

# “Probabilistic inference of ecohydrological parameters using observations from point to satellite scales” by Maoya Bassiouni et al.

## 5 Response to Sally Thompson (Editor)

*This manuscript received four independent reviews, and all of them offered sensible and constructive suggestions. The reviews broadly concur that the manuscript is of interest to the research community, but that a number of methodological and scope issues need to be addressed. I am largely convinced that these points have been taken on board by your author team based on the response to the reviewers - thank you.*

*To summarize, I will be looking for the following changes in the revised manuscript:*

*(1) Clarify the scope of the paper and avoid making overly strong statements about what it achieves. The goals of model calibration and "identifiability" of parameters (it may be best to speak of identifiability rather than speaking of "avoiding equifinality" -- maybe see Wagener and Kollat 2007?) seem more appropriate than strong statements about correctness and accuracy.*

*(2) Clarify the assumptions in the modelling and how they are addressed. In particular assumptions about statistical stationarity versus parameter stationarity versus homogeneity should be considered.*

*(3) Improve the treatment of non-stationarity in the soil water timeseries. As several reviewers noted, the model was inappropriately inverted during a period of time where soil moisture is non-stationary - drawing conclusions about calibration performance in this situation is of highly questionable value. I reiterate the 3rd reviewers suggestion to consider adopting the frameworks of Dralle (which is simpler) or Viola (more complex) in order to address growing season conditions in Mediterranean sites.*

*(4) Improve and justify the goodness of fit metrics used*

*(5) Tread carefully around the treatment of soil depth versus Emax in the modeling.*

**We appreciate your feedback on our manuscript. We have responded to all of the reviewers suggestions below and addressed your major expectations in the revised draft.**

**(1) We have simplified the scope of the manuscript, revisited the questions addressed in the analysis in response to the reviewers' major comments. A portion of the analysis in the previous draft was no longer relevant and removed from the revised manuscript. We have adopted the word 'identifiability' to avoid making overly strong statements about the parameter estimates.**

**(2) We have reworded the manuscript to clarify the concepts of stationarity and homogeneity.**

**(3) We have used the suggested framework in Dralle and Thompson, 2016 in the revised manuscript to improve treatment of non-stationarity in the soil water time series. Results of the model inversions were improved by the use of a full year time series instead of an isolated summer season. We discuss whether the added complexity of a seasonal model versus a steady state model improves the identifiability of the ecohydrological parameters.**

**(4) We have adopted the quantile-level Nash Sutcliffe Efficiency as an improved goodness of fit metric in the revised manuscript and added section 2.4 and 2.5 to define our evaluation criteria**

**(5) We only consider the soil moisture sensing depth, removed the sensitivity test related to soil depth in the revised manuscript and carefully defined Emax.**

# Response to Minghui Zhang (Referee #1)

## I. General comments

5 Thank you for the opportunity to review the paper “Probabilistic inference of ecohydrological parameters using observations from point to satellite scales”. This work introduces a Bayesian inference technique that estimates four ecohydrological parameters from empirical soil moisture pdfs. The paper’s novelty lies in the application of this technique beyond the point scale. In the method, the four ecohydrological parameters, which encompass soil water holding thresholds and evapotranspiration, were related to soil moisture observations through Laio et al. (2001)’s analytical formula. The authors then pose questions about the spatial scale, data availability, and model complexities that are appropriate for such an estimation method, and provide concise answers: estimates are most robust at the satellite scale; the method is accurate with as few as 75 random daily observations; and a specific group of parameters ( $s_w$ ,  $s^*$ ,  $E_{max}$ ,  $E_w = 0.05E_{max}$ ) can be inferred with highest accuracy. In my opinion, this paper, with major revisions, will have important implications in hydrological modeling. Below are my scientific comments, requests for clarification, and technical corrections.

15 **Thank you for your thorough review and constructive suggestions. We have provided responses and corrections below.**

## II. Major comments

### 20 1. Applicability of the method

I appreciated the paper’s use of sensitivity tests to define the method’s applicability in a range of data availability levels, spatial scales, rooting depths, and model complexities. However, I think there’s room for another, broader view of method applicability. The conclusions about method applicability were (naturally) only applied in cases where the simulation converges. It would be important to also define the conditions under which the method does (or does not) behave well. On page 1 lines 15-16, the authors wrote that “parameter estimates were most constrained for scales and locations at which soil water dynamics are more sensitive to the fitted ecohydrological parameters of interest”. Am I correct in concluding that the method does not converge when soil moisture is NOT sensitive to the ecohydrological parameters of interest? I recommend that the authors address the conditions under which the method fails to converge. They have briefly mentioned the effect of dry vs. wet climates, but I would like to see a discussion on the effects of soil and vegetation type as well.

25 **Thank you for this suggestion. We agree that this is an interesting aspect of this study and have revised the results to report the number of sample runs required to obtain converging results (see method in section 2.3.2). This measure quantifies how rapidly converging results are obtained. Only results that met the convergence criteria were reported. We generally concluded that convergence was obtained when model assumptions are appropriately met and the empirical pdf is consistent with the parameters defined in the analytical model. The revised manuscript compared annual pdfs instead of summer season pdfs. This approach was overall more appropriate and model inversions for all sites and datasets converged. There was no evidence of effects of soil and vegetation type on the convergence of the results.**

### 30 2. Choice of estimated parameters

40 On page 3 line 3, the authors state that the method focuses on estimating “vegetation controls on soil water dynamics”. Within this broad category of parameters, four were chosen specifically:  $s_w$ ,  $s^*$ ,  $E_w$ , and  $E_{max}$ . The authors should elucidate their choice of parameters in two ways.

First, there should be a brief explanation of why four was chosen as the maximum number of parameters. If it was out of concern for equifinality, a formal analysis should be included.

45 Second, I was surprised to see that the rooting depth  $Z$  was not among the estimated parameters. From my point of view,  $Z$  could be estimated in the same manner as the four chosen parameters and significantly affects the soil moisture pdf. Porporato’s work indicates that the volume of storage in the rooting zone is a key determinant of the pdf shape, so there is an a priori reason to expect that  $Z$  is an important parameter. In Section 4.2, the authors mentioned that the four estimated parameters aren’t very sensitive to the value of  $Z$ , but I’m not convinced that Figure 5 supports this conclusion. I strongly suggest a practical or theoretical explanation about why  $Z$  was not chosen as an estimated parameter.

50 **Thank you for this comment. Practical reasons determined the choice of the parameters that were estimated. Among all the parameters necessary to compute the analytical soil saturation pdf in Equation 2,  $s_w$ ,  $s^*$ , and  $E_{max}$  are not directly observable and generally difficult to estimate using available data and existing methods. The other parameters including rainfall characteristics ( $\lambda$  and  $\alpha$ ) and physical soil parameters ( $s_{fc}$ ,  $s_h$ ,  $K_s$ , and  $b$ ) were characterized based on readily available data and established methods explained in section 2.2.2. We have added a discussion of this choice in the 3<sup>rd</sup> paragraph of the introduction.**

**Z was not included as a parameter to be estimated because it is most appropriate for Z to be equal to the measurement depth associated with each scale. We have removed the sensitivity test related to soil depth because it is not useful to determine whether estimates of  $s_w$  and  $s^*$  derived from surface soil moisture measurements are relevant to deeper soil depths and does not provide information on the homogeneity assumption. We have defined the choice of setting Z to the measurement depth in the methods section (2.2.2).**

### III. Minor comments

#### Section 2.2.1: Model definition

*In my opinion, ignoring interception is questionable given the differences in forest type (and especially the presence of deciduous forest in some sites). I recommend a defence of the decision to ignore interception in the soil moisture model.*

**We agree that interception is an important component of the soil water balance at forested sites. In this analysis we decided to apply the simplest form of the soil water balance model that would be consistent with the empirical soil saturation pdfs and did not include interception. Results for forested sites were acceptable and did not indicate that the level of model complexity needed to be increased by including interception. The proposed methods can be modified for other studies in which it is important to include interception as a known or unknown parameter (the code associated with this analysis that will be also published included interception as a parameter, here set to 0). Errors due to ignoring interception at the forested sites in this study may have been absorbed in other estimated parameters such as  $E_{max}$  or compensated by uncertainties in observed rainfall characteristics. We added the following sentences of section 2.2.1 to clarify this point.**

For simplification, we assume that the rainfall applied is equal to the amount reaching the ground surface and do not account for rainfall intercepted by vegetation. Interception may be a significant component of the soil water balance at forested sites and may need to be accounted for in other studies.

*Using a date range of April to September might introduce nonstationary behavior in climate parameters as the seasons progress from spring to autumn. I suggest a discussion of the impact of (1) nonstationary  $E_{max}$  within this period due to vegetation growth, particularly leaf out and LAI changes in the deciduous forest sites; and (2) any large changes in rainfall occurrence in summer-dry climates on the method's accuracy.*

**We acknowledge that the date range may not be optimal for stationary behaviour in climate parameters at each site. The revised analysis utilized a full year timeseries and also adopts the framework in Dralle and Thompson (2016) to account for non-stationary dynamics.**

#### Section 2.2.2: Climate, soil and vegetation parameter characterization

*On page 7 lines 17-18, the authors provided a reasonable explanation for why  $s_{fc}$ ,  $s_h$  and  $K_s$  don't significantly affect soil moisture pdf. It would be nice, though not crucial, to support this claim using either a sensitivity analysis or with reference to existing analytical studies from Laio et al., (2001).*

**OK this reference will be added. We also added to Table 1 minimum and maximum observed soil saturation values for comparison with soil saturation threshold estimates.**

#### Section 2.3.1: Application of the Bayes theorem

*The authors have assumed uninformed prior knowledge of each of the soil balance parameters while applying Bayes theorem. However, the soil type, climate, and primary forms of vegetation are known at each site, and soil threshold parameters may be estimated from pedotransfer functions. Therefore, it seems that an informed prior for each of the four parameters was in fact possible. I suggest exploring the influence of including informed priors on the results and, based on this exploration, defend or reject the decision to use an uninformed prior.*

**We acknowledge that some information about the soil type, climate, and primary forms of vegetation are known at each site. We have taken advantage of this knowledge in defining the parameters that were not estimated in the model (see Table 1) and defining the bounds of parameters to estimate. This was useful to better constrain the estimated parameters and avoiding equifinality. The added complexity of informed prior knowledge was unnecessary. Our goal was to develop a method with the minimum level of complexity in order for it to be applied at any location using easily available data, which is particularly important for the satellite scale analysis. If pedotransfers are not well defined and inconsistent with the soil moisture data they unnecessary uncertainty would introduced in the methods.**

#### Section 4: Results and Discussion

*Several times over the course of this section, the authors mentioned that "acceptable results" were obtained in the various sensitivity tests. The authors should define what is meant by "acceptable" earlier on.*

**Section 2.4 and 2.5 was added in the revised manuscript to explicitly describe evaluation goals and metrics used.**

*The Kolmogorov-Smirnov statistic is subject to bias and therefore a problematic way to compare pdfs. I recommend exploring*

measures that compare pdf quantiles, as was done in Muller et al. (2014).

**This is a good suggestion. We agree that the KS test has disadvantages. We reported both the KS and NSE in the revision.**

- 5 *In addition to comparing pdfs, I recommend validating values of the individual estimated parameters. For example, estimations of  $E_{max}$  should be compared to  $E_{max}$  calculated from the Hargreaves equation, and estimates of  $s^*$  and  $sw$  should be compared to results from pedotransfer functions.*

**We agree that it would be useful to validate estimated parameters with other estimates. However, estimated ecohydrological parameters that are generally not directly measured. This is also argued in Miller et al., 2007).**

10 **It is therefore challenging to compare estimated parameter values to site-specific observations and determine their accuracy because these are not directly available. Calibration parameters from previous studies are now cited in the revised manuscript. We have used the wording parameter identifiability instead of accuracy to avoid misleading statements.**

15  **$E_{max}$  is not exactly the atmospheric moisture demand, it is a fraction of the atmospheric moisture demand that can be withdrawn from the soil layer considered.  $E_{max}$  can be equal to the atmospheric moisture demand approximated by potential evapotranspiration (PET) if the full soil column or rooting depth is considered.**

**In this study we cannot assume that  $E_{max} = PET$  because only the surface soil moisture is sensed. It was not meaningful to compare  $s^*$  and  $sw$  to estimates from pedotransfer functions because these functions are highly non-linear and not specifically calibrated for data used at each site/scale.**

20 *Section 4.1: Level of model complexity*

*Based on Figure 4, it looks like certain location-parameter pairs are very sensitive to model complexity, whereas others are not. I recommend that the authors further explore and explain this sensitivity.*

**Figure 4 was removed**

25 *Section 5: Conclusions*

*I suggest including proposed next steps to improve this method, or planned applications using this method.*

**OK, we added the following sentences to the conclusions**

30 *This study provided a method to estimate ecohydrological characteristics that are not directly observable, and for which established estimation methods are not available. This study only used available datasets from sensor networks and global satellite products and methods can therefore be applied to a large range of sites or to full global datasets to improve understanding of spatial patterns in ecohydrological parameters relevant for local and global water cycle analyses.*

*Figures*

- 35 *Figure 1: In general, satellite scale soil moisture seems to fluctuate much more than that of footprint scale under dry climate conditions. The caption should include a comment on why this is so, and on the implications of this on performance at the satellite scale.*

40 **Thank you for noticing this. We are not aware of references that analysed causes of higher noise in the satellite-scale soil moisture observations during dry periods. We are not able to make any clear interpretations of this pattern based on the short observation period and limited sites presented in this study. Data indicates that the noise in the satellite-scale soil moisture observations does not significantly affect the mean of the observed soil moisture but may have increased the kurtosis of the empirical pdfs. We will report the mean, standard deviation and kurtosis of empirical soil moisture pdfs in Table 1. Overall, we do not expect our methods to be affected by the noise in the satellite data at the selected locations. This is an illustration of the advantage of analysing pdfs versus time series (mentioned in our introduction) to estimate ecohydrological parameters from satellite soil moisture data. Often areas with highly uncertain satellite soil moisture observations are masked out data products and should not be an issue. Future studies should always assess data quality related to this potential problem**

50 **We revised the following sentence in section 2.1:**

*Soil saturation and rainfall data at each scale and for each site during the selected analysis period are presented in Fig. 1 and summary statistics are reported in Table 1. The difference in data quality between data sources and sites is not expected to significantly affect empirical soil saturation pdfs and resulting parameter estimates in this study.*

- 55 *Figure 4: In the caption, explain why are there error bars associated with only some data points.*

**Figure 4 was removed**

*Figure 5: In the caption, explain the abrupt changes and “dangling” data points around soil depths of 400m and 600mm for the point and footprint scale plots, respectively.*

60 **Figure 5 was removed**

Figures 4 to 6: please add a legend showing that each of the different colors represents a different location.

**We have changed the location of the legend to increase clarity.**

5 *IV. Technical corrections*

Page 1 line 13: be more specific about what is meant by “footprint” scale.

**The footprint scale is specifically defined in Section 2.1.**

Page 1 line 25: “back to the atmosphere”

10 **OK this was corrected**

Page 2 line 29: “space-borne”

**OK this was corrected**

15 Page 6 line 9: “commonly used in soil water balance”

**OK was corrected**

Page 9 line 20: the run was discarded”

**OK was corrected**

20

Page 9 line 21: “more than 10 run samples”

**OK was corrected**

The paper skips directly from section 2 to section 4.

25 **OK was corrected**

Figure 3 caption: “empirical versus modelled”

**OK was corrected**

30 *Reference*

Muller, M.F, D. N. Dralle, and S. E. Thompson (2014), Analytical model for flow duration curves in seasonally dry climates, *Water Resour. Res.*, 50, 5510-5531, doi: 10.1002/2014WR015301.

## Response to Marc F. Müller (Referee #2)

5 The authors use soil moisture observations in a Bayesian inversion procedure to estimate vegetation-related drivers of soil moisture dynamics in the root zone, as modeled by a simple model of soil moisture distribution. The authors apply the approach to a diverse sample of study regions where soil moisture and climate observations are available at different scales. The presented research is important and innovative in that it investigates the potential for recent remote sensing approaches that monitor spatially aggregated soil moisture to estimate eco-hydrologic parameters that are very challenging to observe in-situ, even in well instrumented basins. The research also bridges the gap between different observation scales, which has potentially interesting implications in poorly gauged regions. While I recommend the paper for publication in HESS, I would also like to raise a few comments/questions that could possibly help the authors during the revision of their paper.

**Thank you for your thorough review and constructive suggestions. We have provided responses and some corrections below.**

### 15 Major comments

1. The authors appear to use the same sample of soil moisture observations to calibrate (via Bayesian Inversion) and validate (KS tests and Fig 3) the approach, which instinctively raised red flags on a first read. After reflecting, it became clear (well, to me at least) that the purpose of the exercise was to show that Bayesian inversion can be used to estimate vegetation-related drivers of soil moisture using soil moisture time series, conditional on the assumed pdf model being an accurate description of soil moisture dynamics. In that case, the research design would be appropriate because the posterior CV portrays estimation uncertainties and the goodness-of-fit shows that the soil moisture model is, indeed, appropriate. Consequently, the purpose of the goodness-of-fit test appears to be to evaluate the functional form of the pdf, not the estimated parameter values, so it is fine to use the same dataset to calibrate parameters and evaluate outcomes. Please clarify the distinct function of these two metrics as appropriate.

20 **Yes, the above comment describes our intentions. Section 2.4 and 2.5 was added in the revised manuscript to explicitly describe evaluation goals and metrics used.**

2. I am having issues with the way you use KS tests to evaluate pdf fits. First off, if I am not mistaken, the null hypothesis of a ks test is that the two tested distributions are identical. If so, the p-value could be interpreted as the probability of obtaining a ks-distance at least as large as the one that would be obtained if the two samples were taken from the same distribution. This is loosely equivalent to the probability of falsely rejecting the null. In other words, a p-value of 5% would mean that one has a 95% chance of being right when stating that the two distributions are different, which is quite a low standard when assessing goodness of fit. Significance levels don't tell anything about type II errors, which is what I would think we are ultimately after when evaluating goodness of fits. More importantly, the KS statistic does not follow the kolmogorov distribution (i.e. estimated p-values are wrong) if the same sample of data is used to calibrate the cdf model and construct the empirical cdf to which it is compared. In my opinion, however, a formal test is not necessary to make your point here (see point 1). The graphs in Fig 3 are sufficient to make the point that the laio model reproduces the shape of the observed empirical histogram. You can then use a distance measure to monitor fits in the sensitivity analysis. The KS-distance is probably not the most appropriate measure for that though, as it only considers the largest distance between the cdfs.  $\hat{A} \tilde{T}$  global distance metrics like the Cramer Van Mises statistic or quantile-level nash sutcliffe efficiency, Muller 2016), or information based criteria (e.g. AIC, Ceola 2010) are useful alternatives to consider.

35 **We reported both KS and NSE values in the revision. We agree that the KS test has disadvantages. We agree that the p-value for the KS test is not always meaningful is not discussed in the revision.**

3. Your sensitivity analysis on soil depth (Section 4.2.) convinces me that the value assumed for Z in eqn 2 has little effect on the modeled soil moisture dynamics. This is of course important, but without actually measuring whole column soil moisture, I fail to see how you test the homogeneity assumption (i.e. that near surface soil moisture observations can be used to estimate whole-column characteristics). Please elaborate.

45 **We agree that it is difficult to test the homogeneity assumption through the sensitivity tests in this analysis. We have removed the sensitivity analysis related to Z. We will only consider Z equal to the actual measurement depth for each sensor in the revision.**

50 4. I would find it interesting to elaborate on the interpretation of convergence in the context of Bayesian inversion. You mention (I think) that MCMC runs do not converge if insufficient information is available in the empirical p(s) to determine the considered model parameters. I would find it interesting to elaborate on when (and why) these non converging runs arise, perhaps in your discussion on data availability (section 4.3).

