Responses to reviewer's comments

We thank the editor and the reviewers for their time and effort to review our manuscript. Please find our replies to all comments below.

Reviewer comments are marked in red.
Responses to the comments are marked in blue.
Changes that will be made in the revised manuscript are marked in *italic*.

Reviewer 2:

The manuscript "Uncertainty estimation for a new exponential filter-based long-term root-zone soil moisture dataset from C3S surface observations" by A. Pasik et al. describes the development of a root-zone soil moisture (RZSM) dataset based on the C3S near-surface soil moisture using the exponential filter method. The newly derived product contains estimates of root-zone soil moisture for different depths, but also their uncertainty estimates considering several sources of uncertainty and their propagation in time. The data product and the code to generate this dataset are available online. I enjoyed reading this well written and clear paper. Please read below my comments which hopefully will help to further improve the manuscript.

We thank the reviewer for their positive feedback and constructive comments.

Major Comments	Reply
1. The root-zone soil moisture is defined here as the water present in the top meter of the soil column (p2, lines 38-39). However, I would argue that the root-zone soil moisture represents the water in the subsurface which is accessible to the roots of the vegetation for transpiration. The depth thereof is highly variable and may depend on climatic (de Boer-Euser et al., 2016; Wang-Erlandsson et al., 2016) and topographic indicators (Fan et al., 2017). Now the derived product provides estimates of soil moisture at different depth intervals, but not really an integrated root-zone soil moisture estimation, which depends on the rooting depth. Would such an addition in the dataset be feasible?	We acknowledge the observation that root-zone soil moisture represents the water in the subsurface which is accessible to the roots of vegetation for transpiration. We also appreciate the potential utility of the suggested integrated root-zone dataset, especially in land surface and hydrological modelling. We indeed plan to investigate the feasibility of producing such an integrated variable in the future, informed by a plant-rooting depth map like the one referenced here (Fan et al. 2017). This is however outside the scope of this study, which is primarily tasked with developing a comprehensive uncertainty estimation scheme for the exponential filter method.

2. When comparing the newly derived product with ERA5L and local data, it would be interesting to see plots of timeseries at specific locations and a spatial map showing where both products have high or low correlations. This would give potential users of the dataset some guidance on where the product may and may not be used. Perhaps the authors can work out some correlations to relate skill with catchment characteristics including climate, land use, topography and soil types.

We will include spatial correlation maps between the C3S SSM and RZSM products with their respective ERA5-Land counterparts in an additional new Figure (please find it included at the end of this document). We believe this will give a spatially more complete understanding of the product's performance than time series could. We will discuss the observed spatial patterns: "*A global SM dataset spanning the 2002–2020 period was computed using the EF method and T-parameters optimized at the point scale with the approach described in section 4.1. Figures Xa–e) show correlation maps of each of the RZSM product layers as well as the input C3S SSM dataset with E5L. The spatial patterns observed in the C3S SSM data (Figure Xa) are strikingly similar to those in RZSM layer 1 (Figure Xb) with slight to moderate deterioration in performance over the high latitudes (> $60°N$). This is not surprising given that both products differ only by a small degree of smoothing applied to RZSM layer 1 and are compared to the same E5L layer (0-7 cm). RZSM layers 2 and 3 (Figure Xc-d) are compared to E5L layers 7-28 and 28-100 cm, respectively, and largely preserve good performance in regions where the input C3S SSM product also performs well, i.e., in Europe (bar Scandinavia), the Caspian and Aral Sea basins, the Eastern United States, India, Southeast Asia, South America, Sub-Saharan Africa, and Australia. At the same time, deterioration of performance is observed in high latitudes and in arid environments such as the Sahara desert and the Arabian Peninsula where the reduced strength of coupling between the surface and root-zone dynamics may hinder the EF performance (Yang et al., 2022). The patterns of good and poor performance visible in RZSM layers 1-3, are not replicated in RZSM layer 4 (Figure Xe) where the agreement with the reference E5L 100-289 cm layer is spatially very heterogeneous and worse overall. The few regions where the good performance observed in shallower layers is preserved include India, Southeast Asia, and the Eastern United States*".

