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Response to the Community

Community comments are presented in italics, while the authors' responses are in blue.

1 Community Comments and Responses

CC – community by Markus Köhli

In their manuscript "Improved representation of soil moisture simulations through incorporation of cosmic-ray neutron count measurements in a large-scale hydrologic model"

the authors Fatima et al. describe the combination of several years of data from CRNS instruments at selected experimental sites and hydrological modeling. The reviewer appreciates the approach of the authors to move towards a more comprehensive picture of how CRNS can help to understand hydrological dynamics however, there are significant concerns about the methodology, data representation, completeness in the representation of CRNS, and lack of transparency in the choice of models and parameters in the paper. The reviewer suggest addressing these issues to improve the quality and validity of the research.

General:

[-] *Without any apparent reason or justification this paper selectively uses the soil depths 0-5 cm, 5-25 cm and 25-60 cm. Except for the top soil layer, none of these classes are representative for either hydrological processes or measurement depths of CRNS. What is the reason for the authors to use that scheme? This sampling is too coarse and not deep enough to be acceptable and needs to be refined. This sampling can and will lead to non-obvious systematics and therefore would create misleading results. Specifically, as the authors focus on statistical analysis methods this whole approach seems questionable.*

We agree that our choice of vertical resolution can appear arbitrary for readers that are not experienced with intricacy of large-scale hydrological modelling and their application in mesoscale settings. While we agree that the vertical resolution could also be critical with respect to capturing small-scale hydrological processes, it has been, however, shown in the past that the chosen depth resolution is reasonably accurate to describe the relevant hydrological processes in the root-zone relevant soil processes for mesoscale hydrological models Al-Shrafany et al. (2014); Crow et al. (2018); Vereecken et al. (2015); Mohajerani et al. (2021); Downer and Ogden (2004). Furthermore, the chosen depth resolution and stratification ensure that the most important supporting points for the description of depth-dependent neutron sensitivity are captured as justified by recent literature. Andreasen et al. (2020); Franz et al. (2020); Baatz et al. (2017); Iwema et al. (2017); Andreasen et al. (2016); Han et al. (2015).

Besides, we have also conducted a set of experiments with varying soil depths, ranging from 3 to 6 layers, specifically (0-5 cm, 5-15 cm, 15-25 cm, 25-30 cm, 30-60 cm, and 60-100 cm). In the model settings, our analysis pointed out that the simulated neutron count results were not significantly influenced by the number of soil layers (see Fig. 1 below for more details). Based on our prior experiences of modelling with mHM, we adopt the same soil layer (0–5 cm, 5–25 cm, and 25–60 cm) depths as utilized in the study by Boeing et al. (2022) - who have extensively evaluated mHM simulations against observed soil moisture across different locations in Germany.

The theoretical measurement depths of CRNS are in the range of 10 to 80 cm according to Zreda et al. (2008), Franz et al. (2012), and Köhli et al. (2015). For intermediate soil moisture conditions (0.1–0.4 m^3/m^3), the average CRNS measurement depth is between 15 and 30 cm, but the highest sensitivity is in the upper layers, 0–5 cm (Schrön et al., 2017). It is correct that the accuracy of numerical calculations (such as our COSMIC model set-up) would benefit from higher resolved soil profiles, however, our experiments demonstrated that varying soil depths from 3 to 6 layers did not have a substantial impact on the simulated neutron count results in our model setting.

Finally, we would like to emphasis past modelling studies that use CRNS measurements in their respective model based investigation where certain modelling choices are inevitable. For example, Iwema et al. (2017) used a land surface model to investigate the impact of reducing the scale mismatch between surface energy flux and soil moisture observations of CRNS point measurement data. The model used with grid cells of 1 km^2, parameters calibrated with eddy-covariance flux data and point-scale soil moisture data. In the study they used point-scale soil moisture data from the soil layers up to 30 cm depth and 2012- 2015 data were simulated. Other factors limit the limited effect of calibrating soil parameters on soil moisture dynamics and surface energy fluxes spatial-temporal stability. Barbosa et al. (2021) study used HYDRUS-1D model for the simulation of soil moisture time series at the 6 different depths of 2, 20, 30, 40, 60, and 100 cm and compared it to independent soil moisture measurements of PR2. HYDRUS 1D is coupled with the COSMIC Operator and Richards nonlinear partial differential equation was used and compared the neutron count rate with soil moisture simulated data and inversely calibrated the soil hydraulic parameters based on CRNS data.Zhao et al. (2021) used the land surface model (the Community Land Model; CLM version 3.5), a coupled land surface-subsurface model (CLM-ParFlow) is applied, and used the soil layer depth of 5cm and 20 cm.