We agree that this is an interesting aspect of this study and will amend the results and discussion section to elaborate on the interpretation of convergences. We have revised the results to report (see table 2) the number of sample runs required to obtain converging results (see section 2.3.2). Only results that met the convergence criteria were reported. We generally concluded that convergence was obtained when model assumptions are appropriately met and the empirical pdf is consistent with the parameters defined in the analytical model. The revised manuscript compared annual pdfs instead of summer season pdfs. This approach was overall more appropriate and model inversions for all sites and datasets converged.

5. Finally, I would find it useful to get a sense of how parameters estimated using SM observations taken at a certain scale are valid at different scales. This would have interesting implications, for instance in terms of using satellite remote sensing SM observations to estimate smaller scale SM dynamics in ungauged regions. You discuss this point a little in the paper, but it would be interesting to substantiate your arguments with some analysis. For instance you could run a goodness of fit analysis between modeled SM distributions using params estimated at one scale to empirical SM pdfs observed at another scale.

**These are interesting questions that may be better answered with a different dataset. Our results indicate that the parameters estimated at one scale are not applicable at other scales. One reason is that soil texture constraints ( $s_n$  and  $s_{fc}$ ) are different. Another point is that when averaging over larger areas, the effects of a large number of plants (as opposed to one in a point measurement) will change the  $s^*$  and  $s_w$ . Ideally soil water retention parameters would be accurately known and soil saturation thresholds could be converted to more universal values such as soil water potentials and therefore be more transferable for scaling analysis, assuming  $E_{max}$  is uniform within the area.**

*Minor comments*

*p3. I would find it useful if you could comment on the advantages of using the Bayesian inversion approach you propose vs more "standard" frequentist approaches such as maximal likelihood, which is the go-to approach I would take to fit a "low dimensional" (4 params) closed form analytical pdf.*

**This comment is addressed by revising the following sentence in the introduction:**

We selected a Bayesian inversion approach instead of a least-squares or maximum likelihood approach because it quantifies the inference uncertainty directly and improves upon the work of Miller et al. (2007), which used a least-squares approach to calibrate soil saturation pdfs. In addition, measures of inference uncertainty and parameter convergence diagnostics provided by the Bayesian approach can be used to evaluate the validity of model inversion and develop criteria to generalize the presented framework.

*p7 l.18. To illustrate your claim, it would be useful if you could present statistics on the frequency of  $s$  in each zone of the pdf (in eqn 2) using your best estimation of  $s^*$  and  $s_w$  at each site.*

**We visualized  $s^*$  and  $s_w$  in Figures 2-5 to address this suggestion. Also, we reported minimum and maximum observed soil saturation for each site and scale in Table 1.**

*p7. Please describe your procedure to compute empirical pdf's from time series observation. If you use kernels to estimate density functions, please specify and justify the chosen shape and bandwidth.*

**Empirical pdfs were visualized with histograms in Figure 3 using 20 bins, evenly spaced between 0 and 1. In the Bayesian inversion, for each observed soil saturation value, we compute the theoretical probability of that value given a set of model parameters. The quantile level NSE evaluates quantiles from 1/365 to 354/365.**

*p9 l.20: 'discarded'*

**This was corrected**

*p10: section 3 is missing*

**This was corrected**

*p11. It would be useful to summarize the results (model, scale, posterior CV, goodness of fit distance) for the different cases of the sensitivity analysis in a table.*

**Table 2 reports the most important summary statistics and results.**

*p12 l.27. "Consistent" has a very specific statistical meaning (asymptotically unbiased), please rephrase if necessary*

**We rephrased to:**

because the mean and standard deviation of the randomly selected subsets of annual data were generally representative of the full record

p13 l 18: "versus"

**This was corrected**

5 p 14 l3. Please elaborate on how you could disentangle confounding effects of scale and observation depths. The way I understand it, your analysis in Section 4.2 shows that the results are insensitive to the assumed root-zone depth, not the actual depth, which appears to be unknown (see point 3 above).

10 **Yes, our analysis shows that estimates of  $s_w$  and  $s^*$  are not very sensitive to the depth assumed in the model inversion. This is important if the sensing depth is not precisely known or is variable in time and space, which is the case for the cosmos and satellite measurements. We removed the sensitivity test related to soil depth because it is not useful to determine whether estimates of  $s_w$  and  $s^*$  derived from surface soil moisture measurements are relevant to deeper soil depths. We have defined the choice of setting  $Z$  to the measurement depth in the methods section (2.2.2).**

15 Fig 5: you state that the Kolmogorov statistic is significant with a 95% confidence levels. Does that mean that the statistic is significantly different from zero? If so, I would interpret that as having a 5% chance of being wrong if I state that the two compared distributions are different (see my point on KS tests above), which I don't think is the point you intended to make.

20 **Yes, that was the point we intended to make, we have removed the details about the KS significance in the figures as response to your comment above.**

#### References

Ceola, Serena, et al. "Comparative study of ecohydrological streamflow probability distributions." *Water Resources Research* 46.9 (2010).

25 Müller, M. F., and S. E. Thompson. "Comparing statistical and process-based flow duration curve models in ungauged basins and changing rain regimes." *Hydrol*



## Response to David Dralle (Referee #3)

*The authors pair in situ and remotely sensed soil moisture data with a Bayesian approach to infer parameters in a 1-d analytical model for soil moisture dynamics.*

5

**Thank you for your thorough review and constructive suggestions. We have provided responses and corrections below.**

*General Comments:*

10 1) *My primary concern is that the authors frequently claim “accurate” results, yet the study does not include any comparison between predicted and measured soil moisture thresholds. I would say that the study is more accurately described as an exercise in Bayesian model calibration. The novelty of the study, in my opinion, lies in comparing parameters of calibrated PDFs across observation scales. This is a useful exercise, though it’s not fully explored in the study.*

15 **We agree that this study is primarily an exercise in Bayesian calibration of the commonly used stochastic soil water balance model. We explore whether a Bayesian inversion of the model can provide plausible estimates of ecohydrological parameters that are generally not directly measured. It is therefore challenging to compare estimated parameter values to site-specific observations and determine their accuracy because these are not directly available. We have adopted the wording ‘identifiability’ to avoid making overly strong statements about the parameter estimates. As suggested in your minor comments, we have cited calibrated parameters from**

20 **previous studies in the revised manuscript.**

**Section 2.4 and 2.5 was added in the revised manuscript to explicitly describe evaluation goals and metrics used.**

25 **A range of different sites was selected to develop and demonstrate methods in varying environmental conditions. However, the purpose of this study is not to compare estimated values at these sites. We limit the scope of this paper to presenting the model inversion methods and deriving criteria to obtain meaningful parameter estimates. A comparison of estimated parameters can be the focus of a future study in which a larger number of sites are considered and provide more insights on the variability of these ecohydrologic parameters. We amended the statement of objectives in the introduction and our conclusions to clarify this scope.**

30

*The authors only go so far as to say that “spatial heterogeneity” explains shifting parameter values across scales. The significance of the study would be greatly increased if the authors worked to address some of these scaling effects. A couple questions include: How transferrable are inferred parameter values between scales? How might the optimal form of the PDF change across scales if heterogeneity is the culprit? And, are there simple in silico exercises that could be performed to explore these questions? For*

35 *example, if the authors generate spatially correlated fields of soil moisture parameters and solve the 1-d model at each point, can aggregation explain (even qualitatively) observed trends in the inferred parameters? What are the implications for applications in sparsely monitored areas, or for making useful predictions at a point using remotely sensed data?*

**These are interesting questions that would require a different dataset.**

40 2) *While I appreciate the authors’ thoroughness, the inclusion of 6 distinct models for soil moisture dynamics somewhat obscures the paper’s results. What intuition does this degree of added complexity provide, other than “model performance increases when there are more parameters to tune”? Could some of these results be relegated to Supporting Information, keeping the two most illustrative models?*

45 **We agree that this section has some information that may be obscuring the main message. We have removed this analysis from the revised manuscript and only present the comparison of the steady state versus seasonal models with unknown parameters  $s_w$ ,  $s^*$ , and  $e_{max}$ .**

50 3) *The authors assume steady-state conditions for application of the stochastic models. While this may be appropriate for MMS and ARM, soil moisture dynamics at the seasonally dry sites Tonzi Ranch and Metolius are highly non-stationary during the dry season study months April – September. One can see this in the bi-modality of the soil moisture PDFs in Figure 3. At the very least, it is important for the authors to address or test the effects of this non-stationarity on inferred parameter values. How might strong non-stationarity affect the interpretability of parameter inferences? Perhaps more appropriately, the authors could consider related models that can accommodate seasonally dry soil moisture dynamics. In particular, Dralle et al. (2016, doi: 10.1002/2015wr017813) develop a seasonal stochastic soil moisture model and apply the model at Tonzi Ranch. The calibrated*

parameter values in that study are exactly comparable to inferred values in the present study. Similarly, Viola et al. (2008, doi: 10.1029/2007WR006371) present a transient formulation of the same stochastic soil moisture model.

**We agree that seasonality at the Tonzi and Metolius sites affect our ability to inverse the soil water balance model with the selected data. The revised analysis utilized a full year timeseries and also adopts the suggested framework in Dralle and Thompson (2016) to account for non-stationary dynamics.**

*Specific Comments:*

*Page 1 Lines 8-9: What is a “hydrologically meaningful” scale?*

**The first sentence of the abstract was changed to**

Vegetation controls on soil moisture dynamics are generally not directly measured directly and not easy to translate into scale and site-specific ecohydrological parameters for simple soil water balance models.

*Page 1 Lines 9-10: Passive voice makes the sentence a little confusing; try, “we hypothesize that pdfs of soil saturation encode sufficient information. . .”*

**The sentence was changed to:**

We hypothesize that empirical probability density functions (pdfs) of relative soil moisture or soil saturation encodes sufficient information to determine these ecohydrological parameters, and that these parameters can be estimated through inverse modelling of the commonly used stochastic soil water balance.

*Page 1 Line 12: When the authors refer to soil “saturation”, do they mean “water content”, or “moisture”? I associate the word “saturation” with a water content equal to porosity.*

**We specify : relative soil moisture or soil saturation**

*Page 1 Line 28: Check spelling of reference.*

**The spelling was fixed**

*Page 1 Line 31: What are the “mean components of the soil water balance”?*

**Sentence was changed to:**

Given this ecohydrological framework, the probability density function (pdf) of soil moisture and the mean components of the soil water balance (rainfall, runoff, evapotranspiration, and leakage losses) are analytically derived

*Page 2 Line 17: Issues with citations*

**The citation was fixed**

*Page 3 Line 18: “interference”?*

**Interference was changed to inference**

*Page 4 Lines 1-2: Usage, “confront pdfs. . .to a commonly used analytical model”?*

**We reworded to match pdfs**

*Page 6 Lines 3-4: I do not believe the model specifies that ET occurs at a constant rate  $E_{max}$ .*

**The word constant was removed and the sentence was changed to:**

The rate of evapotranspiration is assumed to occur at a maximum rate ( $E_{max}$ ), which is independent of the saturation state.

*Page 7 Line 12: Do Rawls (1982) list physical soil characteristics for these sites?*

**The sentence now reads:**

Physical soil characteristics for soil textures associated with each site,  $s_h$ ,  $K_s$ , and  $b$  were taken from Rawls et al. (1982) and are listed for each site in Table 1.

*Page 8 Lines 9-10: It’s not clear to me why values for  $E_w/E_{max}$  must be tested in a separate (not shown) calibration procedure. See General Comment (2).*

**Seer response to General Comment (2). Our results showed that  $E_w/E_{max}$  needs to be smaller than 10% for equifinality to be reduced and that the convergence, goodness of fit and posteriori parameter distributions were not sensitive to values between 1 and 10%. So we picked 5%. We are not including Supplementary material in with this manuscript. However the code associated with the analysis will be published.**

Page 12 Lines 6-7: My understanding of  $E_{max}$  is that it quantifies atmospheric moisture demand. Why should it scale with rooting depth? Typically, I've seen this value computed using Penman-Monteith e.g. Viola et al. (2008, doi: 10.1029/2007WR006371).

**$E_{max}$  is not exactly the atmospheric moisture demand, it is a fraction of the atmospheric moisture demand that can be withdrawn from the soil layer considered.  $E_{max}$  can be equal to the atmospheric moisture demand approximated by potential evapotranspiration (PET) if the full soil column or rooting depth is considered.**

**In this study we cannot assume that  $E_{max} = PET$  because only the surface soil moisture is sensed. In the revised manuscript we will only consider  $Z$  equal to the sensing depth and  $E_{max}$  is always expected to be lower than PET. We clarified definitions in section 2.2.2 with the following sentences**

The soil depth considered corresponded to the measurement sensing depths of 10, 20, and 5 cm for the point, footprint, and satellite scales, respectively. Because the soil depth  $Z$  is more shallow than the rooting depth,  $E_{max}$  is only a fraction of the atmospheric moisture demand (or potential evapotranspiration) contributed by that soil depth and therefore unknown.

Page 13 Line 1: I would suggest that model performance at Tonzi and Metolius suffers primarily due to the stationarity assumption, which is likely not valid at these Mediterranean sites.

**We agree, and revised the analysis to discussion this comment.**

## Response to Xue Feng (Referee #4)

The manuscript titled “Probabilistic inference of ecohydrological parameters using observations from point to satellite scales” by Bassiouni et al. adopts a Bayesian inference approach to estimate parameters from a parsimonious soil moisture model based on readily available data (soil texture, rainfall, soil moisture) at the point, footprint, and satellite scales. This is a worthwhile exercise and paves the way for the evaluation of the utility of soil moisture data from satellite products. I recommend its publication contingent on clarification on a few issues.

**Thank you for your thorough review and constructive suggestions. We have provided responses and corrections below.**

1. A key assumption embedded in the use of this approach requires that the time series of soil moisture capture the whole range of realizable values. This is required to disentangle cases where soil moisture values cannot be observed due to physical constraints (e.g., imposed by saturation thresholds – the point of this study) versus heuristic constraints (e.g., we simply have not measured it under sufficiently wet or dry conditions). Please include this caveat and discuss practical considerations in overcoming this issue.

**We agree. This is an important assumption that should be described more explicitly and addressed in the revision. A number of sections of the introduction and methods section (2.2.2, 2.4 and 2.5 ) have been revised to consider this suggestion.**

2. Relatedly, the study concludes that “model inference at wetter sites... is more successful than at dry sites” because known rainfall parameters have been used to constrain the model at wetter sites, where it is hypothesized to play a stronger role in determining the soil moisture pdf. I think this is true, but does not capture the whole story. The “drier” sites used in this study (Tonzi Ranch and Metolius) are also located in Mediterranean climates where substantial seasonal variations in soil moisture can occur between early summer (April/May) and late summer (Sept), which span the period of study. This is apparent from inspection of Figure 1, where soil moisture undergoes an initial rapid decay in Tonzi and Metolius.

As such, I suspect that this assumption of steady state may impact the following statement which I found very interesting (Page 11, line 15): “sw was more important in the analytical equation for soil saturation pdfs and soil water loss equations than  $s^*$ .” If the time series span a transient period that eventually converge toward a dry state, then the shape of the soil moisture pdf would be less defined around  $s^*$  because there would be relatively fewer soil moisture values near  $s^*$  than near sw. In that case, sw would naturally become a more important parameter because the shape of the soil moisture pdf would be more defined around sw, but this would be purely an artifact of the relative data availability around sw and  $s^*$ . To test this issue, I think it might be useful to divide the time series into more distinct periods of “wet,” “transition,” or “dry” and use those periods to explicitly estimate the relevant parameters  $sfc$ ,  $s^*$ , and sw.

**We agree with your comment. The revised analysis utilized a full year timeseries and also adopts the suggested framework in Dralle and Thompson (2016) to account for non-stationary dynamics.**

And a tangential note on Page 6, line 22 “this framework was derived under the assumption of steady state, wherein parameters are constant for a given period of time.”

Constant parameter values are not sufficient criteria for achieving steady state – as it can also result in a transient period based on initial conditions. Please be careful with this terminology.

**We clarified that the theoretical pdf equation is the steady state solution of the stochastic soil water balance but it does not necessarily imply that the data indicates a steady state.**

3. The role of rooting depth. While the model-data fit was not greatly affected by different rooting depths, the resulting values for  $E_{max}$  certainly was. Thus, the authors were able to demonstrate equifinality of results by using  $E_{max}$  to compensate for changes in Z. If the goal is to ultimately estimate meaningful values of vegetation and hydrological thresholds from data, is model-data fit a sufficient metric for evaluation of this approach? My own take away from this part of the study was that rooting depth can in fact be a very sensitive parameter due to the large amount of change in  $E_{max}$  required to achieve similar fit with data. Perhaps a more useful way of tackling this question would be to include Z as another model parameter and evaluate the site and climate conditions under which its impacts would be limited.

**Z was not included as a parameter to be estimated because it is most appropriate for Z to be equal to the measurement depth associated with each measurement. Our analysis shows that estimates of sw and  $s^*$  are not very sensitive to the depth Z assumed in the model inversion while  $E_{max}$  scales as expected with Z. This is important if the sensing depth is not precisely known or is variable in time and space, which is the case for the**

cosmos and satellite measurements. The model inversion convergence, and the coefficient of variation of posteriori parameter estimates were the more important metrics to detect equifinality than goodness of fit. We have previously tested the model inversion including  $Z$  as a parameter to be estimated. We found in this case, a decreased in convergence and no increase in goodness of fit because there is equifinality between pairs of  $Z$  and  $E_{\max}$ .

In the revised manuscript we only consider  $Z$  equal to the sensing depth. We removed the sensitivity tests related to soil depth because it is not useful to determine whether estimates of  $sw$  and  $s^*$  derived from surface soil moisture measurements are relevant to deeper soil depths.

10 4. A few definitions:

Page 1, line 14: “parameter uncertainties” – how are these defined?

The term “parameter uncertainties” was changed. The sentence reads: the coefficient of variation of posteriori parameter distributions were ...

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Page 11, line 9: “the most successful parameter estimations were obtained. . . with 97, 94, 85 percent converging results” – how are these percentages defined (via GR diagnostics?) and what is the significance of the different levels of convergence? I couldn't find a reference in the text.

We defined in the methods section that the GR diagnostic determines that the algorithm reaches convergence when the within-run variability ( $\sigma_w$ ) is roughly equal to the between-run variability ( $\sigma_b$ ), i.e.  $\sigma_w/\sigma_b$  approaches 1. We considered that a model inversion had appropriately converged if the GR diagnostics was lower than 1.1 for each estimated parameter. See explanation in section 2.3.2 of the revised manuscript.

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Minor point: section 4 (results and discussion) should actually be section 3.

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The numbering was corrected.