The impact of soil type or land cover on the performance of the EF remains ambiguous (e,g., Stefan et al. 2021). External variables could potentially influence the uncertainty estimates, but such detailed analysis is outside of the scope of this study. We will reiterate the focus of this study throughout the MS, e.g., as per major comment #1 and also by adding the following concluding sentences to the MS' Introduction: "*The focus and novelty of this paper lie in quantifying, rather than reducing, the EF model's known limitations by providing a methodology for comprehensive uncertainty*

Minor Comments	Reply
3. line 64: I would specify here: "does not consider the model structural error of the EF method". Although this becomes clear later in the paper, it was not directly clear to me at this stage.	Thank you for the suggestion. We will change L64 to: *"This approach takes into account the uncertainties of both the SSM input data and the EF model parameter, but does not consider the model structural uncertainty (Beven, 2005) of the EF method."*
4. line 85: "uncertainties [..] were then calculated from the law of propagation of uncertainties". Could you explain how this was done in more detail?	It is literally applying the law of the propagation of uncertainties to the merging equation (weighted average), i.e., ${}^{2}_{\varepsilon_m} = \sum_i w_i^2 \, {}^{2}_{\varepsilon_i}$, where ${}^{2}_{\varepsilon}$ is the error variance, m refers to the merged SSM estimate, and i refers to the input SSM products that are being merged. We will make this more clear by extending the sentence in question to: *"Uncertainties of the merged SSM estimates were then calculated from the law for the propagation of uncertainties (i.e., predicting the uncertainty reduction due to the weighted averaging, assuming that merging weights are correct; see Gruber et al. (2017))"*

5. section 3.2.3: could you explain the presented formulas in more detail? What are the units and what are all parameters? E.g. what does G represent? What does delta represent?	Thank you for this suggestion, we believe the reviewer is referring to section 3.2.1. We will add further details to this section to make the formulas and parameters more understandable. *"In De Santis and Biondi (2018), the standard law for the propagation of uncertainties is applied to the EF method, assuming the errors in the SSM inputs and T-parameter to be normally distributed and uncorrelated. We use this approach as a baseline for our analyses. The recursive formulation of this baseline method is as follows:* **(equations 4–7)** *(RZSM) and (T) denote the uncertainty of the RZSM estimates (in m^3=m^3) and the EF model parameter T (a unit of time, in days), respectively. The equation is initialized as $_0$ = (SSM$_0$), @RZSM$_0$ / @T = 0 and G$_0$ = 0. Uncertainties of the SSM input data are considered by the term (in m^3=m^3), which also takes into account the effect of possible prolonged input data gaps dependent on the T-value. The Jacobian term @RZSM/@T assumes high values proportional to the latest SSM input variability on a time scale related to the T-parameter (expressed as m^3=m^3 over time). This is reflected in significant changes in the RZSM value associated with wetting or drying of the soil. Finally, the term G (dimensionless) weighs the contribution of change recorded between the latest and penultimate RZSM estimates".*
6. line 246: could you quantify with numbers in the text how substantial the difference is between the correlation between E5L and RZSM versus E5L and SSM?	The correlation values for E5L/SSM/RZSM are discussed in L242-249 of the submitted MS. We will annotate the median lines in each box in Figure 3 (revised figure included at the end of this document) for a better overview of differences in correlation scores.
7. Figure 5: in the legend I read "GCOS required uncertainty" but it is not entirely clear to me what this threshold refers to exactly, could you please elaborate?	GCOS outlines target accuracy requirements for ECV data products that are determined by the scientific community. These requirements can be found in the so-called "GCOS Implementation Needs" (GCOS, 2022). We will add a clarifying statement to the manuscript: *"The dashed grey line indicates the uncertainty level defined by GCOS (2022) as an accuracy goal for RZSM products."*