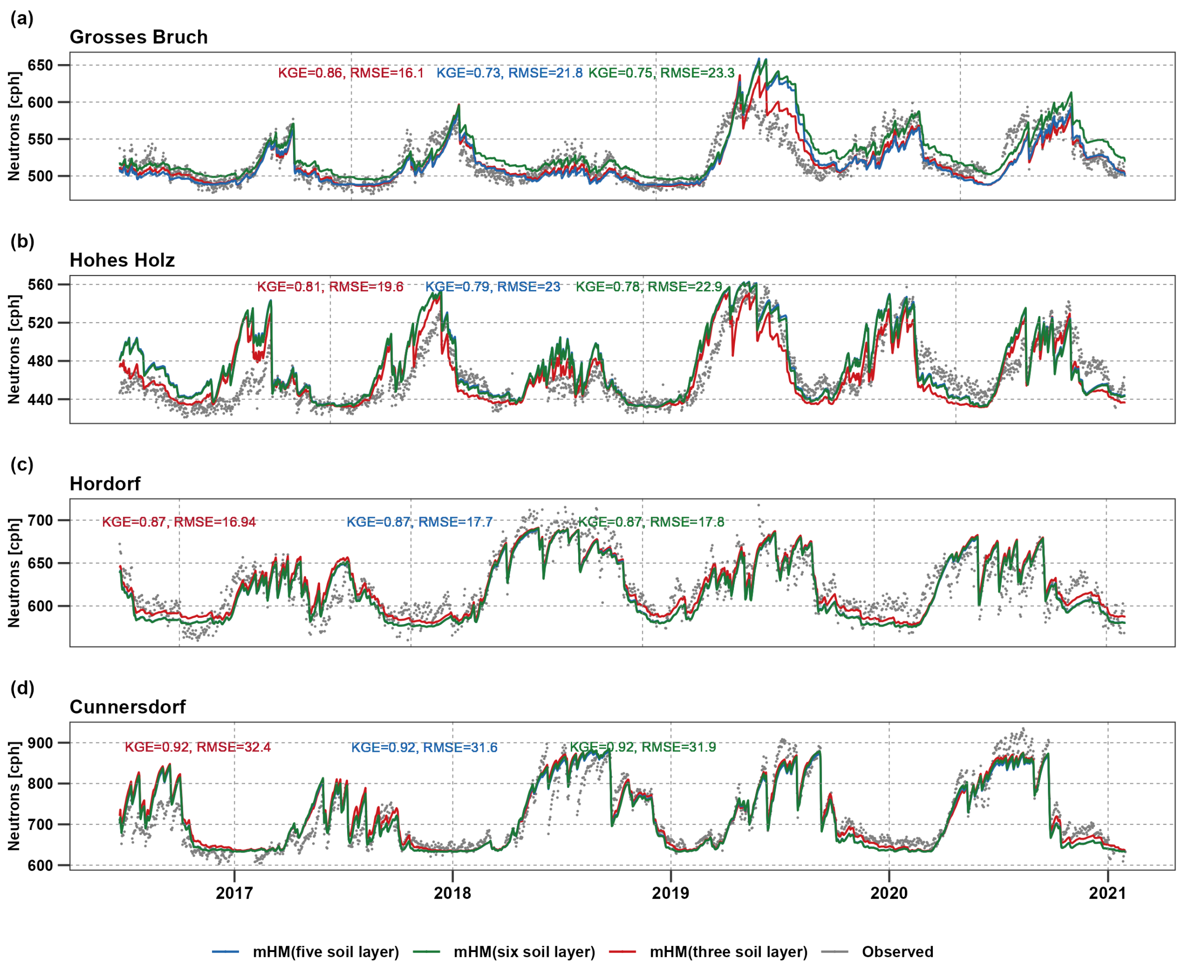


Figure 1. Simulated neutron counts from mHM using different soil horizon depths: three soil layers (5 cm, 25 cm, 60 cm), five soil layers (5 cm, 15 cm, 25 cm, 40 cm, 60 cm), and six soil layers (5 cm, 15 cm, 25 cm, 40 cm, 60 cm, 100 cm).