# Probabilistic inference of ecohydrological parameters using observations from point to satellite scales

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**Abstract.** ~~Ecohydrological parameters that describe vegetation~~ Vegetation controls on soil moisture dynamics are ~~not~~ easy ~~challenging~~ challenging to measure ~~at hydrologically meaningful scales and translate into scale~~ and site-specific ~~values are rarely~~ available ~~eco~~hydrological parameters for simple soil water balance models. We hypothesize that empirical probability density functions (pdfs) of relative soil moisture or soil saturation encodes sufficient information ~~required~~ required to determine these ecohydrological parameters ~~is encoded in empirical probability density functions (pdfs) of soil saturation, and that this information.~~ Further, these parameters can be ~~extracted~~ estimated through inverse ~~modeling~~ modelling of the analytical equation for soil saturation pdfs, derived from the commonly used stochastic soil water balance framework. We developed a generalizable Bayesian inference ~~approach~~ framework to estimate ~~soil saturation thresholds at which plants control soil water losses, based only on soil texture, rainfall and soil moisture data~~ ecohydrological parameters consistent with empirical soil saturation pdfs derived from observations at point, footprint, and satellite scales. ~~The optimal analytical soil saturation pdfs were statistically consistent with empirical pdfs and parameter uncertainties were on average under 10 %.~~ We applied the inference method to four sites with different land cover and climate assuming i) an annual rainfall pattern and ii) a wet season rainfall pattern with a dry season of negligible rainfall. ~~The Nash-Sutcliffe efficiencies of the analytical model's fit to soil observations ranged from 0.89 to 0.99. The coefficient of variation of posterior parameter distributions ranged from <1 to 15 %. The parameter identifiability was not significantly improved in the more complex seasonal model; however, small differences in parameter values indicate that the annual model may have absorbed dry season dynamics.~~ Parameter estimates were most constrained for scales and locations at which soil water dynamics are more sensitive to the fitted ecohydrological parameters of interest. ~~The algorithm convergence was most successful and the best~~ In these ~~cases, model inversion converged more slowly but ultimately provided better~~ goodness-of-fit statistics and lower uncertainty. ~~Results were obtained at the satellite scale. Robust and accurate results were obtained with~~ robust using as little ~~few~~ few as ~~75~~ 100 daily observations randomly sampled from the full records, demonstrating the advantage of analyzing soil saturation pdfs instead of time series. ~~A sensitivity analysis showed that estimates of soil saturation thresholds at which plants control soil water losses were not sensitive to soil depth and near surface observations are valuable to characterize~~ estimate ecohydrological ~~factors driving soil water~~ dynamics at ecosystem scales. ~~This~~ parameters from sparse records. Our work ~~combined modeling~~ combines modelling and empirical approaches in ecohydrology and ~~provided~~ provides a simple framework to obtain scale- and site-specific analytical descriptions of soil moisture dynamics ~~at a range of spatial scales that are~~ consistent with soil moisture observations.

## 1 Introduction

The movement of water from soils, through plants, and back to the atmosphere via transpiration, is a critical component of local and global hydrologic cycles, and is the largest surface-to-atmosphere water pathway (Good et al., 2015). A realistic analytical description of soil moisture dynamics is key to understanding ecohydrological processes that regulate the productivity of natural and managed ecosystems. ~~Rodrigues~~ Rodriguez-Iturbe et al. (1999) introduced a ~~conceptually~~ simple framework using a bucket

model of soil-column hydrology forced with stochastic precipitation inputs, where soil water losses are only a function of relative soil moisture or soil saturation. Given this ecohydrological framework, the analytical equation for the probability density function (pdf) of soil moisture and the mean components of the soil water balance are analytically derived and depends on simple abiotic characteristics such as average climate and soil texture, and biotic characteristics including soil saturation thresholds at which vegetation can influence soil water losses. However, the shapes of analytical soil moisture saturation pdfs are generally not consistent with observations when literature values for model parameters are used (Miller et al., 2007). Analytical pdfs have never been directly compared Some parameters such as field capacity and wilting point do not correspond to conventional definitions, because of simplifications made to describe soil water loss processes in the model, and need to be calibrated (Dralle and Thomsson, 2016a). To our knowledge, parameters of the analytical soil saturation pdfs have not been directly calibrated to empirical pdfs derived from measurements beyond the point scale. Observation networks provide freely available point scale, spatially integrated soil moisture observations, while remotely sensed soil moisture observations are available through satellite products. These data sources create an opportunity to: 1i) evaluate whether analytical soil saturation pdfs are consistent with observations across a range of scales; and 2ii) determine average ecohydrological parameters relevant to each scale.

Estimates of ecohydrological parameters are relevant to used in a large range of applications for which the stochastic soil water balance framework has been used and adapted, including: the effects of climate, soil and vegetation on soil moisture dynamics (Laio et al, 2001a; ~~Rodrigues~~ Rodriguez-Iturbe et al., 2001; Porporato et al., 2004); ecohydrological factors driving spatial and structural characteristics of vegetation (Caylor et al., 2005; Manfreda et al., 2017); soil salinization dynamics (Suweis et al., 2010); biological soil crusts (Whitney et al., 2017); vegetation stress; optimum plant water use strategies and plant hydraulic failure (Laio et al., 2001b; Manzoni et al. 2014; Feng et al., 2017); vertical root distributions (Laio et al., 2006); plant pathogen risk (Thomsson et al., 2013); streamflow persistence in seasonally dry landscapes (Dralle et al., 2016, 2016b); and soil water balance partitioning (Good et al., 2014 ; Good et al., <http://rdeu.be/yqW7>); 2017. A survey of ~~close to~~ approximately 400 ~~ecohydrology~~ ecohydrology publications ~~found~~ revealed that 40% of studies relied heavily on simulation, rarely integrated empirical measurements, and were almost never coupled with experimental studies, suggesting a critical need to combine modeling modelling and empirical approaches in ~~ecohydrology~~ ecohydrology (King and Caylor, 2011). Few Only a few studies have directly confronted the governing equations of the stochastic soil water balance model with observed soil moisture data, and even fewer studies have attempted to optimize model parameters to best fit soil moisture observations. Miller et al., (2007) calibrated soil moisture saturation pdfs to project vegetation stress in a changing climate. Dralle and Thomsson (2016a) developed an analytical expression for annually integrated soil saturation pdfs under seasonal climates and then calibrated soil saturation thresholds between which evapotranspiration is maximum and zero to compare the model to soil moisture observations at a savanna site. Chen et al. (2008) related evapotranspiration observations at the stand scale to soil moisture values using a Bayesian inversion approach, and Volo et al. (2014) calibrated the soil moisture loss curve to investigate effects of irrigation scheduling and precipitation on soil moisture dynamics and plant stress. The functional form of the soil moisture losses was approximated using conditionally averaged precipitation (Salvucci, 2001; Saleem and Salvucci, 2002) and remotely sensed data (Tuttle and Salvucci, 2014). The time scale of soil moisture dry-downs, derived from the soil moisture loss equations, were parameterized using evapotranspiration measured at micro-meteorological stations (Teuling et al., 2006) and space-~~borne~~ borne near-surface soil moisture observations (McColl et al., 2017). These studies indicate that the ecohydrological soil water balance framework is consistent with ground and larger scale remotely sensed measurements.

This study expands upon previous work and presents sensitivity tests. Parameters representative of larger scale observations are necessary to generalize the direct inference of characterize ecohydrological parameters and associated uncertainty, from observed soil moisture pdfs processes at a range of ecosystem scales. We hypothesize that key information required to determine the and are more relevant to ecohydrological factors driving soil moisture dynamics is encoded in empirical soil saturation pdfs, and that this information can be extracted by calculating the inverse of the commonly used stochastic soil water balance. Non-biological modelling. These larger scale parameters integrate a range of ecohydrological interactions that are poorly understood and difficult to measure. Abiotic controlling factors on the of soil water balance including rainfall and soil texture can generally be assessed from readily available data, including site measurements, regionalized maps, and satellite observations. Vegetation, but vegetation controls on soil water dynamics are largely unknown and difficult to measure at hydrologically meaningful scales (Li et al., 2017). Vegetation water-use traits are generally observed at the species level and are not easily translated to the simple parameters necessary in soil-water balance models. The rate of soil water losses from the near-surface soil layer, where soil moisture measurements are generally made, do not precisely correspond to evapotranspiration observed or calculated from meteorological stations. We thus focused on estimating parameters that are not generally directly observable, in particular particularly the soil saturation thresholds at which vegetation controls soil water losses, through and the maximum rate of evapotranspiration from a near-surface soil layer. We use an inverse modelling approach and using data that are commonly collected at environmental monitoring sites. Analysis of soil saturation pdfs is a more robust and integrated approach to investigate ecohydrological factors of soil water dynamics than time series analysis. Soil saturation pdfs are less sensitive to the many sources of uncertainty and common gaps in soil moisture observations or measured from satellites. We present an inference framework that provides a means to quantify and do not require high quality co-located and concurrent hydrologic measurements that are often lacking. compare the sensitivity of soil moisture dynamics at varying scales through estimates of simple ecohydrological parameters.

A number of studies have combined inverse modeling modelling approaches with ground and remotely sensed soil moisture data to successfully extract meaningful hydrologic information (Xu et al., 2006; Miller et al, 2007; Chen et al., 2008; Volo et al., 2014; Wang et al., 2016; Baldwin et al., 2017). In particular, Bayesian inference methods are effective in relating prior pdfs of observations to posterior estimates of model parameters (Xu et al., 2006; Chen et al., 2008; Baldwin et al., 2017). The soil water balance model provides a direct analytical equation for soil moisture saturation pdfs that is convenient to use with the Bayesian paradigm because it is a low parameter model with few data inputs. In this study, we developed We selected a Bayesian inversion approach to directly estimate soil water balance model parameters that best fit soil moisture pdfs derived from observations at point, footprint, and satellite scales. The Bayesian instead of a least-squares or maximum likelihood approach because it quantifies the interference inference uncertainty directly and improves upon the work of Miller et al. (2007), which used a least-squares approach to calibrate soil saturation pdfs. Measures of inference uncertainty and parameter convergence diagnostics provided by the Bayesian approach can be used to evaluate the validity of model inversion and develop criteria to generalize the presented framework.

Parameters that are representative of larger scale observations are necessary to characterize ecohydrological processes at ecosystem scales and are more relevant to ecohydrological modelling. In addition, the resulting inference framework provides a means to compare the sensitivity of soil moisture dynamics at varying scales to simple ecohydrological parameters. The generalization of the proposed approach was evaluated using co-located and concurrent soil moisture observations at the point, footprint, and satellite scales. To our knowledge, this is the first study to infer parameters for the analytical model of soil saturation pdfs for scales beyond point observations. We sought to evaluate 4 key questions necessary to generalize the inference of ecohydrological parameters: (1) What is the minimum level of model complexity needed to obtain consistent analytical and empirical soil saturation pdfs, and which



parameters can be inferred with the most certainty? (2) Are ecohydrological parameter estimates sensitive to the soil moisture sensing depth, and can we assume a homogenous soil column of a depth greater than the sensing depth? (3) What is the minimum amount of data necessary to estimate ecohydrological parameters through a Bayesian inversion of soil saturation pdfs? (4) At which scales and sites are ecohydrological parameter estimates most accurate and pertinent?

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~~The goal of this study was to confront empirical soil moisture~~ We assume that if a sufficient range of soil moisture values are observed at a site, the shape of the empirical soil saturation pdf is constrained by the ecohydrological factors driving soil moisture dynamics. We hypothesize that key information required to determine these ecohydrological factors is encoded in empirical soil saturation pdfs and that this information can be extracted by calculating the inverse of the commonly used stochastic soil water balance. The analysis of soil saturation pdfs is a more robust and integrated approach to investigate ecohydrological factors of soil water dynamics than is time series analysis. Soil saturation pdfs are less sensitive to the many sources of uncertainty, sensor noise, and common gaps in soil moisture observations and do not require high-quality, co-located and concurrent hydrologic measurements that are often lacking. We tested three key assumptions embedded in the proposed method. (i) The analytical soil saturation pdfs properly describe empirical soil saturation pdfs observed in annual data. Annual soil moisture records can be affected by transitional dynamics between wet and dry seasons, and the appropriate level of model complexity must be used. We compare parameter identifiability using an annual and a seasonal formulation of the analytical soil saturation pdfs. (ii) Parameter estimates and their uncertainty at point-, footprint-, and satellite- scales are different and reflect variability in soil water dynamics. We determine whether the inference approach can be applied at point-, footprint-, and satellite-scales to provide appropriate scale-specific parameters for ecohydrological modelling. (iii) The range of realizable soil moisture values is captured by the selected time series and the soil saturation pdf determined from these observations is not truncated. We determine whether the inference method based on soil saturation pdfs is robust against reduced data availability by repeating the model inversions on subsets of the soil moisture time series and show that the method can be applied to sparse datasets.

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~~Our goal was to match empirical soil saturation~~ pdfs derived from point-, footprint-, and satellite-scale observations to a commonly used analytical model. We demonstrate the use of a Bayesian inversion framework to ~~infer~~calibrate the ecohydrological parameters of a simple stochastic soil water balance model that best fit empirical soil ~~moisture~~saturation pdfs. We first present data sources, define the analytical model for soil ~~moisture~~saturation pdfs including parameter assumptions, and detail the algorithm used in the Bayesian inversion. Then, we present a summary of the goodness of fit of optimal analytical soil ~~moisture~~saturation pdfs and estimated parameter uncertainty ~~for a range of sensitivity tests. Results of sensitivity tests were used. We evaluated results to define criteria for a generalization of the presented approach to future applications~~test key method assumptions including model complexity and data availability. Finally, we discuss the potential of the approach to provide a simple means to investigate variability in ecohydrological controlling factors at varying spatial scales. ~~This~~Our work combines modelling and empirical approaches in ~~ee~~hydrologyeco hydrology to provide more realistic analytical descriptions of soil moisture dynamics. Estimates of ecohydrological parameters that are consistent with observed soil ~~moisture~~saturation pdfs, from point- to ecosystem- scales, are needed to better characterize site-specific ecohydrological processes.

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## 2. Data and Methods

### 2.1 Data analysed

~~Daily~~We used ~~daily~~ soil moisture observations from three data products at three ~~different~~ spatial scales ~~were~~. We used ~~in this study~~. ~~Point~~point-scale soil moisture ~~data~~ at ~~10-cm~~ depth ~~was taken of~~ 10 cm from the FLUXNET2015 data product (http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/). ~~Footprint~~We used ~~footprint~~-scale soil moisture ~~was taken~~data from the Cosmic-ray Soil Moisture Observing System (COSMOS) (http://cosmos.hwr.arizona.edu/Probes/probelist.html). The COSMOS soil moisture footprint measures soil moisture at an average depth of 20 cm with a radius ranging from 130 to 240 m, depending on site characteristics (Köhli et al., 2015). Near-surface soil moisture observations at a spatial resolution of 0.25° were taken from the European Space Agency's (ESA) Climate change Initiative (CCI) project. ~~The~~We used ~~the~~ combined soil moisture product (ECV-SM, version 0.2.2) that merges soil moisture retrievals from four passive (SMMR, SMM/I, TMI, and ASMR-E) and two active (AMI and ASCAT) coarse resolution microwave sensors ~~was used~~(Liu et al., 2011; Liu et al., 2012; Wagner, 2012). Although the ECV-SM sensing depth is ~~less than~~ <5 ~~centimeters~~centimetres, it has been shown to have a close relation to ground-based observations of soil moisture in the upper 10 ~~centimeters~~centimetres (Dorigo et al., 2015). ~~Daily~~We compiled ~~daily~~ rainfall time series ~~were compiled~~ from the FLUXNET2015 dataset for the point- and footprint-scale analysis, and ~~the~~ National Aeronautics and Space Administration's (NASA) Tropical Rainfall Measuring Mission (TRMM) dataset (Huffman et al., 2007) for the satellite-scale analysis. ~~The growing season of May to September 2012 was selected for analysis because concurrent rainfall and soil moisture observations for each soil moisture and rainfall data product were available during this time period for a maximum number of sites.~~

~~In total~~,We selected 4 sites with ~~soil moisture and rainfall~~ data available ~~during April to September for the~~ 2012 ~~were selected for this analysis (calendar year (Figure 1, Table 1)).~~ Selected sites ~~spanned~~ a range of land cover types including crop and grasslands, oak savanna, deciduous forest and pine forest. ~~For each site, the~~We determined dominant soil texture of the upper soil layer ~~was determined~~ from the Harmonized World Soil Database (HWSD) (version 1.2) (FAO/IIASA/ISRIC/ISS-CAS/JRC, 2012). ~~Soil~~ for each site. We used soil porosity values, derived from the HWSD available as ancillary data through the ESA-CCI data product ~~were used~~, for the satellite-scale analysis. ~~For point- and footprint-scale data products, we used~~ the maximum soil moisture observation during the year 2012 ~~was used~~ as a site-specific soil porosity estimate. ~~Soil- for point- and footprint-scale data products, we used soil porosity for each site was applied to compute the relative soil moisture content or calculate~~ soil saturation  $s$  ( $0 \leq s \leq 1$ ) from each observed soil moisture value. ~~Soil saturation and rainfall- We do not expect the differences in data at each scale and for each site during the selected analysis period are presented in Fig. 1-quality between data sources and sites to significantly affect empirical soil saturation pdfs and resulting parameter estimates.~~ All sites had ~~183~~full records of daily point- and footprint-scale observations ~~except for US-Me2, which had 55 missing footprint-scale observations during winter when the ground was saturated and between 109 and 153 frozen. The number of~~ daily satellite-scale observations. ~~We consider that during in the selected analysis period May to September 2012 the steady state assumption is met. records ranged from 202 to 283.~~

### 2.2 Analytical model for soil saturation probability density functions (pdfs)

#### 2.2.1 Model definition

~~The~~Our framework ~~used in this study~~ is based on a standard bucket model of soil column hydrology at a point forced with stochastic precipitation inputs and in which soil water losses are a function of soil saturation. We ~~follow~~followed the simple formulation of

soil water losses in Laio et al. (2001a) and apply the). We applied two associated analytical formulations for the soil saturation pdf detailed below. However, the methodology described in Sect. 2.3 can be customized to characterize site-specific and derived under the assumption of steady state, wherein parameters are constant for a given period of time. The annual model assumed an annual rainfall pattern and test consistency between observed the seasonal model accounted for a wet season rainfall pattern and analytical soil saturation pdfs for any application or adaptation of the stochastic ecohydrological framework a dry season of negligible rainfall.

The soil water balance model is defined at a point scale and a daily time scale step, for a soil with porosity  $n_s$  and depth  $Z$ , and assumes assuming that soil saturation is uniform in the rooting zone considered soil column of depth  $Z$ . Rainfall, the only input to the soil water balance, is treated as a Poisson process distribution characterized by an average event frequency,  $\lambda$ , and average event intensity,  $\alpha$ . For simplification simplicity, we assume assumed that the rainfall applied is was equal to the amount reaching that reached the ground surface and do not account for rainfall intercepted that interception by vegetation, was negligible. Interception may be a significant component of the soil water balance at forested sites and may need to be considered in future extensions of this work. The daily soil water balance is written as the difference between  $\phi$ , the rate of rainfall infiltration from rainfall  $\phi$  and  $\chi$ , the rate of soil moisture losses  $\chi$ :

$$nZ \frac{ds(t)}{dt} = \phi[s(t); t] - \chi[s(t)] \quad (1)$$

$$nZ \frac{ds(t)}{dt} = \phi[s(t); t] - \chi[s(t)] \quad (1)$$

$\phi[s(t); t]$  is both a stochastic process controlled by rainfall and is also a state-dependent process, because excess rainfall relative to available soil storage is converted to surface runoff.  $\chi[s(t)]$ , the soil moisture loss curve, is summarized in Fig. 2a and  $\chi[s(t)]$ , includes leakage losses due to gravity and evapotranspiration and is described in stages determined by five soil saturation thresholds (Laio et al., 2001a). These stages are: (1i) the saturation point ( $s = 1$ ), at which all pores are filled with water; (2ii) the field capacity ( $s_{fc}$ ), at which soil-gravity drainage becomes negligible compared to evaporation; (3iii) the point of incipient stomata closure ( $s^*$ ), at which plants begin to reduce transpiration from water stress; (4iv) the wilting point ( $s_w$ ), at which plants cease to transpire; and (5v) the hygroscopic point ( $s_h$ ), at which water is bound to the soil matrix. Soil water losses are controlled by physical soil properties for saturation states above  $s_{fc}$ . The rate of leakage due to gravity is assumed maximum when the soil is saturated ( $K_s$ ) and decays exponentially to a value of  $\theta$  zero at  $s_{fc}$  (Brooks and Corey, 1964). Soil water losses are controlled by micro-meteorological conditions for saturation states between  $s_{fc}$  and  $s^*$ . The rate of evapotranspiration is assumed to occur at a constant maximum rate ( $E_{max}$ ), independent of the saturation state. Soil water losses are controlled primarily by vegetation for saturation states between  $s^*$  and  $s_w$ . Plants close their stomata in response to soil water deficits that drive leaf water potential gradients, as well as to atmospheric vapor pressure deficits, and evapotranspiration decreases linearly from  $E_{max}$  to  $E_w$  at  $s_w$ . Soil water losses are controlled by soil diffusivity for soil saturation states below  $s_w$ , and soil evaporation decreases linearly from  $E_w$  to  $\theta$  zero at  $s_h$ . Soil water losses are negligible for soil saturation states below  $s_h$ . The piece-wise linear relation between soil saturation and evapotranspiration is a simplifying assumption commonly used in soil water balance models.