8. line 280: could you elaborate more on why we expect uncertainties to be amplified during transitions between wet and dry conditions? Which processes play a role which are not well represented in the EF method? Now you briefly refer to Fig6, but it does not provide a clear explanation on why this is expected.	Essentially, the EF method operates by smoothing the variations in the SSM signal, therefore the sudden changes are attenuated and delayed while in reality they can be more significantly transmitted to the deeper layers. This simplistic nature of the model results in its limited ability to capture the wetting/drying accurately and, for that reason, in larger uncertainties. We will further clarify this by adding a sentence following the one referred to here. Together, this will read: *"Compared to the baseline (Figure 5a), this yields an increased overall magnitude of the uncertainties, a more realistic increase in (temporal average) uncertainties with depth, and an amplified temporal variability in all layers during transitions between dry and wet conditions (see Figure 6). The latter effect is caused by the simplistic nature of the model, which essentially operates as a smoother and therefore attenuates sudden variations in the SSM signal which in reality may be transmitted into the deeper layers in a more significant manner. The reduced accuracy of the EF method during soil wetting and drying phases was also observed by others (Ford et al. 2014)."*
9. line 292 "and highlighting 20% of data with the highest uncertainty". At this stage, this reads a bit confusing as the previous paragraph describes masking out data with the highest uncertainty and here (if I understood correctly) you are instead plotting data with high uncertainty. Perhaps good to clarify what you mean with "highlighting 20% of data with the highest uncertainty".	We will edit the referenced sentence (L303-304) to read: *Figure 6a) and d) indicate (in magenta shading) 20% of RZSM layer 2 data with the highest uncertainties masked out in the experiment described above based on uncertainties estimated with the baseline (b), and our method (d), respectively.*
10. line 299: the described difference in uncertainty from 0.008 m3/m3 to 0.004 m3/m3 is very hard to see in the Figure using the applied scale.	Figure 6 will be redesigned for more clarity by removing the not relevant in situ signal and placing uncertainties on independent scales where their temporal dynamics are better visible (please see its revised version at the end of the document).

11. line 302: why are the uncertainties related to structural breaks not clearly seen in the MAD Topt approach. Can you reflect (here or later in the discussion) a little bit more on this result. It seems to me that the change in uncertainty related to a change in sensor is an important change that you would also want to see in the improved methodology for uncertainty estimation.	Thank you for this comment. Indeed, the uncertainties of the input data are an important element here and their sudden shifts should be reflected in the propagated values. We observe that in this particular aspect, the difference between the baseline and our methods is driven solely by the value assumed by the (T). A higher value of (T) places more weight on the impact of significant changes in RZSM values (represented by the Jacobian term @RZSM$_0$ / @T), while lower (T) favors the impact of the input uncertainty values ( ). The former better reflects the sudden changes in input uncertainty due to sensor changes, while the latter is more suited to resolving day-to-day uncertainty variations. This seems to be somewhat of a trade-off with this approach as it cannot do both at the same time. We will extend the discussion of this result in Section 5 **Summary and Conclusions** by adding the following sentences to the existing comparison of the used (T) values (L335-340 of the submitted MS): *"A higher value assumed by (T) (in this case $MAD(Topt)$) places more weight on short-term significant variations in RZSM values (accounted for by the Jacobian term @RZSM/@T) and overshadows the contribution of the input uncertainties ( ) to the overall uncertainty budget. This approach results in higher uncertainty outputs paralleling significant changes in RZSM signal (e.g., soil wetting/drying events) and is generally better suited to describe day-to-day uncertainty variations. Meanwhile, lower value of (T) (here $Topt$=10) favors the impact of the input uncertainties and appears to be more skillful in detecting sudden shifts in the magnitude of the input uncertainties due to C3S SSM sensor changes. While both the significant variations in RZSM values and the magnitude shifts in the input uncertainties are crucial elements of the overall uncertainty budget, there appears to be a trade-off in favoring the impact of one or the other based on the value assumed by (T)"*.

12. line 314-320: here, it is not clear to me why using Topt/10 as T parameter uncertainty yields more realistic estimates of temporal uncertainty variations than using MAD Topt in the case of using the time series which includes a structural break (and the opposite in case a shorter time series is used). Which aspects in figure 7 suggest these findings?	In fact, both approaches yield realistic temporal variations as they mostly assign highest uncertainty values to the same RZSM estimates (this is evident in Figure 6). In the context of Figure 7, we describe the uncertainties which yielded better results in improving R with the in situ reference as *"more realistic estimates of temporal uncertainty variations"*. Indeed in reference to Figure 7 this sentence could be more clear. We will rephrase it: *"In case of the full product period (Figure 7a–d), using* $(T) = Topt$=10 *as T parameter uncertainty seems to yield more consistent improvements in correlation with the in situ reference after removing a percentage of the most uncertain data, than using* $(T) = MAD(Topt)$*."* The so called structural breaks are sudden shifts in the magnitude of the input uncertainties and the value assumed by (T) either increases or decreases the weight of their contribution to the total uncertainty budget. Please see our response to the previous comment (#11).
13. line 320-324: Again, could you elaborate why the uncertainty estimations of temporal uncertainty variations are no longer accurate for deeper layers?	Thank you for the comment, we will elaborate on the challenges of capturing the temporal uncertainty variations in deeper layers by including the following sentences at the end of section 3.5 **Assessment of uncertainty estimates**: *"At greater depths, the contribution of the model structural uncertainty on the total uncertainty budget has been shown to increase. In the circumstances where the EF model appears to be inadequate, for example due to poor coupling between the root zone in consideration and the surface layer, it can be assumed that the model structural uncertainty is so predominant as to make the temporal patterns of the other uncertainty components marginal in practice. However, in circumstances where the magnitude of the real uncertainty is such as to make the EF-based RZSM so unreliable, the lack of ability to reproduce the temporal variations of the estimated uncertainty becomes less relevant."*
14. line 351: here, you forgot to add the units of the mentioned uncertainties.	Thank you for pointing this out, we will add the missing units.

