects that are relevant on ecosystem scale at this point. For the latter, leaf to canopy scaling, micrometeorological conditions, and boundary layer dynamics might contribute to the observed relationship between ecosystem scale water use efficiency and radiation. Thus, further research is needed to reconcile our empirical findings with detailed ecosystem-scale modeling and theory on the one hand and plant-physiological research under controlled conditions on the other hand.

Finally, we caution against prematurely interpreting the between-site variability of underlying water-use efficiency (uWUE). We showed that estimates of uWUE derived with the Zhou model explained only a third of the observed variability of ecosystem uWUE derived from our empirically superior model formulation. The dependence of uWUE estimates on the chosen model formulation makes the interpretation of uWUE as an ecosystem property problematic. This concern would

also hold for assessing temporal dynamics of uWUE such as long-term trends. For example, the unexpectedly large global trend of WUE across FLUXNET sites (Keenan et al., 2013) would need to be tested for its omission of radiation in the model that was used. Overall, this study highlights the importance of model structure uncertainty for interpretations of parameter variability.

References

Baldocchi, D., Falge, E., Gu, L., Olson, R., Hollinger, D., Running, S., Anthoni, P., Bernhofer, C., Davis, K., Evans, R., Fuentes, J., Goldstein, A., Zhou, G., Law, B., Lee, X., Malhi, Y., Meyers, T., Munger, W., Oechel, W., Paw U,K.T.,

5   Pilegaard, K., Schmid, H., Valentini, R., Verma, S., Vesala, T., Wilson, K., and Wofsy, S.: FLUXNET: A new tool to study the temporal and spatial variability of ecosystem-scale carbon dioxide, water vapor, and energy flux densities, Bulletin of the American Meteorological Society, 82, 2415–2434, 2001.

Ball, J. T., Woodrow, I. E. and Berry, J. A.: A Model Predicting Stomatal Conductance and its Contribution to the Control of

10   Photosynthesis under Different Environmental Conditions, in: Progress in Photosynthesis Research (Eds. Biggins, J.), Springer Netherlands, Dordrecht, 221–224, 1987.

Beer, C., Ciais, P., Reichstein, M., Baldocchi, D., Law, B. E., Papale, D., Soussana, J.-F., Ammann, C., Buchmann, N., Frank, D., Gianella, D., Janssens, I. A., Knohl, A., Köstner, B., Moors, E., Roupsard, O., Verbeeck, H., Vesala, T., Williams,

15   C. A., and Wohlfahrt, G.: Temporal and among-site variability of inherent water use efficiency at the ecosystem level, Global Biogeochemical Cycles, 23, GB2018, 2009.

Churkina, G., Running, S. W., and Schloss, A. L.: Comparing global models of terrestrial net primary productivity (NPP): the importance of water availability, Global Change Biology, 5, 46–55, 1999.

20

Ciais, P., Sabine, C., Bala, G., Bopp, L., Brovkin, V., Canadell, J., Chhabra, A., DeFries, R., Galloway, J., Heimann, M., et al.: Carbon and Other Biogeochemical Cycles, in: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change (Eds. Stocker T. F., Qin D., Plattner G. K., Tignor M., Allen S. K., Boschung J., Nauels A., Xia Y., Bex V., Midgley P. M.), Cambridge University

25   Press, Cambridge, United Kingdom and New York, NY, USA, 465–570, 2014.

Conley, M. M., Kimball, B., Brooks, T., Pinter, P., Hunsaker, D., Wall, G., Adam, N., LaMorte, R., Matthias, A., Thompson, T., et al.: CO2 enrichment increases water-use efficiency in sorghum, New Phytologist, 151, 407–412, 2001.

30   Cowan, I. R. and Farquhar, G. D.: Stomatal function in relation to leaf metabolism and environment, in: Integration of Activity in the Higher Plant, edited by Jennings, D. H., pp. 471–505, Cambridge University Press, 1977.

Elzhov, T.V., Mullen, K.M., Spiess, A.N., and Bolker B.: minpack.lm: R Interface to the Levenberg-Marquardt Nonlinear Least-Squares Algorithm Found in MINPACK, Plus Support for Bounds. R package version 1.2-0. 2015

Farquhar, G.D., von Caemmerer, S. and Berry, J.A.: A biochemical model of photosynthetic CO_2 assimilation in leaves of C_3 species, Planta, 149, 78–90, 1980.

Gerten, D., Schaphoff, S., Haberlandt, U., Lucht, W., and Sitch, S.: Terrestrial vegetation and water balance – hydrological evaluation of a dynamic global vegetation model, Journal of Hydrology, 286, 249–270, 2004.

Ito, A. and Inatomi, M.: Water-use efficiency of the terrestrial biosphere: a model analysis focusing on interactions between the global carbon and water cycles, Journal of Hydrometeorology, 13, 681–694, 2012.

Jarvis, P. G. and McNaughton, K.: Stomatal control of transpiration: scaling up from leaf to region, Advances in ecological research, 15, 49, 1986.

Jasechko, S., Sharp, Z. D., Gibson, J. J., Birks, S. J., Yi, Y., and Fawcett, P. J.: Terrestrial water fluxes dominated by transpiration, Nature, 496, 347–351, 2013.

Katul, G., Manzoni, S., Palmroth, S., and Oren, R.: A stomatal optimization theory to describe the effects of atmospheric CO2 on leaf photosynthesis and transpiration, Annals of Botany, p. mcp292, 2009.