For this simplified theoretical description of the soil water loss curve and stochastic rainfall forcing, the analytical solution of the steady-state probability distributions of soil saturation,  $p(s)$ , was given by Laio et al. (2001a) is:

$$p(s) = \begin{cases} 0, & 0 < s \leq s_h, \\ \frac{C}{\eta_w} \left( \frac{s-s_h}{s_w-s_h} \right)^{\frac{\lambda(s_w-s_h)}{\eta_w}-1} e^{-\gamma s}, & s_h < s \leq s_w, \\ \frac{C}{\eta_w} \left[ 1 + \left( \frac{\eta}{\eta_w} - 1 \right) \left( \frac{s-s_w}{s^*-s_w} \right) \right]^{\frac{\lambda(s^*-s_w)}{\eta-\eta_w}-1} e^{-\gamma s}, & s_w < s \leq s^*, \\ \frac{C}{\eta} e^{-\gamma s + \frac{\lambda}{\eta}(s-s^*)} \frac{\eta}{\eta_w} \frac{\lambda(s^*-s_w)}{\eta-\eta_w}, & s^* < s \leq s_{fc}, \\ \frac{C}{\eta} e^{-(\beta+\gamma)s + \beta s_{fc}} \left( \frac{\eta e^{\beta s}}{(\eta-m)e^{\beta s_{fc}} + m e^{\beta s}} \right)^{\frac{\lambda}{\beta(\eta-m)}+1} \frac{\eta}{\eta_w} \frac{\lambda(s^*-s_w)}{\eta-\eta_w} e^{\frac{\lambda}{\eta}(s_{fc}-s^*)}, & s_{fc} < s \leq 1, \end{cases} \quad (2)$$

where

$$\frac{1}{\gamma} = \frac{\alpha}{nZ},$$

$$\eta_w = \frac{E_w}{nZ},$$

$$5 \quad \eta = \frac{E_{max}}{nZ},$$

$$m = \frac{K_s}{nZ(e^{\beta(1-s_{fc})}-1)},$$

$$\beta = 2b - 4.$$

where  $b$ , is an experimentally determined parameter used in the Clapp and Hornberger, (1978) soil water retention curve, and the constant  $C$  can be obtained numerically to ensure the integral of  $p(s)$  is equal to 1. We used a simplifying relation  $E_w = 0.05E_{max}$  to 1. This framework was derived under the assumption of steady state, wherein parameters are constant for a given period of time.

We adopted Dralle and Thompson's (2016a) framework to account for transient dynamics between wet and dry seasons. We defined the dry season as a period of duration  $t_d$  in which precipitation was negligible and assumed to not contribute to soil moisture. During that period, we assumed soil saturation decayed from an initial value  $s_0$  to  $s(t_d, s_0)$ , given by Laio et al. (2001). For simplicity, we determined  $t_d$  using rainfall records at a monthly step (see Sec 2.2.2) and  $s_0$  was the soil saturation value on the last day of the wet season. Note that we did not define  $s_0$  as the soil saturation following the last significant storm of the wet season as was done in prior studies (Dralle and Thompson 2016a). We then calculated the annual soil saturation pdf ( $p_{wd}(s)$ ) as the weighted sum of the wet and dry season pdfs,  $p_w(s)$  and  $p_d(s)$ , respectively.

$$20 \quad p_{wd}(s) = \left(1 - \frac{t_d}{365}\right) p_w(s) + \frac{t_d}{365} p_d(s) \quad (3)$$

The steady state solution in Eq. (2) was used for the wet season pdf and the dry season pdf is numerically determined by

$$p_d(s) = \int_{s_0}^1 p_{s_d|s_0}(s, s_0) p_0(s_0) ds_0 \quad (4)$$

where  $p_0(s_0)$  is the pdf of the initial dry season soil saturation, equal to  $p_w(s)$ , and  $p_{s_d|s_0}(s, s_0)$  is the pdf of dry season soil saturation given an initial condition  $s_0$ .

$$p_{S_d|S_0}(s, s_0) = \frac{C_d}{t_d} \begin{cases} \frac{e^{\beta(s_0-s)}}{(\eta^d-m)e^{\beta(s_0-s)} - \eta^d + m + me^{\beta(s_0-s_{fc})}}, & s_{fc} < s \leq 1, \\ \frac{1}{\eta^d}, & s^* < s \leq s_{fc}, \\ \frac{1}{\eta^d - \eta_w^d} \left( \frac{s^* - s_w}{(\eta^d - \eta_w^d)(s - s_w) + \eta_w^d(s^* - s_w)} \right), & s_w < s \leq s^* \\ \frac{1}{\eta_w^d} \left( \frac{s_w - s_h}{s - s_h} \right), & s_h < s \leq s_w \\ 0, & s_0 \leq s, \\ 0, & s \leq s_h, \\ 0, & s \leq s(t_d, s_0) \end{cases} \quad (5)$$

where  $\eta^d$  and  $\eta_w^d$  are equivalent to  $\eta$  and  $\eta_w$  relative to  $E_{max}^d$ , the maximum evapotranspiration rate during the dry season, and  $C_d$  is a normalization constant. We used the analytical expression for soil saturation decay,  $s(t, s_0)$ , in absence of rainfall given by

5 [Laio et al. \(2001\)](#) to derive  $p_{S_d|S_0}(s, s_0)$ .

### 2.2.2 Climate, soil and vegetation parameter characterization

~~The We chose readily available data for rainfall characteristics ( $\lambda$  and  $\alpha$ ), length of the dry period ( $t_d$ ), and physical soil parameters ( $s_{fc}$ ,  $s_h$ ,  $K_s$ , and  $b$ ) used needed in the analytical models of soil saturation pdfs (Eq. (2)) are based on readily available data. We chose values based on our best estimates of the driving climate and physical soil controls on the soil water balance. We thus Eq. (3)). We focused on estimating the ecohydrological parameters  $s^*$ ,  $s_w$ , and  $E_{max}$ , and  $E_w$ , which describe vegetation controls/control on soil water losses and are not easily observable.~~

We acknowledge that the pre-defined-calculated rainfall characteristics and physical soil parameters based on observations or literature values may not be perfectly representative of the processes at each location or scale and could create biases and uncertainties in our fitted parameters of interest.

~~Rainfall characteristics  $\lambda$  and  $\alpha$  were calculated for the year and wet season months for each site from the FLUXNET2015 and TRMM rainfall records during the selected 2012 growing season following Rodriguez-Iturbe et al. (1984). The (Table 1). We used FLUXNET2015 rainfall characteristics were used for the point- and footprint-scale analysis, while the analyses, and we used TRMM rainfall characteristics were used for the satellite-scale analysis. Physical soil characteristics,  $s_h$ , TRMM rainfall records were generally consistent with ground-based measurements. For each location, we evaluated monthly FLUXNET2015 rainfall depth and categorized consecutive months contributing <5 % of the site's annual rainfall as dry season months (Fig. 1). We then calculated length of the dry period ( $t_d$ ) as the number of days in those dry months. We used physical soil characteristics for soil textures at each site ( $s_h$ ,  $K_s$ , and  $b$  were taken) from Rawls et al. (1982) and are listed for each site in Table 1. To be most (Table 1). We estimated  $s_{fc}$  from each soil saturation record (Table 1) to be consistent with the assumption that drainage losses are generally insignificant compared to evapotranspiration losses the day following a rain event,  $s_{fc}$  was estimated from each soil saturation record and listed in Table 1. All. We identified all days in the 2012 record immediately following an observed increase/decrease in soil saturation were identified and  $s_{fc}$  was estimated  $s_{fc}$  as the 95th percentile of the soil saturation values on these value of the selected days. The Daily soil saturation pdfs in this study generally indicate that soil moisture states below  $s_w$  and above  $s^*s_{fc}$  are rare, therefore (Laio et al., 2001), so we did not expect the pre-defined average soil texture values for  $s_{fc}$ ,  $s_h$  and~~

$K_s$  to significantly affect the results. Soil depths  $Z$  are 10, 20, and 5 cm for the point-, footprint-, and satellite-scales, respectively.  $E_{max}$  results. The is only a fraction of the atmospheric moisture demand (or potential evapotranspiration) contributed by that soil depth because we used a soil depth that is shallower than the rooting depth. Consequently our framework we present thus considers 4 includes 4 (or 3 if seasonality is ignored) unknown soil water balance parameters,  $s^*$ ,  $s_w$ ,  $E_{max}$ , and  $E_w$ . Our goal is estimate  $E_{max}^d$ .

5 We estimated these parameters, as defined over the following intervals:

$$\begin{cases} s_h \leq s^* \leq s_{fc}, \\ s_h \leq s_w \leq s_{fc}, \\ 0 \leq E_{max} \leq 10, \\ 0 \leq E_w \leq 5 \end{cases} \quad (3)$$

$$\begin{cases} s_h \leq s^* \leq s_{fc}, \\ s_h \leq s_w \leq s_{fc}, \\ 0 \leq E_{max} \leq 10, \\ 0 \leq E_{max}^d \leq 10 \end{cases} \quad (6)$$

where 10 and 5 mm day<sup>-1</sup> are the pre-defined upper possible bounds boundary for potential evapotranspiration and actual evapotranspiration at the wilting point. Estimates of  $s^*$  and  $s_w$  can be converted to soil matrix potential if soil water retention parameters are well known. The Clapp and Hornberger, (1978) soil water retention curve is highly non-linear and estimates of soil water potential at which stomata fully are open or closed were not evaluated in this study.

### 2.2.3 Model complexity descriptions

We considered the following 4 levels of complexity for the soil water loss curve model:

- 15 (i) evapotranspiration decreases linearly from  $E_{max}$  to 0 between  $s_{fc}$  and  $s_h$ ,
- (ii) evapotranspiration is maximum between  $s_{fc}$  and  $s^*$ , then decreases linearly from  $E_{max}$  to 0 between  $s^*$  and  $s_h$ ,
- (iii) evapotranspiration decreases linearly from  $E_{max}$  to  $E_w$  between  $s_{fc}$  and  $s_w$ , then decreases linearly from  $E_w$  to 0 between  $s_w$  and  $s_h$ . We also test a variation of model (iii), assuming  $E_w = 0.05E_{max}$  and call this model (iii')
- 20 (iv) evapotranspiration is maximum between  $s_{fc}$  and  $s^*$ , decreases linearly from  $E_{max}$  to  $E_w$  between  $s^*$  and  $s_w$ , then decreases linearly from  $E_w$  to 0 between  $s_w$  and  $s_h$ . We also test a variation of model (iv), assuming  $E_w = 0.05E_{max}$  and call this model (iv').

The simplest model (i) has one unknown parameter, and the most complex model (iv), equivalent to the Laio et al., 2001 model, has 4 unknown parameters. We used the simplifying relation  $E_w = 0.05E_{max}$  to reduce the number of model parameters in models (iii') and (iv'). For iii' and iv' a range of  $E_w/E_{max}$  fractions were tested (not shown), and although overall the method was not sensitive to this parameter, 0.05 was selected to provide converging results with low uncertainty. Models (i)–(iv) are defined in Table 2 and illustrated in Fig. 2. We evaluated models (i)–(iv) to determine which level of complexity is consistent with soil moisture observations and which parameters could be estimated with most certainty.

## 30 2.3 Bayesian inversion approach

### 2.3.1 Application of the Bayes theorem

Bayes' theorem, Eq. (4) is used to relate We related  $p(S)$ , the empirical soil saturation pdf of the  $j = [1, \dots, m]$  soil saturation observations ( $s_j$ ) and the analytical soil saturation pdfs in Eq. (2) or Eq. (2),3) derived from the simple soil water balance model

in Eq. (1) with 4 up to four unknown soil water balance parameters  $\theta = [s^*, s_w, E_{max}, E_w]$  using the Bayes' theorem defined as:

$$p(\theta|S) = \frac{p(S|\theta) p(\theta)}{p(S)} \quad (47)$$

~~The~~ where the posterior distribution,  $p(\theta|S)$ , is the solution of the inverse problem and describes the probability of model parameters  $\theta$  given the set  $S = [s_1, s_2, \dots, s_m]$  of soil saturation observations. Assuming uninformed prior knowledge, the prior distribution of model parameters  $\theta$ ,  $p(\theta)$ , are defined by uniform distributions over the intervals ~~in~~ (Eq. (3-6)). The conditional probability of observations  $S$  given model parameters  $\theta$ ,  $p(S|\theta)$ , is the likelihood function of model parameters  $\theta$ .

### 2.3.2 Parameter estimation and evaluation

~~The~~ We used the Metropolis-Hasting Markov chain Monte Carlo (MH-MCMC) technique ~~is used~~ to estimate the posterior distribution of  $p(\theta|S)$  by drawing random model samples  $\theta_i$  from  $p(\theta)$  and evaluating  $p(S|\theta_i)$  (Metropolis et al., 1953; Hastings, 1970; Xu et al., 2006). The We defined the likelihood function of a model  $i$ ,  $p(S|\theta_i)$  defined by as:

$$p(S|\theta_i) = \prod_{j=1}^m p(s_j|\theta_i) \quad (58)$$

where  $p(s_j|\theta_i)$  is the probability of observation  $s_j$  given ~~the model in~~ Eq. (2) or Eq. (3) using parameters  $\theta_i$ .

~~The~~ MH-MCMC technique converges to a stationary distribution according to the ergodicity theorem in Markov chain theory. The sampling algorithm ~~consists~~ consisted of repeating two steps: ~~(1)~~ (1) a proposing step, in which, the algorithm generates a new model  $\theta_i'$  using a random function that is symmetric about the previously accepted model  $\theta_i$ , and ~~(2)~~ (2) a moving step, to determine if the model should be accepted or rejected, in which,  $\theta_i'$  is tested against the Metropolis criterion ~~(a) to estimate if it should be accepted or rejected~~ defined as:

$$a = \frac{p(S|\theta_i')}{p(S|\theta_i)} \quad (69)$$

If  $a > 1$ , ~~then~~  $\theta_i$  is ~~was~~ accepted and  $\theta_{i+1} = \theta_i'$  is ~~was~~ used for the next sample. If  $a < 1$ , a random number  $p_* \in [0,1]$  is ~~was~~ drawn from a uniform distribution and compared to  $a$ . If  $p_* < a$ , ~~then~~  $\theta_i'$  is ~~was~~ accepted and  $\theta_{i+1} = \theta_i'$  is ~~was~~ used for the next sample. If  $p_* > a$ ,  $\theta_i'$  is ~~was~~ rejected and  $\theta_{i+1} = \theta_i$  is ~~was~~ used for the next sample. If  $\theta_i'$  is ~~was~~ an inconsistent model in which ~~the~~ soil saturation thresholds ( $s_w, s_*$ ) are ~~were~~ ranked incorrectly or any of the soil water balance parameters ( $s^*, s_w, E_{max}$  ~~and~~  $E_w$ ) are

~~$E_{max}^d$~~  were outside of their defined physical bounds, the model likelihood ~~is~~ was zero and  $\theta_i'$  is ~~was~~ never accepted. ~~In this study,~~ The log-likelihood was more convenient to compute than the likelihood. The symmetric function used in the proposing step was a Gaussian distribution with a mean value equal to the accepted model  $\theta_i$  and a standard deviation of 1 percent% of interval range for which each parameter is defined in Eq. (3).

~~The~~ (6). We selected this value of the standard deviation of each model parameter ~~was set~~ after a number of test runs to generally ensure an acceptance rate between 20 and 50% (Robert and Rosenthal, 1998). Statistics We obtained statistics of the estimated parameters in  $\theta$  ~~are obtained~~ from the union of 5 ~~three~~ run samples of 20 ~~thousand,000~~ simulations each. The burn-in period is the number of simulations after which the running mean and standard deviation are stabilized. We considered a burn-in period of 10 ~~thousand,000~~ simulations, which were discarded for each run sample. If the acceptance rate of a run sample ~~is below~~ was <1% or greater than 80 ~~>90%~~ after the burn-in period, we discarded the run ~~was discard~~ and ~~we~~ concluded that the algorithm ~~converged~~ was stuck in a local minimum that may ~~might~~ be physically impossible. ~~If more than 10 run sample were performed without retaining 5 run samples, we concluded that the soil saturation record did not contain enough information to estimate  $\theta$ . Convergence~~

~~was-We~~ evaluated convergence by the Gelman-Rubin (GR) diagnostic (Gelman and Rubin, 1992) on the ~~final 5~~-run samples. The GR diagnostic determines that the algorithm reaches convergence when the within-run variability ( $\sigma_w$ ) is roughly equal to the between-run variability ( $\sigma_b$ ), ~~i.e. that is, when~~  $\sigma_w/\sigma_b$  approaches 1. ~~For records that obtain 5 converging run samples, one.~~ We verified that the GR diagnostic for each estimated parameter was  $<1.1$ . If the GR diagnostic did not indicate that the three run samples converged, we discarded the run with the lowest likelihood and re-initiated a new run sample until convergence was attained. We counted the number of attempts to quantify how rapidly convergence occurred. We computed mean and standard deviation ~~offor~~ for each parameter from ~~thea~~ total of ~~50 thousand~~30,000 simulations of  $\theta$  ~~were computed resulting from the three converging run samples.~~ A mean analytical model of soil saturation pdf was determined by applying Eq. (2) or Eq. (3) with the mean values of the ~~50 thousand posterior~~30,000 posterior parameter estimates. ~~The Kolmogorov-Smirnov statistic and Quantile-Quantile plots were used to evaluate the consistency of the mean analytical model and the empirical soil saturation pdfs. Calculations in this study relied on supercomputer resources through the Extreme Science and Engineering Discovery Environment (XSEDE) (Towns et al., 2014). Custom scripts in the Python computing language associated with this analysis are available through a gitHub repository (citation TBD).~~

## 2.4 ~~Description~~ Model evaluation criteria

~~We did not have direct measurement to validate the parameters  $s^*$ ,  $s_{w,2}$  and  $E_{max}$  estimated through the Bayesian inversion methods. We therefore analysed convergence and uncertainty metrics of sensitivity tests~~ the model inversion and goodness of fit between empirical and analytical soil saturation pdfs to evaluate the identifiability of the ecohydrological parameters. We compared the optimum analytical pdf derived from the mean parameter estimates and the empirical pdfs derived from observations. We evaluated the model inversion using the following criteria:

- ~~(i) This study investigates questions of model complexity.~~ Convergence of the Bayesian inversion: a GR diagnostic  $<1.1$  for all unknown parameters is obtained from the union of three run samples and within  $\leq 10$  sample runs.
- ~~(ii) Low uncertainty in parameter estimation, estimates: the posterior distributions of parameter estimates are physically plausible and have coefficients of variations  $<20\%$ .~~
- ~~(iii) Goodness of fit: a quantile-level Nash-Sutcliffe efficiency (NSE) (Müller et al., 2016)  $> 0.85$  and a Kolmogorov-Smirnov statistic  $<0.2$ .~~