15. In addition, I also downloaded the netcdf files and checked the github page. The nc files contain all the necessary meta data. However, the github page does not include extensive documentation on how to use the different methods within the package. Would it be feasible to elaborate on this further?	We appreciate the thoroughness. While the package includes basic examples of the application of the package, we agree that a more extensive documentation would be beneficial and intend to expand it in the future. We made the code package public also in hopes that it will attract contributions from the user community.

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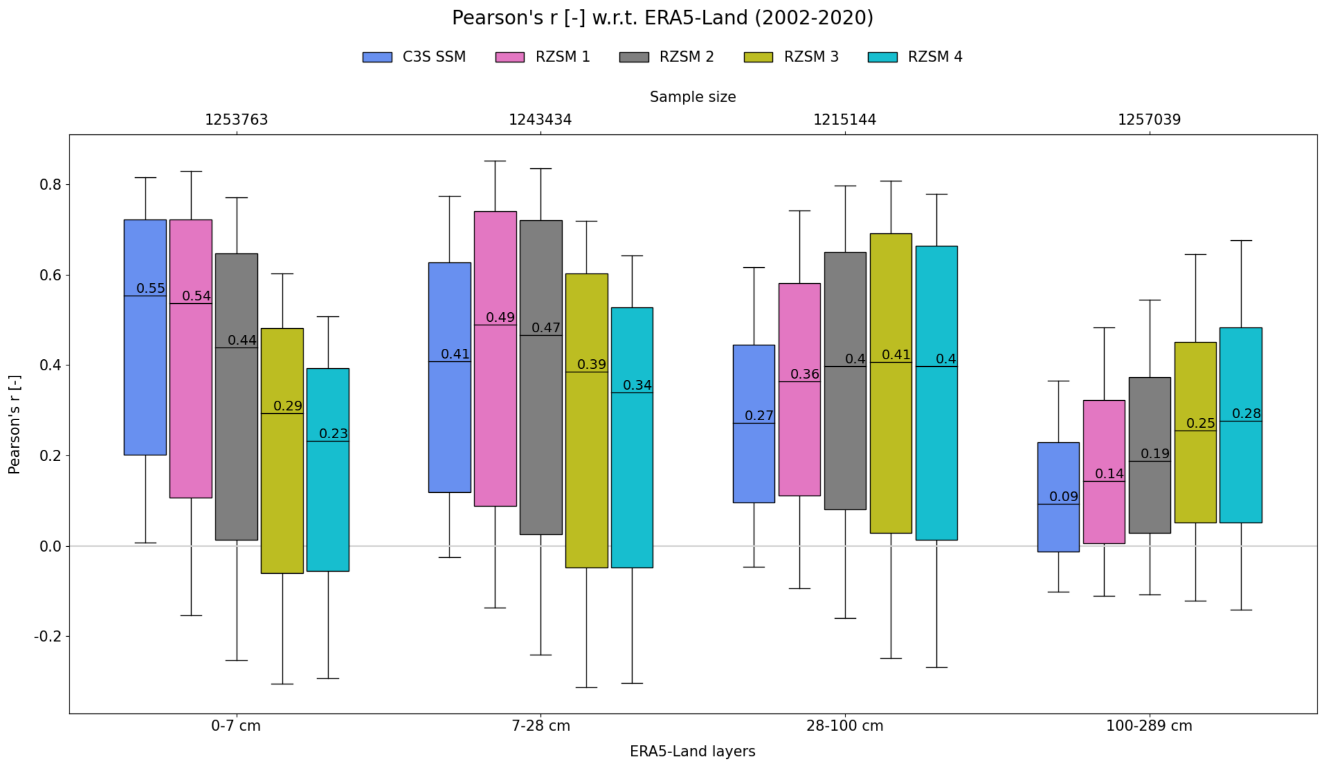
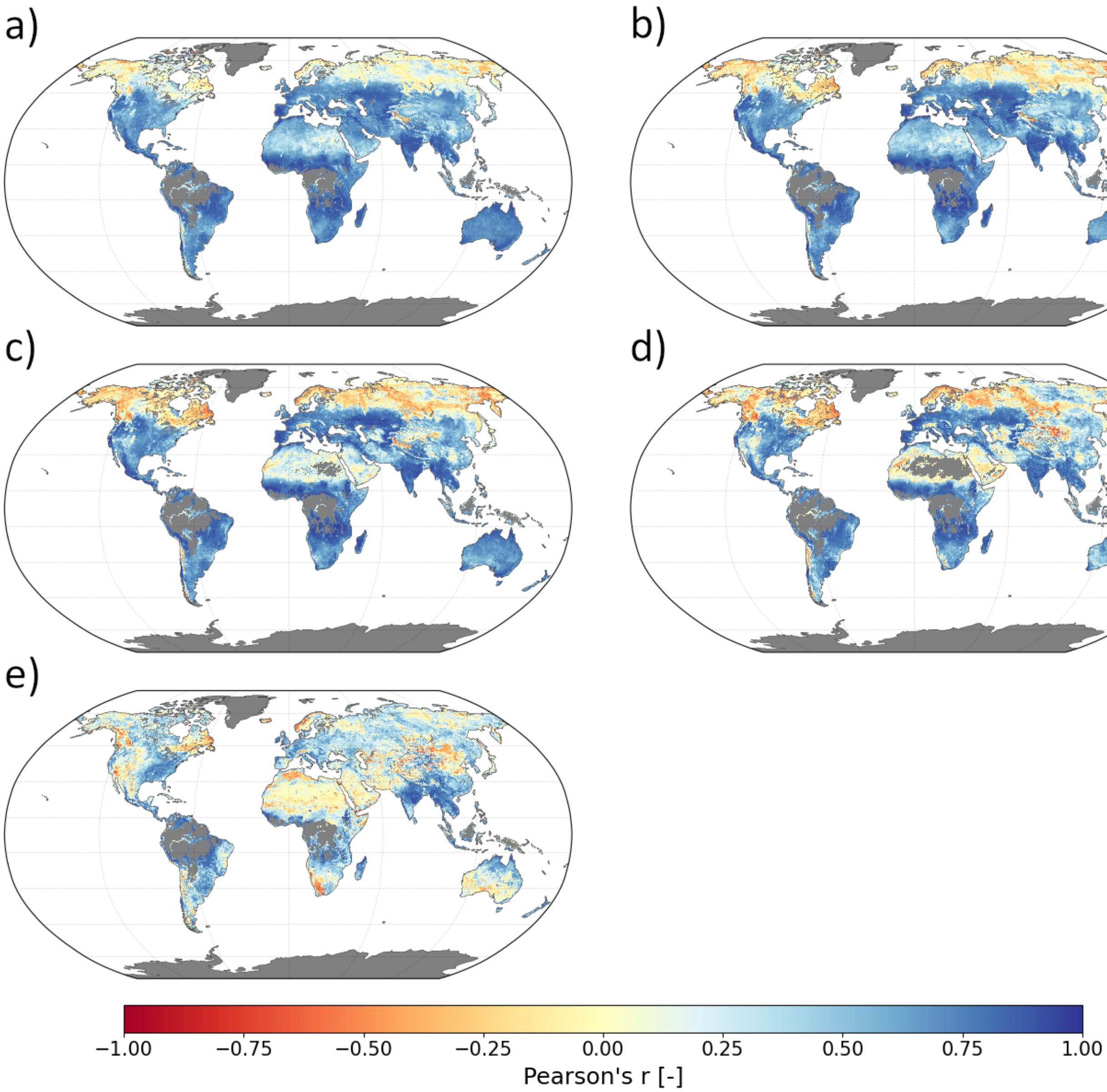


Figure 3: Product intercomparison of the C3S SSM and RZSM products against E5L SM.



Spatial correlation maps of the C3S SSM (a) and RZSM products (b-e) with E5L layer 0–7 cm (a-b), 7–28 cm (c), 28–100 cm (d) and 100–289 cm (e).