Keeling, C. D., Bacastow, R. B., Bainbridge, A. E., Ekdahl, C. A., Guenther, P. R., Waterman, L. S., and Chin, J. F.: Atmospheric carbon dioxide variations at Mauna Loa observatory, Hawaii, Tellus, 28, 538–551, 1976.

Keenan, T. F., Davidson, E., Moffat, A. M., Munger, W., and Richardson, A. D.: Using model–data fusion to interpret past trends, and quantify uncertainties in future predictions of terrestrial ecosystem carbon cycling, Global Change Biology, 18, 2555–2569, 2012.

Kendall, M.: A New Measure of Rank Correlation, Biometrika, 30, 81–89, 1938.

Koster, R. D., Dirmeyer, P. A., Guo, Z., Bonan, G., Chan, E., Cox, P., Gordon, C. T., Kanae, S., Kowalczyk, E., Lawrence, D., Liu, P., Lu, C.-H., Malyshev, S., McAvaney, B., Mitchell, K., Mocko, D., Oki, T., Oleson, K., Pitman, A., Sud, Y. C., Taylor, C. M., Verseghy, D., Vasic, R., Xue, Y., and Yamada, T.: Regions of Strong Coupling Between Soil Moisture and Precipitation, Science, 305, 1138–1140, 2004.

Leuning, R., Zhang, Y., Rajaud, A., Cleugh, H., and Tu, K.: A simple surface conductance model to estimate regional evaporation using MODIS leaf area index and the Penman-Monteith equation, Water Resources Research, 44, 2008.

Medlyn, B. E., Duursma, R. A., Eamus, D., Ellsworth, D. S., Prentice, I. C., Barton, C. V. M., Crous, K. Y., de Angelis, P.,
5 Freeman, M., and Wingate, L.: Reconciling the optimal and empirical approaches to modelling stomatal conductance, Global Change Biology, 17, 2134–2144, 2011.

Miralles, D. G., Gash, J. H., Holmes, T. R. H., de Jeu, R. A. M., and Dolman, A. J.: Global canopy interception from satellite observations, Journal of Geophysical Research, 115, D16122, 2010.
20

Morison, J. I.: Sensitivity of stomata and water use efficiency to high CO2, Plant, Cell & Environment, 8, 467–474, 1985.

Nash, J. E. and Sutcliffe, J. V.: River flow forecasting through conceptual models part I — A discussion of principles, Journal of Hydrology, 10, 282–290, 1970.
25

Oki, T. and Kanae, S.: Global hydrological cycles and world water resources, Science, 313, 1068–1072, 2006.
Omlin, M. and Reichert, P.: A comparison of techniques for the estimation of model prediction uncertainty, Ecological Modelling, 115, 45–59, 1999.

30 Papale, D., Reichstein, M., Aubinet, M., Canfora, E., Bernhofer, C., Kutsch, W., Longdoz, B., Rambal, S., Valentini, R., Vesala, T. and Yakir, D.: Towards a standardized processing of Net Ecosystem Exchange measured with eddy covariance technique: algorithms and uncertainty estimation, Biogeosciences, 3, 571-583, 2006.

Reichstein, M., Falge, E., Baldocchi, D., Papale, D., Aubinet, M., Berbigier, P., Bernhofer, C., Buchmann, N., Gilmanov, T.,
35 Granier, A., Grünwald, T., Havránková, K., Ilvesniemi, H., Janous, D., Knohl, A., Laurila, T., Lohila, A., Loustau, D., Matteucci, G., Meyers, T., Miglietta, F., Ourcival, J.-M., Pumpanen, J., Rambal, S., Rotenberg, E., Sanz, M., Tenhunen, J., Seufert, G., Vaccari, F., Vesala, T., Yakir, D. and Valentini, R.: On the separation of net ecosystem exchange into assimilation and ecosystem respiration: review and improved algorithm, Global Change Biology, 11, 1424–1439, 2005.

40 Tenhunen, J., Serra, A. S., Harley, P., Dougherty, R., and Reynolds, J. F.: Factors influencing carbon fixation and water use by Mediterranean sclerophyll shrubs during summer drought, Oecologia, 82, 381–393, 1990.

Whitehead, D., Okali, D., and Fasehun, F.: Stomatal response to environmental variables in two tropical forest species during the dry season in Nigeria, Journal of Applied Ecology, pp. 571–587, 1981.

Wythers, K. R., Lauenroth, W. K., and Paruelo, J. M.: Bare-soil evaporation under semiarid field conditions, Soil Science Society of America Journal, 63, 1341–1349, 1999.

5   Zhou, S., B. Yu, Y. Huang, and Wang, G.: The effect of vapor pressure deficit on water use efficiency at the subdaily time scale, Geophysical Research Letters, 41, 5005–5013, 2014.

Zhou, S., Yu, B., Huang, Y., and Wang, G.: Daily underlying water use efficiency for AmeriFlux sites, Journal of Geophysical Research: Biogeosciences, 120, 887–902, 2015.

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Data Availability

For this study, we used observations of the FLUXNET initiative from sites with an *open and fair use data policy*[2]. The data

sets can be downloaded at http://fluxnet.fluxdata.org//data/download-data/

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[2] http://www.fluxdata.org/Shared%20Documents/Policy_Free_Final.pdf