## 2.5 Method assessment

~~Major assumptions and limitations embedded in the proposed inference framework were tested through the analysis detailed below. We assume, for each scale and location, that the shape of empirical the soil saturation pdfs is controlled by the physical constraints used to parameterize the analytical model of soil saturation pdfs, these parameters can be determined with some certainty and reflect variability in soil water dynamics. We expect that estimated soil saturation thresholds have greater certainty when the empirical soil saturation pdf is defined around those values and greater uncertainty when fewer soil saturation values are observed around the thresholds. We acknowledge that pre-defined rainfall characteristics and physical soil parameters based on observations or literature values may not be exactly representative of the processes at each location or scale and could also create biases and uncertainties in the fitted parameters of interest. We used model evaluation criteria (Section 2.4) to investigate the applicability of the inference framework with varying model complexities, scales, locations and data availability, and scales of applicability through the following four levels of sensitivity analysis. Each level of analysis was repeated 10 times using.~~



(i) ~~Analytical expressions for soil saturation pdfs were derived under the assumption of steady state. Annual soil moisture records at each scale and site to obtain robust median results can be affected by transitional dynamics between wet and dry seasons, and the appropriate level of model complexity must be used. We applied the inversion framework to annual soil saturation using variations of the analytical model for soil saturation pdfs of increasing complexity: (i) the annual model in Eq. (2) and (ii) the seasonal model in Eq. (3). We determined whether the added complexity of the dry season pdf increases the identifiability of ecohydrological parameters or if the simpler annual model is sufficiently consistent with annual empirical soil saturation pdfs.~~

~~(1) We compared co-located parameter estimates and their uncertainty at We applied the inversion framework to variations of the analytical model for soil saturation pdfs (Eq. 3) of increasing complexity from one to four unknown parameters (Table 1, Fig. 2). We determined which parameters can be estimated with acceptable certainty and if more parsimonious analytical models for soil saturation pdfs are consistent with empirical pdfs and may be more robust to use.~~

(ii) ~~point-, footprint-, and satellite- scales for each site. We determine whether the inference approach can provide appropriate scale-specific parameters for ecohydrological modelling at each location.~~

~~(2) We assumed that the whole range of realizable soil saturation values was captured within the selected time series at each scale and that the resulting soil saturation pdf was not truncated. If the range of observed values is not representative of the soil saturation pdf because it is truncated or affected by noise in the data, parameter estimates may be biased. Minimum and maximum observed soil saturation values during 2012 (Table 1) indicate the range of observed soil saturation values we used to estimate ecohydrological parameters. We determine whether the inference method based on soil saturation pdfs is robust against reduced data availability by repeating the model inversions on subsets of the soil saturation time series and show that the method can be applied to sparse datasets. We performed the model inversion with a range of rooting depths between 5 cm and 1 m. We determined whether the approach using near surface soil saturation observations can evaluate the soil water balance over a range of deeper rooting depths  $Z$ . We tested the assumption of a homogenous soil column and evaluated the sensitivity of the rooting depth on the estimation of soil water balance parameters. This analysis also determined whether it is necessary to input the exact soil moisture sensing depth, which is often unknown for larger-scale observations, to accurately perform the model inversion.~~

~~(3) We performed the model inversion with using subsets of each soil saturation record by randomly resampling fractions of the data down to 20% of the 10% of the annual timeseries and computed goodness of fit statistics between the resulting analytical models and the empirical models based on the full annual record (April and September 2012). We determined the number of data points necessary to infer converging model parameters that best match observations and which data availability criteria influence the convergence and accuracy of the model inversion.~~

~~(4)(iii) We compared co-located parameter estimates and their uncertainty at a range of scales for each site by integrating findings from the above levels of analysis. We determine whether the soil saturation pdf model inversion framework is applicable to point, footprint, and satellite scale observations and whether inferred parameters can be appropriate for ecohydrological modelling at all scales and locations. Co-located and concurrent soil saturation pdfs at a range of scales and their associated model parameter estimates were used to understand whether average ecohydrological parameters vary with scale the~~

proposed inference method based on soil saturation pdf can be reliably used to identify ecohydrological parameters from sparse datasets.

4

### 3. Results and discussion

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#### 3.1 Level of model complexity

For each of the ~~4 selected~~ four locations (Table 1), we obtained optimal analytical soil saturation pdfs consistent with the empirical pdfs derived from soil saturation observations ~~were successfully obtained through using~~ the Bayesian inversion framework and ~~using~~ a MH-MCMC algorithm. Model inversions for each site and scale and for both annual and seasonal models met the evaluation criteria (see Sec 2.4). Our results indicated that the framework of Dralle and Thompson (2016a) can be applied to sites with low (US-MMS) and high (US-TON) seasonality in rainfall patterns. Posterior probability distributions of soil water balance parameters ( $s_w$ ,  $s^*$ ,  $E_{max}$ ) ~~Figure 3 presents~~ were well-constrained overall. The parameter estimates and their coefficient of variation as well as the model goodness of fit statistics are summarized in Table 2. Figures 2 through 5 present a comparison between empirical ~~and as well as~~ analytical pdfs ~~with and~~ associated quantile-quantile plots for point-, footprint-, and satellite-scales at the ~~4~~ four study sites. ~~The (iv') model variation and for both annual and seasonal models. The goodness of fit between empirical pdfs and analytical models was used (see Sect. 4.2) with Z equal to the sensing depths of 10, 20, and 5 cm for the only slightly better for the seasonal model than for the annual model. However, the coefficient of variation of the posterior parameter distributions was smaller for the annual model and it converged more rapidly. The Bayesian inversion of the annual model is therefore more computationally efficient. The parameter identifiability was not greatly improved by the more complex seasonal model. The estimated soil saturation threshold  $s_w$  was consistently smaller for the annual model than for the seasonal model and  $s^*$  was often higher, which may indicate that  $s_w$  and  $s^*$  in the annual model could be biased and may have absorbed dry season dynamics. Previous studies calibrating soil saturation pdf models found ecohydrological parameters values comparable to ours (Table 2). For example, using point-, footprint-, and satellite-scales scale observations at US-Ton, best fit values of  $s_w$  and  $s_{fc}$  were 0.26 and 0.82, respectively. The Kolmogorov-Smirnov statistic ranged from 0.05 to 0.11; associated p-values were greater than 5 percent statistical significance except for the point and footprint scale results at US Ton, which had a p-value of (Dralle and Thompson, 2016a), and best-fit values of  $s^*$  and  $E_{max}$  were 0.02. Posterior  $s_w$  and 1.9 mm d<sup>-1</sup> probability distributions of soil water balance parameters ( $s_w$ ,  $s^*$ ,  $E_{max}$ ) were overall well constrained. The coefficient of variation of posterior distributions were on average 7%, and ranged between 1 and 23 % for all sites and scales.~~

#### 4.1 Level of model complexity

For each spatial scale and site, the 6 model variations in Table 2 were each inversed using 8 Z-values ranging from 5 cm to 40 cm, with 10 repeats for each case. Results were used to determine how many and which soil water loss parameters can be inferred from soil saturation pdfs with most certainty. Only the converging model inversions among the 80 model-site-scale combinations were retained and their median results were summarized in Fig. 4. The most successful parameter estimations were obtained using model variations (iii'), (i), and (iv') with 97, 94, and 85 percent converging results, respectively, compared to model variations (ii), (iii), and (iv) with 52, 44, and 42 percent converging results. The model goodness of fit generally increased with model complexity. The

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average Kolmogorov Smirnov statistic for all model (iv') results was 0.08 with 64 percent that were statistically significant, compared to 0.2, with only 11 percent that were statistically significant for model variation (i). Soil saturation pdfs were therefore more accurately described if  $s_w$  and  $s^*$  soil threshold parameters are included in the soil water loss equation. Convergence and goodness of fit results were generally better for model variation (iii') than (ii), suggesting that  $s_w$  was more important in the analytical equation for (Miller et. al. 2007). We did not compare soil saturation pdfs and soil water loss equations than  $s^*$ . The mean coefficient of variation of the posteriori parameter values, converging cases combined, were, 5, 6, 9, and 30 percent for  $s_w$ ,  $s^*$ ,  $E_{max}$ , and  $E_w$ , respectively. The coefficient of variation of *a posteriori* thresholds  $s^*$  and  $s_w$  with literature values of a parameter was directly related to how sensitive the theoretical shapes soil water potential at which stomata are fully open or closed because the conversion of soil saturation is to that parameter and inversely related to how accurately that parameter can be estimated. Models (iii) and (iv), in which  $E_w$  was an unknown were the least successful. Information may be missing to accurately estimate  $E_w$  for most sites. Results indicate that the goodness of fit of soil saturation pdfs and values of other fitted parameters were not very sensitive to the exact value of  $E_w$ . The simplifying relation  $E_w = 0.05E_{max}$  prevented equifinality in the analytical equation for soil saturation pdfs and reduced uncertainty in the inference of the other soil water loss parameters. We conclude that all parameters except  $E_w$  can be inferred with high certainty. Given the soil matrix potential is non-linear (Clapp and Hornberger, 1978) and site and scale specific soil water retention parameters were unknown. Average parameters derived from soil texture (Rawls et al., 1982) were not compatible with soil moisture data available in this study, model (iv') is the most appropriate, and only this model variation was used to obtain results described in the following paragraphs.

#### 4.2 Soil depth sensitivity

For each spatial scale and site, the (iv') model variation was inverted for Z values ranging from 5 cm to 1 m, with 10 repeats for each case. Results were used to determine whether the inference of soil water balance parameters was sensitive to the sensing depth and if the resulting analytical model for soil saturation pdfs can be relevant to evaluate the soil water balance for a greater soil depth. Only the converging model inversions among the 10 site scale depth combinations were retained and their median results were summarized in Fig. 5. The soil depth used in the analytical equation for soil saturation pdfs didn't generally impact model inference, parameter uncertainty, and goodness of fit. The influence of soil depth decreased as scale increased and was lowest at satellite scales. For the two drier sites (US-Ton and US-Me2), acceptable results were only obtained for shallower soil depths (below 40 cm) at the point and footprint scales. The Kolmogorov-Smirnov statistic was generally optimal for Z values between 15 and 60 cm. Estimated values for  $s_w$  and  $s^*$  were generally not sensitive to the considered soil depth and remained relatively stable. It is expected that  $E_{max}$  would scale with soil depth to account for daily soil water losses from a deeper soil reservoir. Although it is conceptually more consistent to consider the actual sensing depth to infer a best fit model for soil saturation pdfs, we conclude that the model used was not very sensitive to soil depth and methods can be applied with Z values around actual rooting depths. These findings are consistent with discussion related to the sensitivity of the mean soil water components to soil depth in Laio et al. (2001), and indicate that near surface soil moisture can be used reliably to relate inferred model results to soil water dynamics in the rooting zone. These results also indicate that parameter estimates are not sensitive to the soil moisture sensing depth. This is particularly relevant to larger scale soil moisture observations, particularly from satellites, when the sensing depth is not accurately quantified.

### 4.3 Data availability

For each spatial scale and site, the (iv<sup>2</sup>) model was inverted with Z-values ranging from 5 cm to 40 cm, using random subsamples of 100 to 20 percent of the April–September, 2012 record, and with 10 repeats for each case. Results were used to determine the minimum number of observations necessary to obtain an accurate model inversion. Only the converging model inversions among the 80 subsampled site-scale combinations were retained and their median results were summarized in Fig. 6.

~~3.2 For all sites and scales the number of observations did not significantly impact model inference. Although the Kolmogorov-Smirnov statistic, parameter uncertainty and number of non-converging results increased slightly with decreasing number of observations, acceptable results were always obtained and parameter values were stable. The Kolmogorov Smirnov statistic generally indicated that best agreement between analytical and empirical pdfs were obtained with over 75 observations. For subsamples with more than 75 daily observations the average fraction of converging model inversions was 85%. Model parameter values were not sensitive to the number of observations used. Results indicate that there wasn't a limiting number of observations necessary to obtain accurate parameter estimates when the mean and standard deviation of the randomly selected observations were most consistent with the full record and therefore representative of the rainfall characteristics. The MH-MCMC algorithm was also more likely to not reach convergence when the pdfs of the subsample and the full record were inconsistent.~~

### 4.4 Site and scale considerations

~~Soil saturation-Parameter estimates were most constrained for scales and locations at which soil water dynamics are more sensitive to the fitted ecohydrological parameters of interest. In these cases, convergence of the model inversion was attained less rapidly but ultimately provided better goodness of fit. Soil saturation states at drier sites may be more controlled by soil water loss parameters, while soil saturation states at wetter sites may also be more controlled by rainfall characteristics. Model inference at wetter sites, where the rainfall characteristics are known in this study, is therefore more successful than at dry sites. Although modeled pdfs are in good agreement with empirical pdfs for the wetter sites ( Estimated soil saturation thresholds had greater certainty if the empirical soil saturation pdf were defined around those values and had greater uncertainty if there were fewer soil saturation values observed around the thresholds. For example, uncertainty of  $s_w$  was greater for the humid subtropical deciduous forest site (US-MMS) than for the Mediterranean savanna sites (US-Ton, US-ARM and US-MMS), parameter estimates can have higher uncertainty because the shape of the soil saturation pdfs are less sensitive to the soil water loss equation parameters. For the drier sites (US-Ton and US-Me2), the shapes of the soil saturation pdfs are more sensitive to the soil water loss equation parameters, the range of plausible parameters is reduced, and uncertainty can be lower. The MH-MCMC algorithm can be adjusted, if more information were available, to account for the smaller parameter space at drier sites and improve the efficiency of the algorithm. In this study, we discarded results for which the MH-MCMC efficiency was lower than 5% or greater than 80%.~~

~~of  $s^*$  was greater for US-Ton than US-MMS. Similarly, soil saturation states representing larger spatial scales were less sensitive to specific site characteristics, and this study showed model inference at the satellite scale was generally more successful, while parameter uncertainty was greater than for point and footprint scales. Overall a greater number of analytical pdfs were statistically equal (with 95% confidence) to empirical pdfs derived from satellite data than from ground-based data.~~

~~Parameter uncertainty for satellite- and footprint-scales was greater than for the point-scale. Estimates of larger scale soil water balance parameters are more relevant to regional ecohydrological dynamics. Differences in parameter estimates between among scales within a site may be associated with differences in soil texture properties, such as porosity and field capacity, that were determined separately for each record. Figure 3 also shows that co-located and concurrent soil saturation pdfs are different at~~

each scale (Fig 2-5) and suggest variability in observed soil water dynamics ~~that are inferred~~ at each scale. Differences in ~~controlling/driving~~ processes ~~between/among~~ scales were specifically determined from the model inversion for each scale, and provided robust scale-specific parameters for ecohydrological modelling. ~~This study also demonstrated the benefits of analyzing soil saturation pdfs verses time series to understand soil water dynamics, and in particular the appropriateness of the approach for using intermittent data such as satellite-scale observations.~~

5

### 3.3 Data availability

#### 10 For each spatial scale. ~~Conclusions~~

~~Empirical pdfs derived from soil saturation observations provided key information to determine unknown ecohydrological parameters  $s^*$ ,  $s_w$ ,  $E_{max}$ , and site, the annual model was inverted, using random subsamples of 100 to 10 % of the 2012 time series (Fig 6). For all sites and scales the number of observations did not significantly impact model inference. The NSE, Kolmogorov-Smirnov statistic and parameter estimates were stable down to about 100 observations. Fitted model parameter values and the variability of parameter estimates among the 10 repetitions in each subsample category were not sensitive to the number of observations used. Results indicate the identifiability of ecohydrological parameters through the inversion of the analytical model of soil saturation pdfs was robust because the mean and standard deviation of the randomly selected subsets of annual data were representative of the full record. There was no correlation between the small differences in the mean and standard deviations of the subsamples and the model goodness of fit. The proposed inference method based on soil saturation pdfs can therefore reliably be used to identify ecohydrological parameters from sparse datasets. Inference methods, which do not require continuous data are particularly relevant to large scale soil moisture measurements, such as satellite products, that are not continuous.~~

### 4. Conclusions

~~$E_w$ . This study documented~~ We document a generalizable Bayesian inversion framework to ~~accurately infer parameters~~ parameter values of the stochastic soil water balance model and their associated uncertainty using freely available rainfall and soil moisture observations at point-, footprint- and satellite-scales. ~~Empirical pdfs derived from soil saturation observations provided key information to determine unknown ecohydrological parameters  $s^*$ ,  $s_w$ , and  $E_{max}$ . Model assumptions were appropriately met, and optimal satellite scales. Optimal~~ analytical soil saturation pdfs were consistent with empirical pdfs. Uncertainty in parameter estimates ~~was smallest when the number of unknown parameters was reduced to three, assuming a constant relation between  $E_{max}$  and  $E_w$  among sites. The proposed framework was found to be robust. Accurate results were obtained using sparse subsets of the datasets, demonstrating the advantage of analyzing soil saturation pdfs instead of time series. The Bayesian framework was also used to evaluate~~ were small and reflected the sensitivity of the soil water balance model to ecohydrological parameters at varying scales and locations. We ~~demonstrated~~ demonstrate that the form of the simple ecohydrological model for soil saturation pdfs was ~~in agreement~~ consistent with observations from point-, footprint-, and satellite-scales; ~~however,~~ However, optimal parameters were different at each scale because co-located and concurrent soil saturation pdfs are different at each scale ~~and,~~ which may result from spatial heterogeneity in soil water dynamics. ~~Methods developed~~ We demonstrate the advantage of analyzing soil saturation pdfs instead of time series. We obtained stable results using sparse subsets of the datasets, indicating that the proposed framework

is robust and can be used with non-continuous data. Although the seasonal model was conceptually more consistent with our physical understanding of annual soil water dynamics, the annual model provided satisfactory results matching annual empirical pdf sites we analysed. We were not able to determine if some differences in parameters estimated using the seasonal model are physically meaningful because wet and dry season dynamics were better characterized in this study more complex model. Our methodology can be customized to characterize site-specific parameters and to test consistency between observed and analytical soil saturation pdfs for any other adaptation of the stochastic ecohydrological framework with more or less complexity depending on the study objectives.

We provide a method based on a parsimonious soil water balance model, requiring a minimum level of data inputs to estimate ecohydrological characteristics that are not directly observable and for which established estimation methods are not available. Our methods can be applied in future studies to better understand differences in soil water dynamics at different scales and to improve the scaling of ecohydrological processes. Estimates of  $s^*$  and  $s_w$  were generally not sensitive to the soil depth at which data were measured. Results demonstrate the value of large scale near-surface soil moisture observations to improve the characterization of soil water dynamics at ecosystem scales. Relations between the soil saturation threshold values inferred from the near surface soil moisture data and dynamics in the full active rooting zone are unknown. The datasets we used are freely available from sensor networks and global satellite products, and methods can therefore be applied to a large range of sites or to global analyses to improve understanding of spatial patterns in ecohydrological parameters relevant for local and global water cycle analyses.

## 20 Data and code availability

All datasets used in this study were We downloaded all datasets from publicly available sources: point. Point-scale soil moisture and rainfall data are available through FLUXNET2015 (<http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/>); footprint-scale soil moisture data are available through COSMOS (<http://cosmos.hwr.arizona.edu/Probes/probelist.html>); remotely-sensed soil moisture data are available through ESA CCI (<http://www.esa-soilmoisture-cci.org/node/145>); remotely sensed rainfall data are available through NASA TRMM (<https://pmm.nasa.gov/data-access/downloads/trmm>); global soil texture data are available through FAO HWSD (<http://www.fao.org/soils-portal/soil-survey/soil-maps-and-databases/harmonized-world-soil-database-v12/en/>). Custom scripts in the Python computing language associated with this our analysis are available upon request through a private gitHub repository and will be made publicly available after revisions of this manuscript. (Citation and doi TBD).