[-] Using just the N_0 method and the COSMIC operator in order to draw the general conclusions the authors would like to present is with respect to the state of the art not justified. Either narrow down the scope to a more exemplary analysis or include other models like the UCF method from Franz et al. or the UTS method from Köhli et al., which are both not even mentioned in the overview, yet mentioned in the discussion.

Thank you for hinting at the other N-SM conversion functions, we will make it clearer that this is an exemplary study and other methods could be tested in future research. Our choice for COSMIC and Desilets was based on their widespread use in past/recent studies: e.g., Desilets method Desilets et al. (2010) by Baroni and Oswald (2015); Schreiner-McGraw et al. (2016); Zreda (2016); Avery et al. (2016); Vather et al. (2019, 2020); González-Sanchis et al. (2020); Power et al. (2021); Barbosa et al. (2021); Chen et al. (2022) and COSMIC Method Shuttleworth et al. (2013); Rosolem et al. (2014) used by Baatz et al. (2014); Iwema et al. (2015); Han et al. (2015, 2016); Brunetti et al. (2019); Mwangi et al. (2020); Patil et al. (2021). The UCF method from Franz et al. (2013) has its own limitation as has been shown low experimental performance in the past (McJannet et al. 2014, Baatz et al. 2014). The recent UTS method from Köhli et al. (2021) was published after the start of our study, it still requires sound experimental validation, and it adds further complexity (such as air humidity dependency) which is not feasible for mHM at this state. In fact, the cited paper shows that the UTS function behaves very similar to the COSMIC approach. Hence, we believe that we have covered the main processes of the N-SM conversion approaches. Nevertheless, we will mention the recent developments of N-SM conversion functions in the revised manuscript as an opportunity for future elaborated studies.

[-] The study heavily focuses on modeling and statistical analysis. Throughout the manuscript, the reader encounters a large amount of seemingly arbitrary choices, which in the end provides the impression that results are selected and tinkered in order provide a realistic picture. The authors want to show that they uses methods which are accepted in the community, from the statistical and the modeling perspective, then, however, they introduce a significant amount of modifications and ad hoc assumptions which may put the whole approach into question. Examples are: In which way should a sophisticated hydrological model help, if the authors choose to simply take only three layers, for which the choice of hydrological parameters is also not really transparent? What is the reason to take only the 1% of the model runs with the best KGE (that number clearly depends on the initial parameter ranges the authors arbitrarily chose)? As the choice of the neutron model and their parametrization is not at all according to any standard, what does such tight constraint say other than the whole analysis is tuned to fit one specific ad hoc assumption. In which way is the KGE modified by the authors introducing a bias on this analysis? Why are 99 % of the model runs excluded if there are significant deviations from the models and the data, even visible in the plots presented? To be clear on that point: If significant deviations can be observed between model and data, any tight statistical constraint (in matching them incongruently) will lead inevitably to wrong results.

As stated above, we have analysed different soil depths ranging from 3 to 6 layers (0-5 cm, 5-15 cm, 15-25 cm, 25-30 cm, 30-60 cm, and 60-100 cm) but found that the number of layers did not significantly affect neutron count results. As a result, we adopted the same layer depths used in Boeing et al. (2022).

We selected 1% of the model run with the best $KGE_{\alpha,\beta}$ because this simulation yielded neutron counts that captured well towards observed values. Increasing the number of simulations is certainly possible but this could introduce another level of complexity.