## Competing interests

30 Authors declare that they have no conflict of interest.

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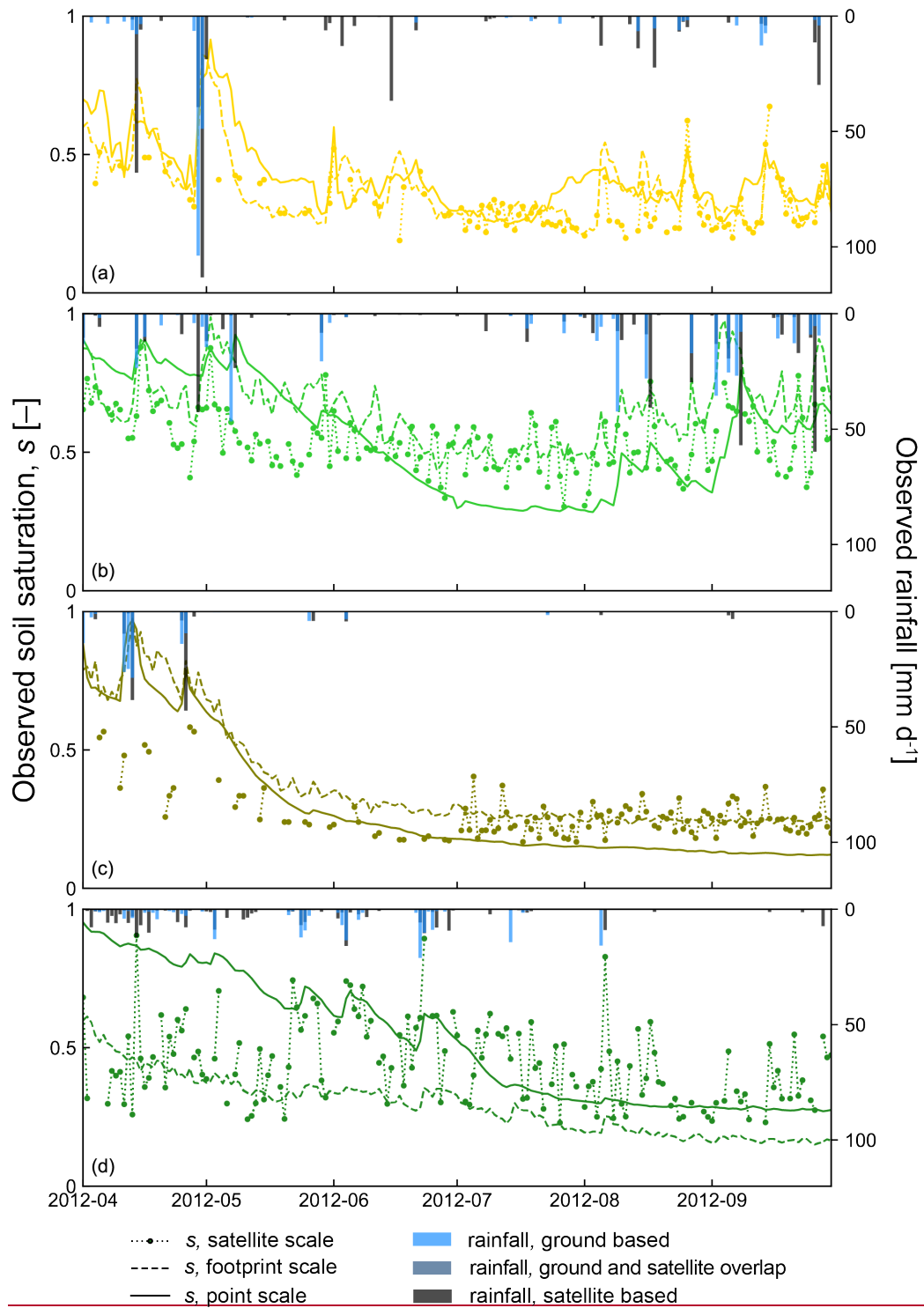


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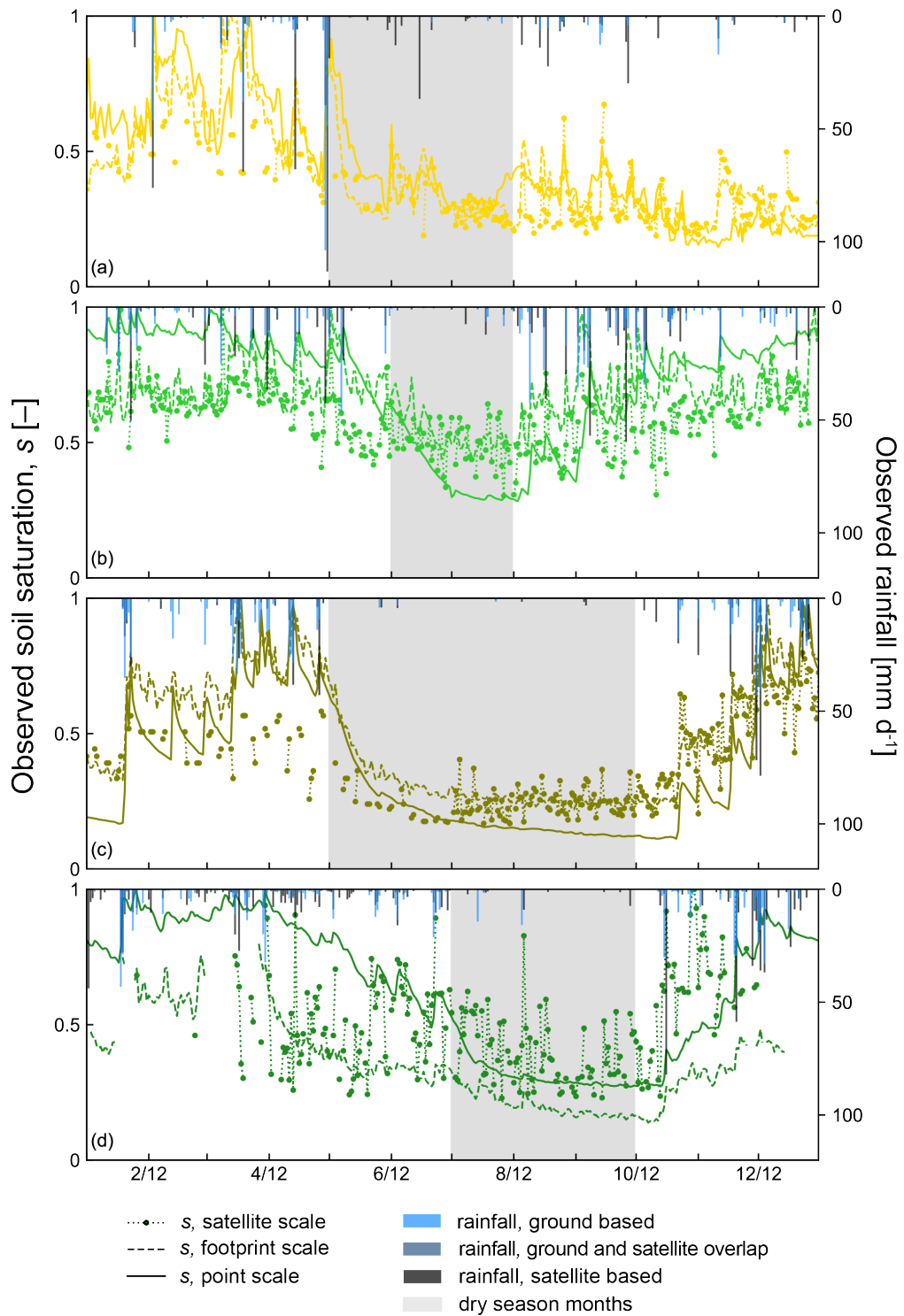
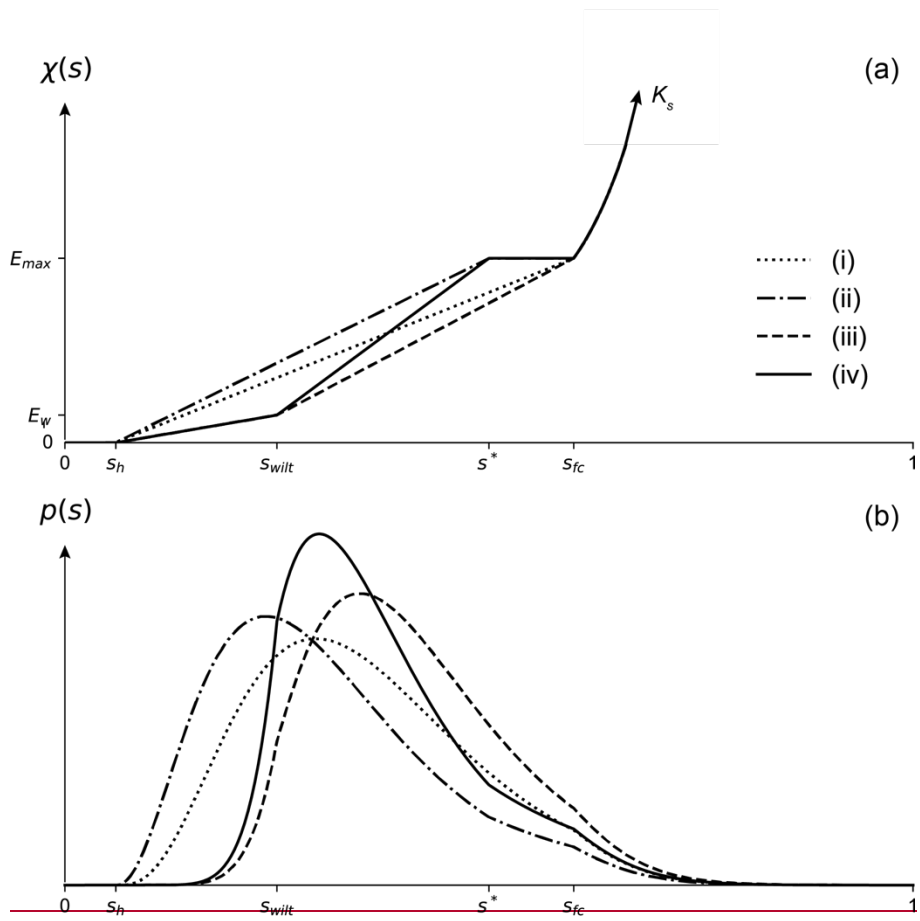
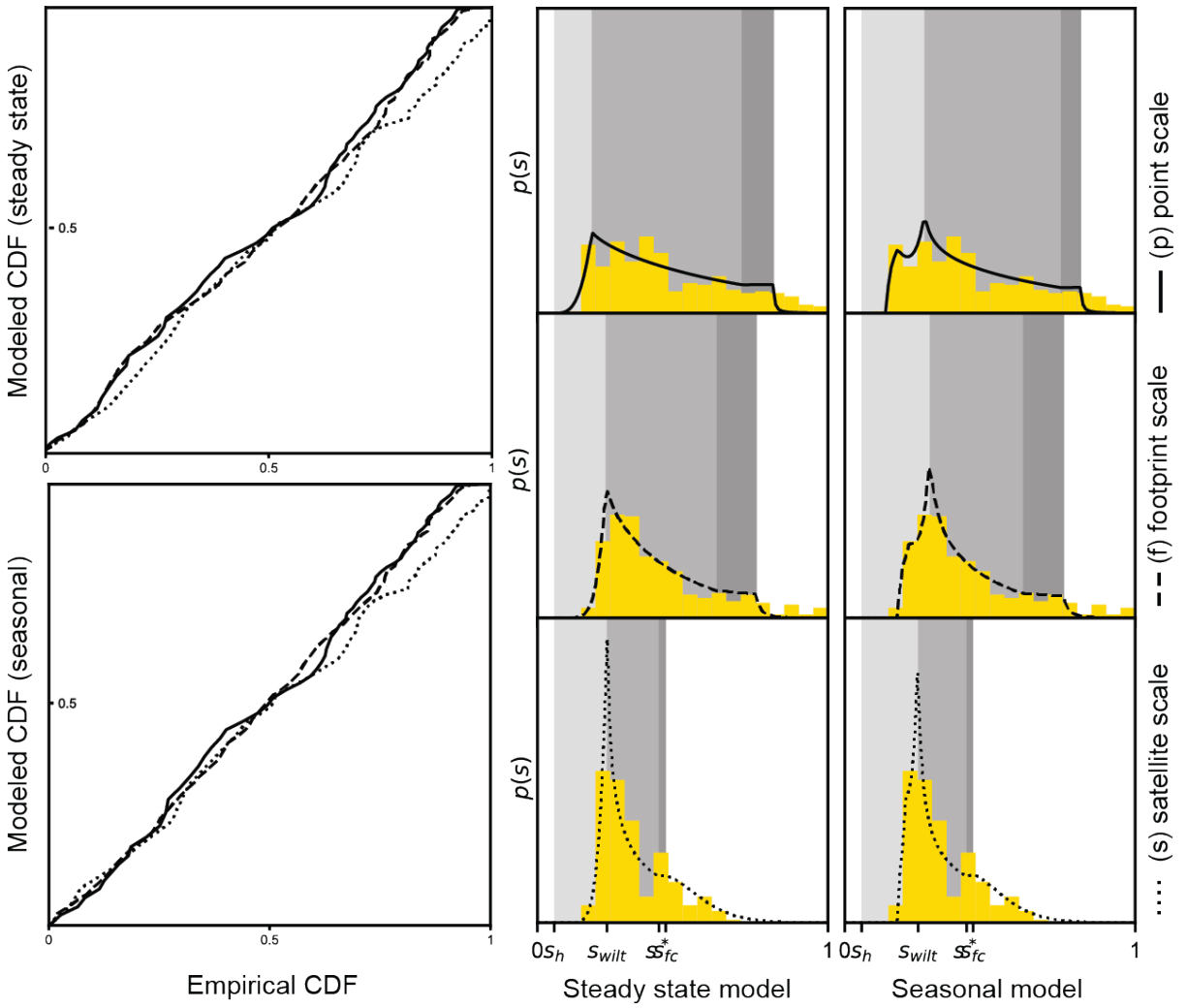
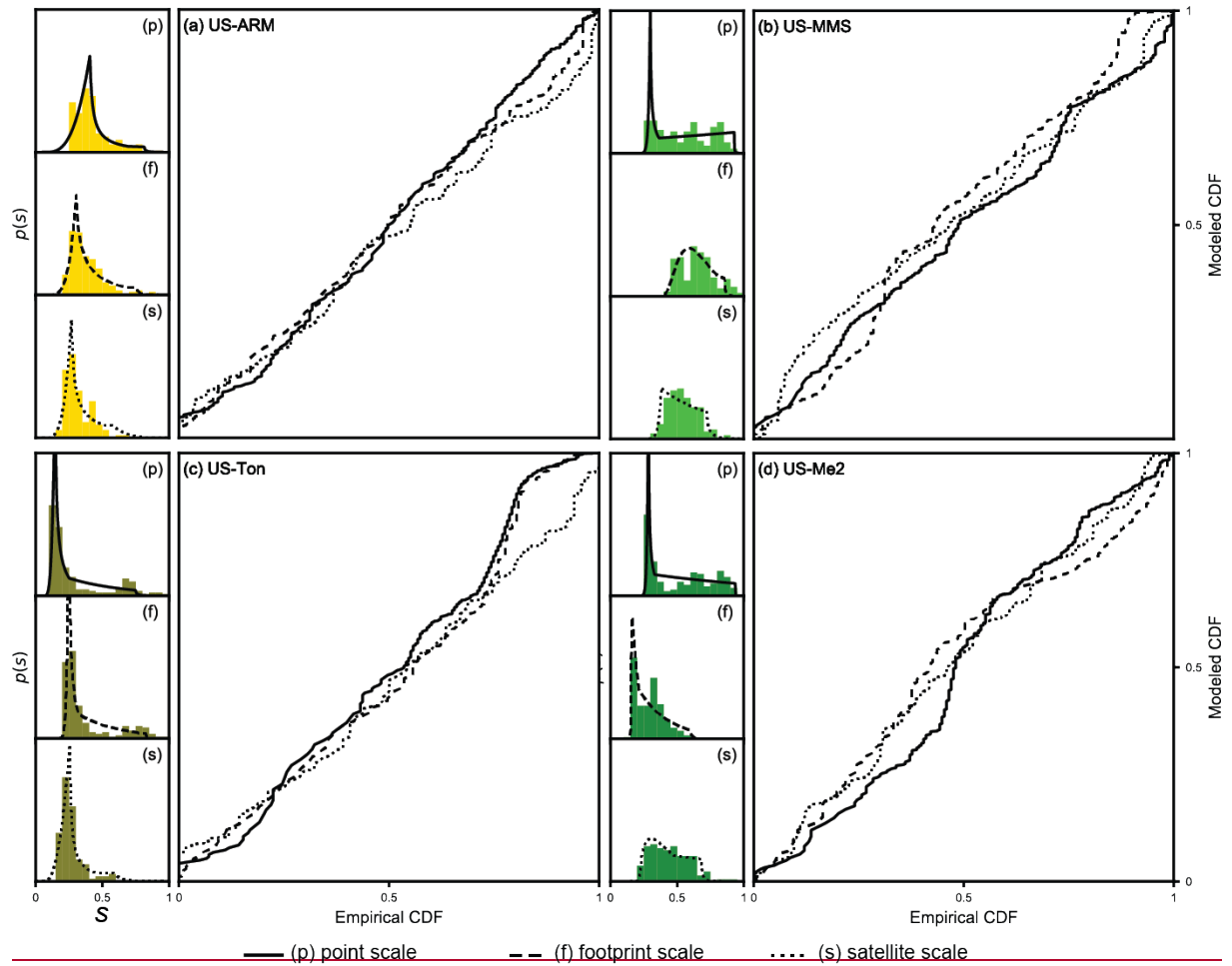


Figure 1: Soil saturation and rainfall time series from (a) US-ARM, (b) US-MMS, (c) US-Ton, and (d) US-Me2.



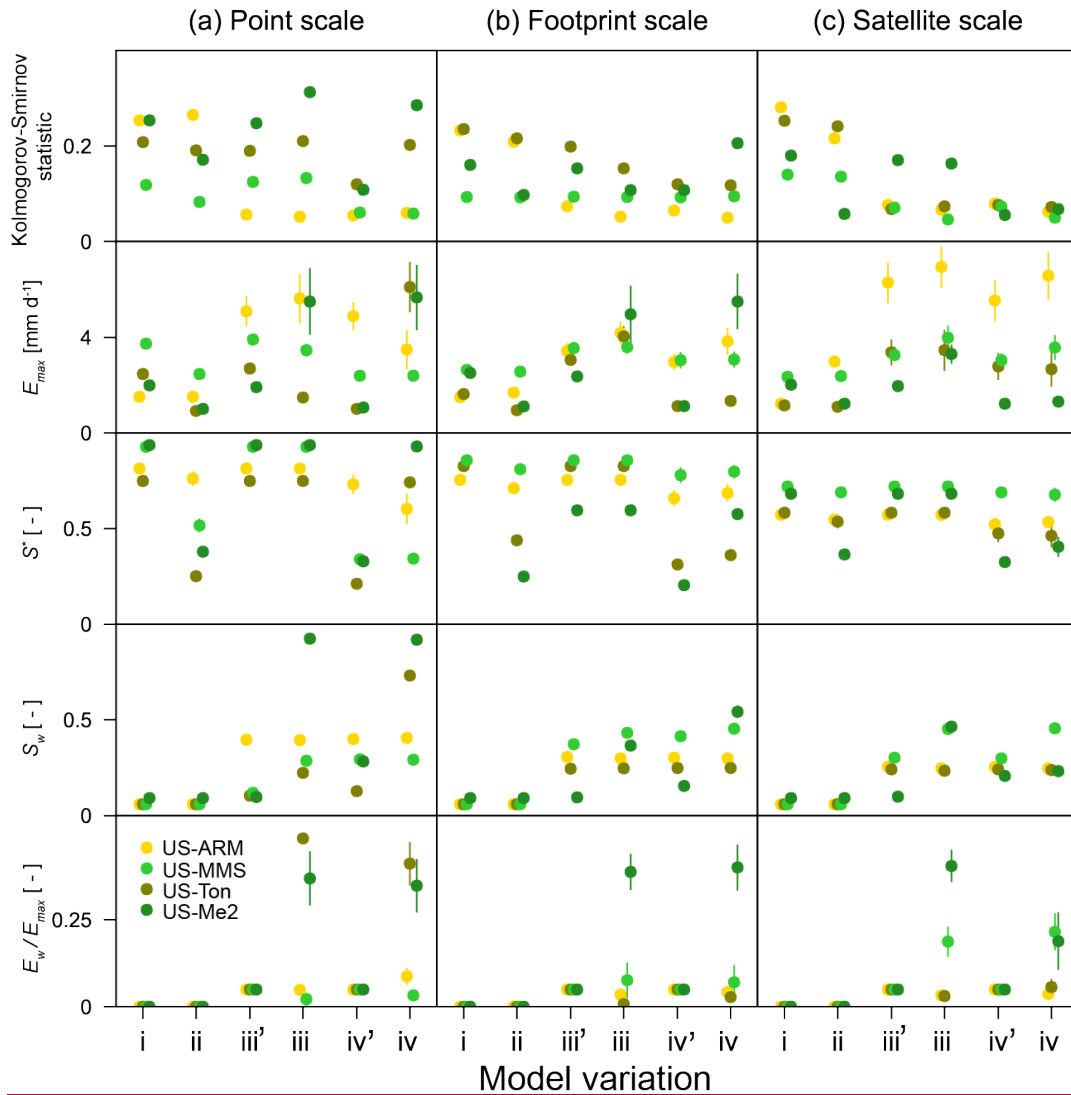


**Figure 2:** Conceptual illustration of (a) soil water losses as a function of soil saturation states,  $\chi(s)$ , for a loamy soil and (b) associated probability density functions of soil saturation,  $p(s)$ , for a sub-tropical climate. Increasing levels of model complexity (i–iv) are defined in Table 2.



**Figure 3:- Empirical versus modelled cumulative density functions (CDF) and soil saturation probability distribution ( $p(s)$ ) and cumulative density functions (CDF) for (a) for US-ARM; (b) US-MMS; (c) US-TON; (d) US-Me2; (p) point scale; (f) footprint scale; (s) satellite scale. The mean values of the posterior parameter distributions were used with model variation ( $\sigma^2$ ) and each spatial scale's sensing depth.**

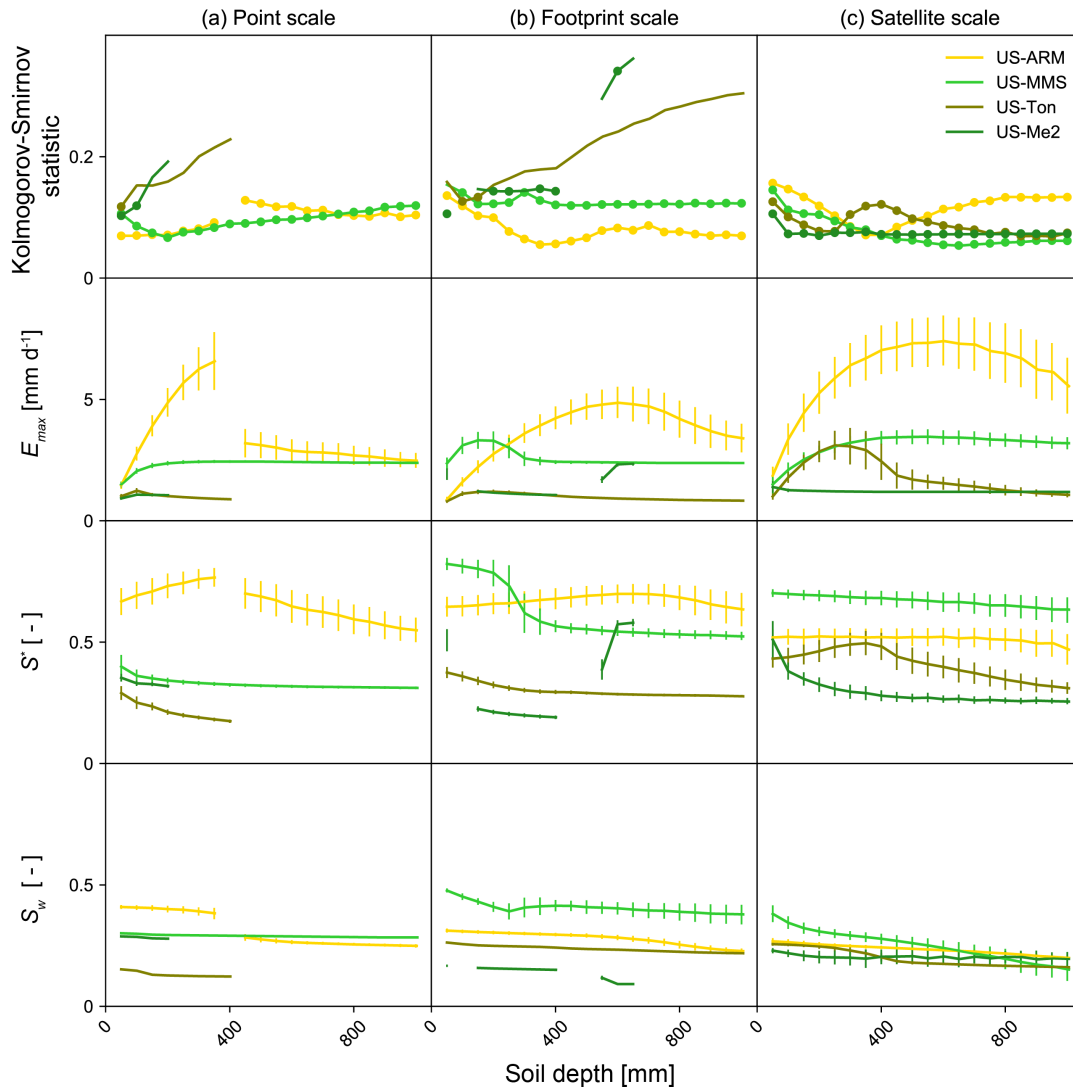
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5 **Figure 4: Goodness of fit and ecohydrological model parameters inferred with increasing model complexity. Model variations i–iv are defined the analytical model in Eq (3) in Table 2; the median results of the converged model inversions are plotted; error bars represent annual model and Eq (6) in the standard deviations of the posteriori distribution of 50 thousand random parameters samples resulting from seasonal model. The grey shaded areas correspond to the soil saturation thresholds ( $S_{hs}$ ,  $S_{ws}$ ,  $S^*$ ,  $S_{fc}$ ) in the MH-MCMC algorithm. water balance model.**

10





**Figure 5: Goodness of fit and ecohydrological model parameters inferred with soil depths ranging from 5 cm to 1m. The median results of the converged model inversions are plotted; circular markers indicate that the Kolmogorov-Smirnov statistic is significant with a 95 % confidence level; error bars represent the standard deviations of the posteriori distribution of 50 thousand random parameters samples resulting from the MH-MCMC algorithm.**

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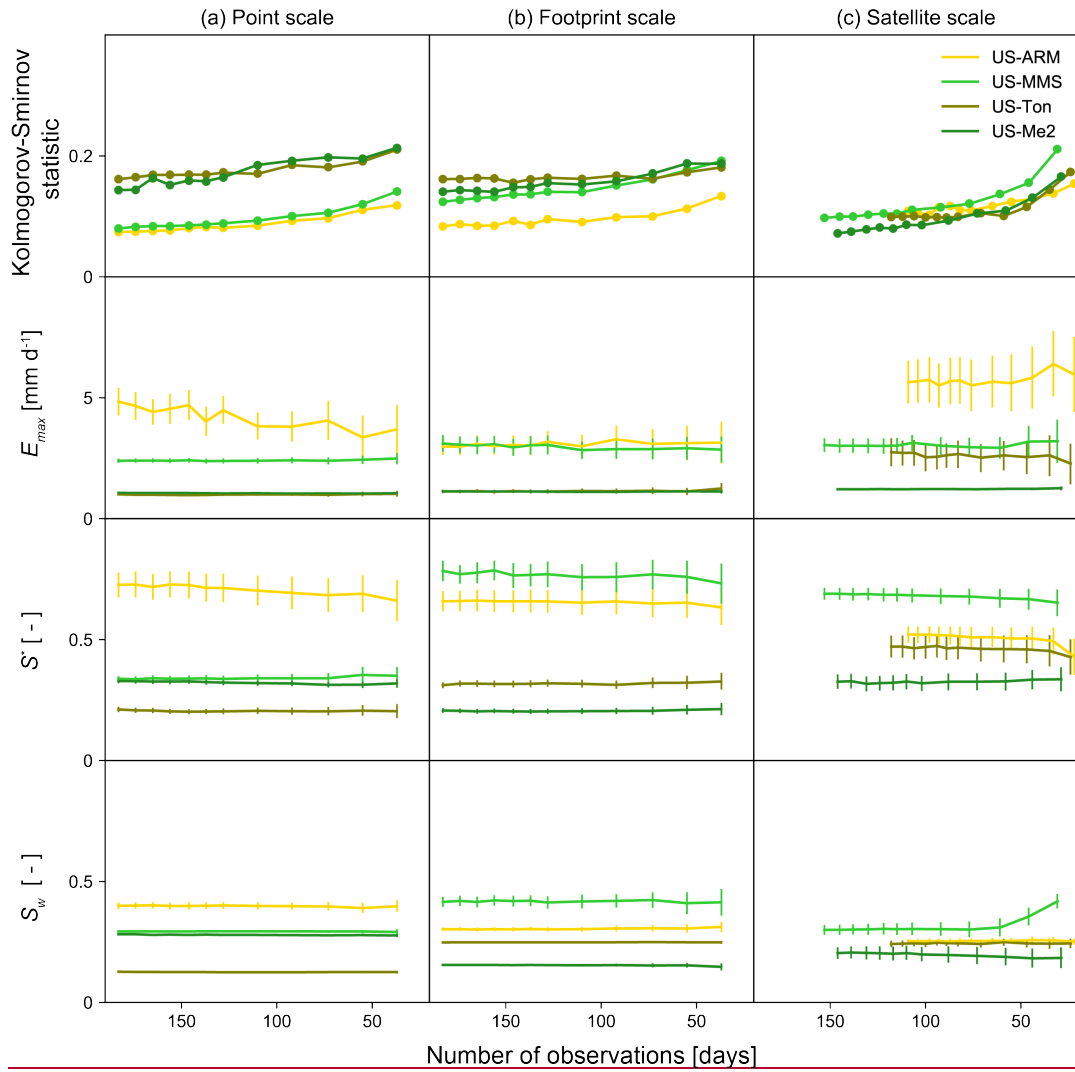
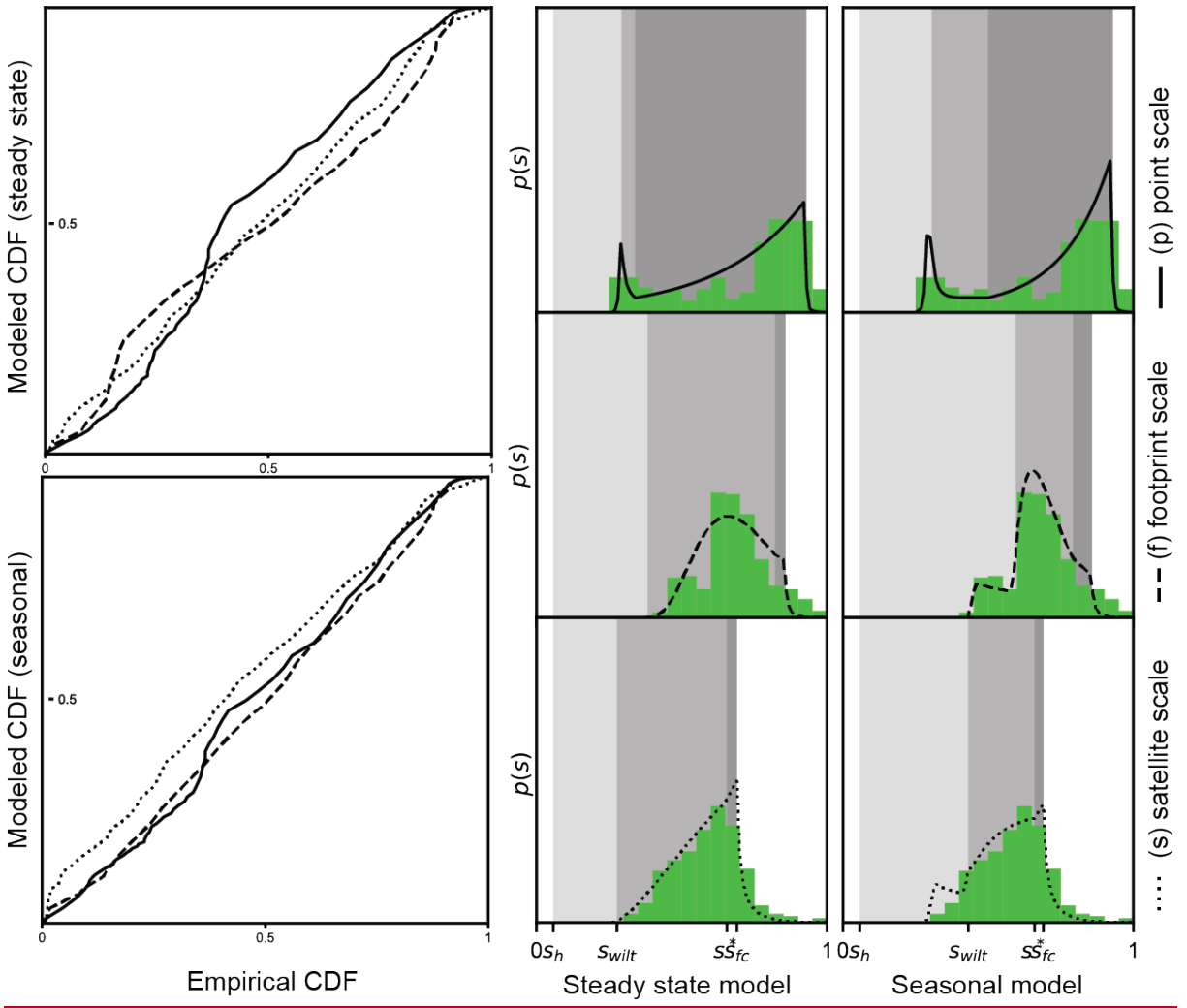
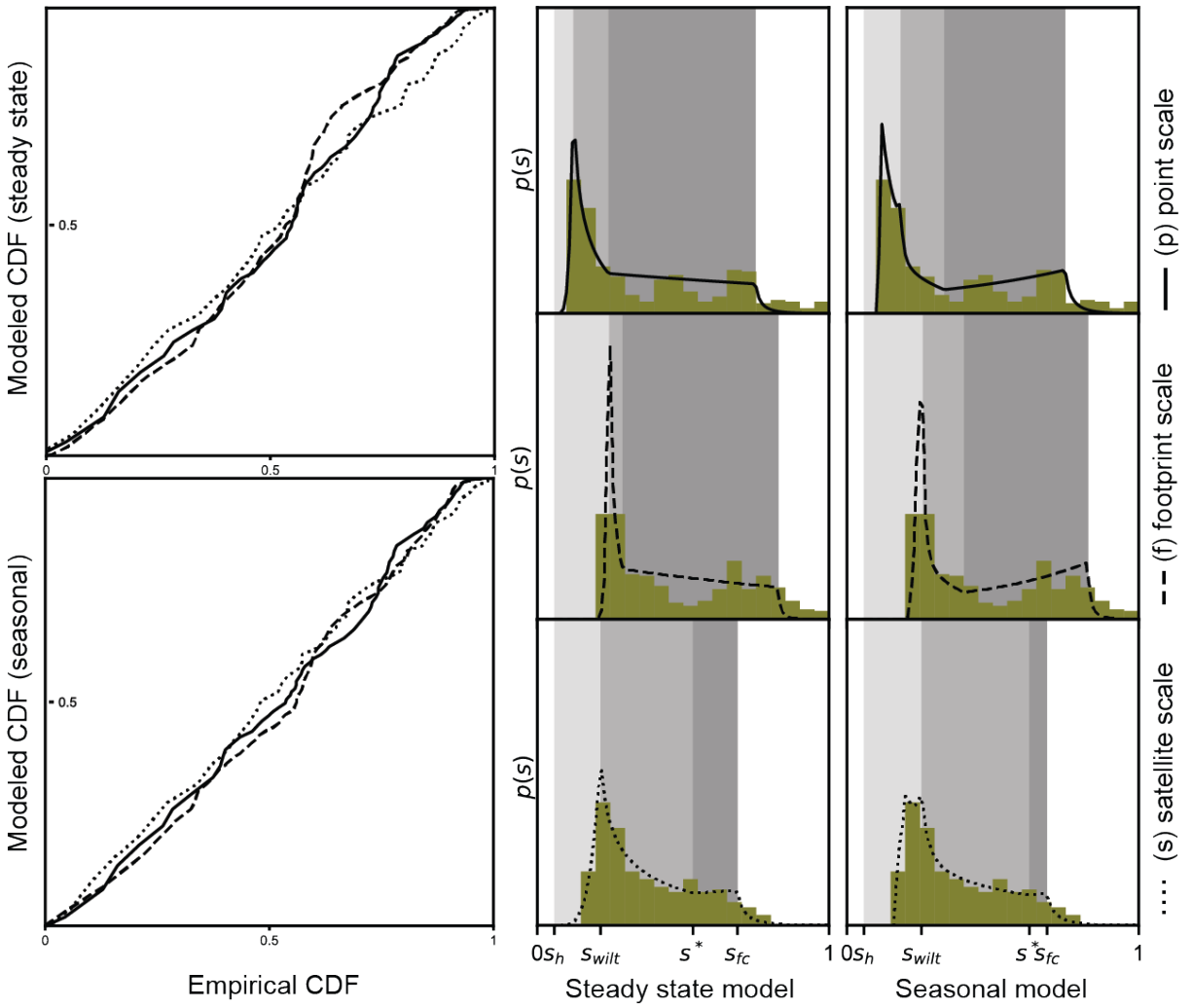