Regarding the revision of KGE, Gupta et al.2009 proposed the KGE as a weighted combination of the three components (bias, variability, and correlation terms). We opted not to consider it in our assessment (objective function), as it accounted for 33% of the total weighting in the overall KGE score. High correlation values stem from the fact that the seasonality of SM is an inherent characteristic in the northern hemisphere, where precipitation minus evaporation is mostly driven by evapotranspiration. Evapotranspiration is higher in summer and lower in winter, and soil moisture indirectly will result from low ET values in winter and high values in summer. This aspect is inherent, and we do not want to emphasis in our optimization these characteristics. That does not mean we are neglecting seasonality, but do not want our parameters to capture the seasonality aspects. Even if a random parameter is selected, the correlation will always be higher because the meteorological forcing is the precipitation - evaporation is seasonal, and seasonal is coming from forcing. Previous studies have also introduced revisions to KGE Mizukami et al. (2019).

The COSMIC model is the established standard for Cosmic-Ray Neutron Sensor (CRNS) forward modeling. There are several studies in the literature that have utilized COSMIC as the recognized model for CRNS simulations. These studies include (Baatz et al. 2014), (Iwema et al.2015), (Han et al. 2015), (Han et al. 2016), (Brunetti et al. 2019), (Mwangi et al. 2020), and (Patil et al. 2021).

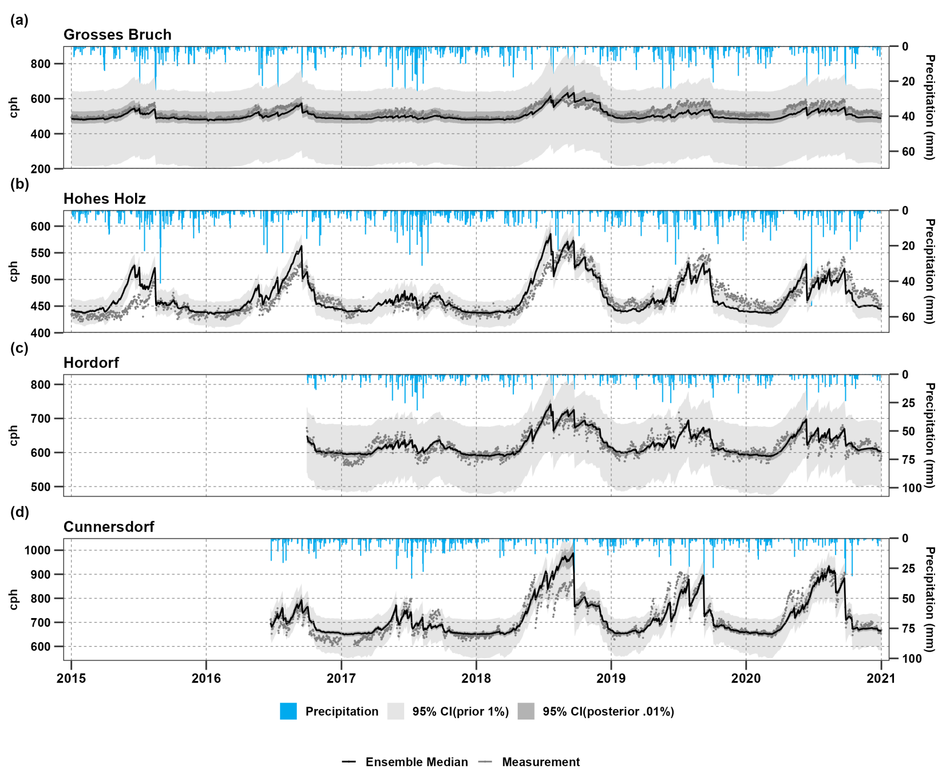
[-] Instead of overloading the manuscript with a multitude of different statistical measures, the authors should focus on providing a reasonable basis for comparing model and data. The authors rather present in the manuscript their own struggles and the reader does not learn anything from that way of analyzing a problem the authors fabricated in an intransparent way.