Figure 6: Goodness of fit and ecohydrological model



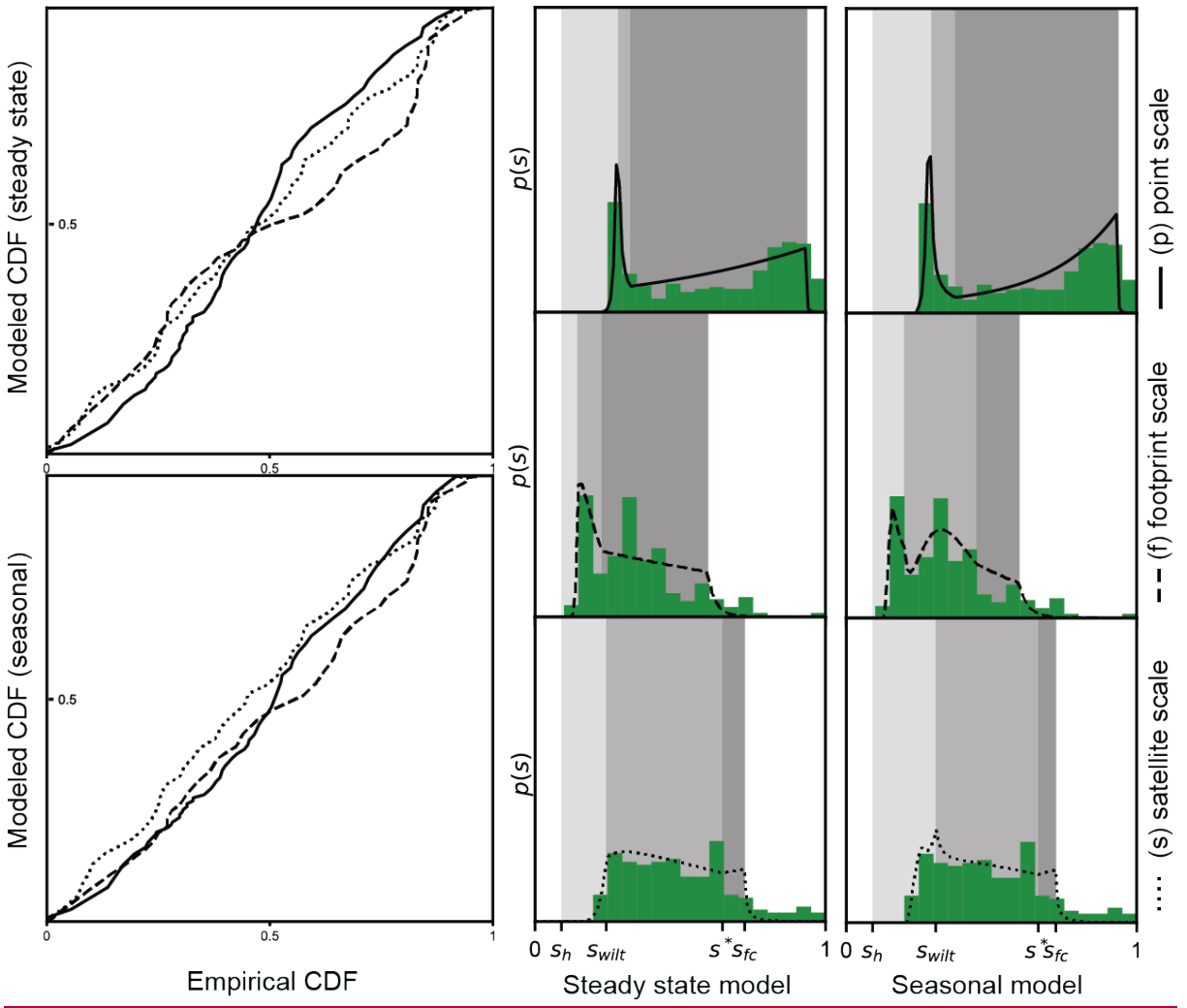
**Figure 3: Empirical versus modelled cumulative density functions (CDF) and soil saturation probability distribution ( $p(s)$ ) for US-MMS. The mean values of the posterior parameter distributions were used with the analytical model in Eq. (3) in the annual model and Eq. (6) in the seasonal model. The grey shaded areas correspond to the soil saturation thresholds ( $s_{wilt}$ ,  $s_{fc}^*$ ,  $s_{fc}$ ) in the water balance model.**

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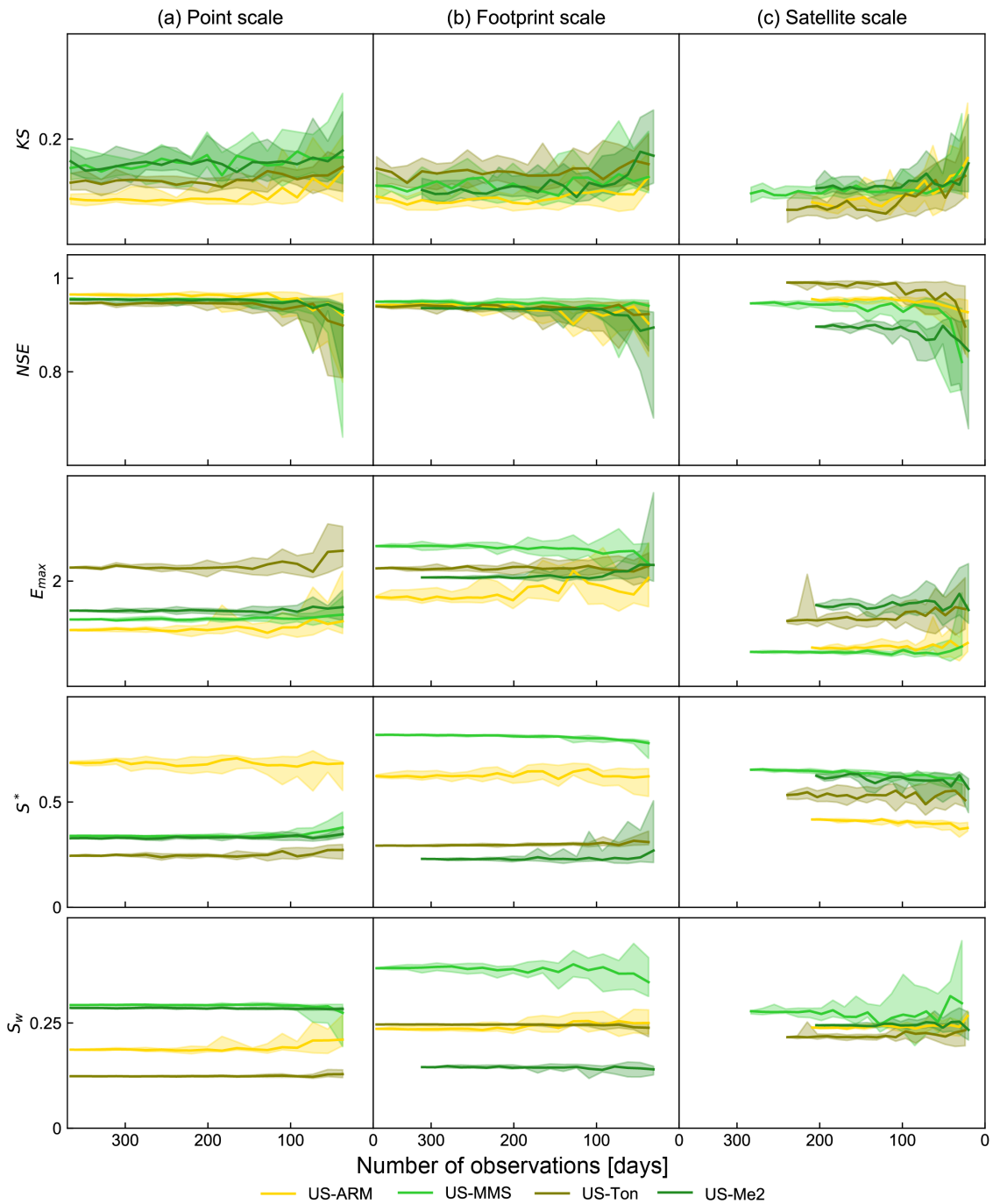
**Figure 4: Empirical versus modelled cumulative density functions (CDF) and soil saturation probability distribution ( $p(s)$ ) for US-Ton. The mean values of the posterior parameter distributions were used with the analytical model in Eq (3) in the annual model and Eq (6) in the seasonal model. The grey shaded areas correspond to the soil saturation thresholds ( $s_h, s_w, s^*, s_{fc}$ ) in the water balance model.**

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**Figure 5: Empirical versus modelled cumulative density functions (CDF) and soil saturation probability distribution ( $p(s)$ ) for US-Me2. The mean values of the posterior parameter distributions were used with the analytical model in Eq (3) in the annual model and Eq (6) in the seasonal model. The grey shaded areas correspond to the soil saturation thresholds ( $s_h, s_w, s^*, s_{fc}$ ) in the water balance model.**

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**Figure 6 - Goodness of fit and ecohydrological parameters inferred with decreasing number of soil saturation observations: The median results (annual model). For each subsample category, the median results of 10 repeats are plotted and results between the 90<sup>th</sup> and 10<sup>th</sup> percentiles are shaded. Colors correspond to the four sites in the legend. KS, Kolmogorov Smirnov statistic; NSE, quantile-level Nash Sutcliffe efficiency;  $E_{max}$ , maximum evapotranspiration in mm d<sup>-1</sup>;  $s^*$ , point of the converged model inversions are plotted; circular markers indicate that the Kolmogorov Smirnov statistic is significant with a 95 % confidence level; error bars represent the standard deviations of the posteriori distribution of 50 thousand random parameters samples resulting from the MH-MCMC algorithm;  $s_{ys}$ , incipient stomatal closure;  $s_{ys}$ , wilting point.**

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Table 1 – Selected study sites

Site Name	ARM Southern Great Plains	Morgan Monroe State Forest	Tonzi Ranch	Metolius Mature Ponderosa Pine
FLUXNET2015 ID	US-ARM	US-MMS	US-Ton	US-ME2
COSMOS ID	15	27	32	38
Latitude	36.6058 (36.625)	39.3232 (39.375)	38.4316 (38.375)	44.4523 (44.375)
Longitude	-97.4888 (-97.375)	-86.4131 (-86.375)	-120.966 (-120.87)	-97.4888 (-97.375)
Elevation [m]	314	275	177	1253
Vegetation	Crops and grassland	Deciduous forest	Oak savanna	Ponderosa pine forest
<b>Soil Texture</b>	<b>Loam</b>	<b>Loam</b>	<b>Loam</b>	<b>Sandy Loam</b>
MAT [°C]	14.8	10.9	15.8	6.3
MAP [mm]	843	1032	559	523
<b><math>\alpha_w</math> [mm day<sup>-1</sup>]</b>	<b>Loam 21.0<sup>(p, f)</sup>, 24.4<sup>(s)</sup></b>	<b>Loam 9.04<sup>(p, f)</sup>, 11.8<sup>(s)</sup></b>	<b>Loam 9.3<sup>(p, f)</sup>, 16.9<sup>(s)</sup></b>	<b>Sandy Loam 8.1<sup>(p, f)</sup>, 11.6<sup>(s)</sup></b>
<b><math>\lambda_w</math> [day<sup>-1</sup>]</b>	<b>21.4<sup>(p, f)</sup>, 26.8<sup>(s)</sup></b>	<b>9.1<sup>(p, f)</sup>, 11.9<sup>(s)</sup></b>	<b>8.7<sup>(p, f)</sup>, 16.7<sup>(s)</sup></b>	<b>7.9<sup>(p, f)</sup>, 11.6<sup>(s)</sup></b>
<b><math>t_d</math> [days]</b>	<b>0.05<sup>(p, f)</sup>, 0.08<sup>(s)</sup></b>	<b>0.24<sup>(p, f)</sup>, 0.20<sup>(s)</sup></b>	<b>0.22<sup>(p, f)</sup>, 0.10<sup>(s)</sup></b>	<b>0.24<sup>(p, f)</sup>, 0.21<sup>(s)</sup></b>
<b><math>n</math> [-]</b>	<b>0.07<sup>(p, f)</sup>, 0.08<sup>(s)</sup></b>	<b>0.27<sup>(p, f)</sup>, 0.23<sup>(s)</sup></b>	<b>0.39<sup>(p, f)</sup>, 0.17<sup>(s)</sup></b>	<b>0.31<sup>(p, f)</sup>, 0.27<sup>(s)</sup></b>
<b><math>K_s</math> [mm day<sup>-1</sup>]</b>	<b>92</b>	<b>61</b>	<b>153</b>	<b>92</b>
<b><math>b</math> [-]</b>	0.35 <sup>(p)</sup> , 0.34 <sup>(f)</sup> , 0.46 <sup>(s)</sup>	0.46 <sup>(p)</sup> , 0.66 <sup>(f)</sup> , 0.43 <sup>(s)</sup>	0.53 <sup>(p)</sup> , 0.39 <sup>(f)</sup> , 0.43 <sup>(s)</sup>	0.36 <sup>(p)</sup> , 0.59 <sup>(f)</sup> , 0.41 <sup>(s)</sup>
<b><math>s_h</math> [-]</b>	317	317	317	622
<b><math>s_{fc}</math> [-]</b>	4.55	4.55	4.55	3.11
<b><math>s_{min}</math> [-]</b>	0.06	0.06	0.06	0.09
<b><math>s_{max}</math> [-]</b>	0.81 <sup>(p)</sup> , 0.75 <sup>(f)</sup> , 0.5744 <sup>(s)</sup>	0.93 <sup>(p)</sup> , 0.86 <sup>(f)</sup> , 0.7269 <sup>(s)</sup>	0.9475 <sup>(p)</sup> , 0.6083 <sup>(f)</sup> , 0.6869 <sup>(s)</sup>	0.94 <sup>(p)</sup> , 0.60 <sup>(f)</sup> , 0.6872 <sup>(s)</sup>
<b><math>\alpha</math> [mm day<sup>-1</sup>]</b>	0.15 <sup>(p)</sup> , 0.19 <sup>(f)</sup> , 0.19 <sup>(s)</sup>	0.28 <sup>(p)</sup> , 0.44 <sup>(f)</sup> , 0.30 <sup>(s)</sup>	0.11 <sup>(p)</sup> , 0.22 <sup>(f)</sup> , 0.17 <sup>(s)</sup>	0.27 <sup>(p)</sup> , 0.14 <sup>(f)</sup> , 0.23 <sup>(s)</sup>
<b><math>\lambda</math> [day<sup>-1</sup>]</b>	26.91.0 <sup>(p, f)</sup> , 1.0 <sup>(f)</sup> , 24.50.67 <sup>(s)</sup>	10.71.0 <sup>(p, f)</sup> , 1.0 <sup>(f)</sup> , 13.31.0 <sup>(s)</sup>	9.71.0 <sup>(p, f)</sup> , 1.0 <sup>(f)</sup> , 14.60.80 <sup>(s)</sup>	4.81.0 <sup>(p, f)</sup> , 1.0 <sup>(f)</sup> , 31.0 <sup>(s)</sup>
<b>Mean <math>s</math> [-]</b>	0.0544 <sup>(p, f)</sup> , 0.42 <sup>(f)</sup> , 0.4933 <sup>(s)</sup>	0.2271 <sup>(p, f)</sup> , 0.68 <sup>(f)</sup> , 0.2959 <sup>(s)</sup>	0.0738 <sup>(p, f)</sup> , 0.49 <sup>(f)</sup> , 0.0438 <sup>(s)</sup>	0.2064 <sup>(p, f)</sup> , 0.35 <sup>(f)</sup> , 0.3950 <sup>(s)</sup>
<b>Standard deviation <math>s</math> [-]</b>	0.21 <sup>(p)</sup> , 0.19 <sup>(f)</sup> , 0.11 <sup>(s)</sup>	0.21 <sup>(p)</sup> , 0.11 <sup>(f)</sup> , 0.12 <sup>(s)</sup>	0.25 <sup>(p)</sup> , 0.23 <sup>(f)</sup> , 0.17 <sup>(s)</sup>	0.25 <sup>(p)</sup> , 0.16 <sup>(f)</sup> , 0.18 <sup>(s)</sup>

Latitude and longitude in parenthesis correspond the centroid of the satellite area associated with the site location; MAT, mean annual temperature from long-term FLUXNET2015 data; MAP, mean annual precipitation from long-term FLUXNET2015 data; **Soil** soil texture taken from the HWSD;  $n$ , porosity;  $K_s$ , saturated soil hydraulic conductivity;  $b$ , pore size distribution index;  $s_h$ , hygroscopic point;  $s_{fc}$ , field capacity;  $\alpha$ , observed average daily rainfall depth (April–September, in 2012); the subscript  $w$  indicates that  $\alpha$  was computed for only the wet season months;  $\lambda$ , observed average daily rainfall frequency (April–September, in 2012, the subscript  $w$  indicates that  $\lambda$  was computed for only the wet season months;  $t_d$ , number of days in the dry season; superscripts <sup>(p)</sup>, <sup>(f)</sup>, and <sup>(s)</sup> correspond to values used for the point-, footprint-, and satellite-scale analysis. Citations for each FLUXNET2015 site: Sebastien Biraud (2002–) AmeriFlux US-ARM ARM Southern Great Plains site- Lamont, 10.17190/AMF/1246027; Kim Novick, Rich Phillips (1999–) AmeriFlux US-MMS Morgan Monroe State Forest, 10.17190/AMF/1246080; Bev Law (2002–) AmeriFlux US-Me2 Metolius mature ponderosa pine, 10.17190/AMF/1246076; Dennis Baldocchi (2001–) AmeriFlux US-Ton Tonzi Ranch, 10.17190/AMF/1245971



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Table 2. Model variations Table 2 Estimated ecohydrological parameters and goodness of fit of analytical soil saturation pdfs

Site name	Scale	$s_{fs}$		NSE		KS		$E_{max}$		$E_i$	$s^*$		$s_w$		
		$p$	$p_{wd}$	$p$	$p_{wd}$	$p$	$p_{wd}$	$p$	$p_{wd}$		$p$	$p_{wd}$	$p$	$p_{wd}$	
US-ARM	point	4	4	0.96	0.96	0.07	0.07	1.1 (11)	$s_{fs} 1.3$ (14)	$s_{fs}$	-0.7 (8)	0.74 (5)	0.19 (4)	0.27 (7)	
	(ii)	2													
	(iii)	footprint	3	3	0.94	0.94	0.08	0.06	1.7 (11)	2 (12)	-	$s_{fs} 0.62$ (7)	-0.61 (9)	$E_{max} 24$ (3)	0.05 0.29 (2)
	(iii)	3													
US-Ton	satellite	3	-3	-	0.05 0.96	$E_{max}$ 97	0.08	0.09	0.7 (13)	0.5 (13)	0.42 (4)	0.42 (4)	0.24 (3)	0.25 (2)	
	point	3	4	0.95	0.97	0.09	0.08	2.3 (4)	1.9 (10)	0.24 (6)	0.33 (7)	0.12 (1)	0.18 (6)		
	footprint	3	3	0.94	0.98	0.13	0.08	2.2 (3)	1.8 (8)	0.29 (2)	0.4 (10)	0.25 (0)	0.26 (1)		
US-MMS	satellite	3	2	0.99	0.99	0.06	0.07	1.2 (15)	1 (13)	0.53 (12)	0.62 (6)	0.22 (3)	0.26 (3)		
	point	3	4	0.96	0.98	0.12	0.08	1.3 (3)	1.1 (6)	0.34 (3)	0.5 (8)	0.29 (0)	0.31 (2)		
	footprint	3	3	0.95	0.95	0.13	0.08	2.7 (6)	4.5 (10)	0.82 (2)	0.79 (3)	0.38 (5)	0.59 (1)		
US-Me2	satellite	3	6	0.95	0.88	0.1	0.14	0.7 (8)	0.9 (10)	0.65 (4)	0.66 (3)	0.28 (9)	0.43 (2)		
	point	3	8	0.95	0.97	0.16	0.1	1.4 (3)	1.1 (7)	0.33 (3)	0.37 (8)	0.29 (0)	0.29 (1)		
	footprint	3	6	0.94	0.94	0.09	0.1	2.1 (2)	2.9 (10)	0.23 (4)	0.45 (5)	0.15 (2)	0.2 (6)		
(iv)	satellite	3	4	-	0.89	0.89	-	0.12	0.1	1.6 (12)	1.4 (15)	0.64 (8)	0.66 (8)	0.25 (3)	0.31 (4)

$i$ , number of unknown parameters; -, indicates that a parameter is not estimated. Values in parenthesis correspond to the coefficient of variation of the posterior parameter in percentage.

$p$ , analytical model inversion;  $s_{fs}$ , field capacity for the soil saturation pdf without seasons,  $p_{wd}$ , analytical model for the soil saturation pdf including wet and dry seasons;  $n$ , number of simulation runs needed to obtain 3 converging results (see Sect. 2.3.2); NSE, quantile-level Nash Sutcliffe efficiency; KS, Kolmogorov Smirnov statistic;  $E_{max}$ , maximum evapotranspiration in mm d<sup>-1</sup> (the weighted average wet and dry season  $E_{max}$  is reported for the  $p_{wd}$  model);  $s^*$ , point of incipient stomatal closure;  $s_{fs}$ , field capacity;  $E_{max}$ , maximum evapotranspiration;  $E_w$ , evaporation at the wilting point.