We are using the five most established measures in hydrology to evaluate the model performance on observations (KGE, modified KGE, NSE, R^2, and PBIAS). As it is well known from the literature Nash and Sutcliffe (1970); Gupta et al. (2009), each of these measures has its own justification to assess the quality of the performance in terms of bias, dynamics, temporal and static errors, etc. The fact that our results are not only based on a single measure but rather in agreement across the many different measures shows that our conclusions are particularly robust (see Table 4). We believe that this procedure strengthens our study and demonstrates that neutron counts could improve hydrological model results not only in terms of correlation but also in reducing biases and improving overall performance measures.

General figure layout:

[-] the neutron data is plotted as quite large dots, which scatter significantly. Either smaller dots should be chosen or some type of smoothing.

Thank you for your suggestion. We will consider using smaller dots in the neutron data plots to improve their clarity and readability.



[l88:] "the physics-based model COSMIC" - COSMIC is not physics-based, it is not based on a comprehensive physical interaction picture. It selectively takes specific processes and invents arbitrary mathematical representations for them.

As was demonstrated in a large number of accepted literature, COSMIC is an analytical-based model incorporating key physics-based processes important for CRNS applications in conjunction with models. COSMIC simplifies the physical process tailored to CRNS applications by mimicking a similar neutron transport behavior at the vertical axis as compared to more complex Monte Carlo models that actually implemented detailed physical interaction processes in three dimensions Shuttleworth et al. (2013); Rosolem et al. (2014). The model includes descriptions of various physical processes, such as neutron flux degradation with soil depth, creation of fast neutrons within the soil, and scattering of fast neutrons, all depending on soil composition and water content. It has been validated with detailed physics-based simulations and has been empirically confirmed in many subsequent studies i.e., Baatz et al. (2014), Iwema et al. (2015), Han et al. (2015), Han et al. (2016), Brunetti et al. (2019), Mwangi et al. (2020), Patil et al. (2021)). Naturally, not all detailed physical processes can be represented by a mathematical model, particularly the 3D neutron transport at scales of 1 to 300 meters. However, at the scale of interest in hydrological and land surface modeling (1 km), COSMIC can be considered adequate. In this study, we rely on the published model structure, while any model improvement with regard to additional physical processes will have to be discussed in a dedicated separate paper.

[l99+:] "What is the best approach to simulate CRNS neutron counts in a hydrological model considering the heterogeneity of vertical soil moisture profiles?" - This paper provides an exemplary data analysis which is insufficient for generalizations of the mentioned type.

Thank you for your comment. In our study, we checked the capability of a mesoscale hydrological model that can simulate the neutron counts by taking into account the vertical heterogeneity of different soil layers and comparing them with the measured neutron counts based on hector scale footprint. To account for sub-grid heterogeneity, which is captured with the multiscale parameter regionalization (MPR) technique in mHM (Samaniego et al., 2010), it allows us to study how model parameters vary across different scales of modeling.

[l159+:] "Simulations from mHM revealed that the sensitivity to the highest soil water content was observed at 5 cm depth (...)" - this sentence is highly confusing, grammatically and in the context of the manuscript as for example there is no information provided anywhere about a layer specifically at 5 cm depth.

Thank you. We will revise the sentence.

[l165+:] Theoretically, the N_0 parameter, which represents the neutron count rate level of the particular CRNS probe used for rather dry soil at the local conditions, should be site-specific" - please describe theories which underline the theoretical reasoning that N_0 is site specific. The mentioned references do not provide that information. In case the N_0 equation is an inadequate representation of the neutron count rate a site-specific behavior would be a result.

Thank you for this remark. The site-specific nature of the N_0 parameter is a well-recognized aspect within the Cosmic-Ray Neutron Sensor (CRNS) community, though there may be other future approaches for N_0 accounting directly for various site-specific influences. Currently, N_0 is typically calibrated for each sensor at each location via in-situ soil sampling campaigns or local soil moisture networks. Many authors have confirmed this observation (Zreda et al. 2012, Hawdon et al. 2014), while others investigated data from several different sensors and found non-identical N_0 values even if the detectors are similar (Fersch et al. 2019, Heistermann et al. 2021, Bogena et al. 2022). This indicates that the influencing factors on N_0 are not yet fully understood though a recent study has outlined that a minimal info from the site could be sufficient to determine the N_0 even without local soil moisture data (Heistermann et al., HESSD, 2023, https://doi.org/10.5194/hess-2023-169). Since the mHM model does not include these effects, we infer the value of N_0 through the calibration procedure.

[l172:] "may be impacted by factors such as soil chemistry" - within the field of CRNS researchers claim that this method would be independent of soil chemistry. The reviewer is curious how the authors come to this assumption.

Regarding CRNS data, the absolute neutron intensity varies by location due to varying soil chemical compositions, although these variations are generally small for epithermal and fast neutrons (ranging from 1 eV to 10^6 eV) because neutron absorption is insignificant. Thermal neutrons have a different sensitivity to varying soil moisture content than do fast and epithermal neutrons because thermal neutrons are highly dependent on on chemical composition of the soil matrix and soil water (Zreda et al. 2008, Andreasen et al. 2019, Rasche et al. 2021). This effect often is negligible, but we still mention it here since the variation of soil chemistry within our four sites is significant, particularly due to a high range of organic input below, on, and above the surface. We will better express this aspect by changing the formulation to “additional hydrogen pools (e.g., from organic material)”.

[l172:] “heterogeneity” - which type of ’heterogeneity’ do the authors refer to? In case ’heterogeneity’ refers to topographical heterogeneity the whole approach of this analysis is questionable.

Thank you for pointing out this part. We would like to clarify the type of ’heterogeneity’ we refer here is related to not only terrain (topography) but also local soil and vegetation characteristics. We will revise the sentence to better capture this aspect e.g, through “... neutrons are sensitive to all kinds of hydrogen in the footprint, hence the variable θ denotes not only soil moisture, θ_{sm}, but is rather assumed to also include lattice water, θ_{lw}, as well as water equivalent from soil organic carbon, θ_{org}, and vegetation biomass, θ_{bio}.”

[l182:] "derived from neutron particle physics modeling" - in which way are these parameters derived from particle physics and empirical (as mentioned above) at the same time?

Thank you for pointing this out. In the revised manuscript, we will formulate the sentence as follows: “parameters a_i were determined empirically by Desilets et al. (2010) who derived $a_0 = 0.0808$, $a_1 = 0.372$, and $a_2 = 0.115$ for values of $\theta > 0.02\ gg^{-1}$."

[l200:] The weighting scheme as presented is incomplete. (5)-(7) only take into account the weight of one depth. As to the model the authors used, the weight needs to be calculated by an integral over the depth weighting function for the height of the soil profile, not just the weighting function by itself.

Thank you for your valuable feedback. We implemented the weighting procedure properly but have not adequately explained the procedure in the manuscript. This will be fixed in the revision. In the weighted-averaging approach, the weights are determined following Schrön et al. (2017), where the vertical contribution of layer i is:

$$N_{\text{Des},W} = N_{\text{Des}}(\theta_{\text{avg}}(w_i)) \tag{1}$$

$$\text{where} \quad w_i = \int_{z_{i,\text{min}}}^{z_{i,\text{max}}} e^{-2\,z/D}\,\mathrm{d}z \tag{2}$$

$$\propto e^{-2\,z_{i,\text{min}}/D} - e^{-2\,z_{i,\text{max}}/D}$$

Here, the integral goes through each horizon from $z_{i,\text{min}}$ to $z_{i,\text{max}}$ in 1 mm steps and summes up the weight over the whole layer. The fact that the integral over an exponential function is again an exponential function is the reason for our simplified description using only z_i in the original manuscript.

[l203:] What is the depth z_i? As the authors use soil horizons of considerable height, how do the authors calculate z_i?

Thank you for your remarks. To calculate the influence of soil moisture in different depths, the soil horizons were subdevided into smaller fractions and integrated over smaller steps of z_i. We will better clarify this in the manuscript in the revised manuscript.

[l210+:] The COSMIC model only mimicks the mentioned subset of physical processes, in no way it represents them. Analytically COSMIC only represents an exponential N(theta) function, with an arbitrary parameter adaptation (8). The underlying mentioned physical processes are not responsible for the signal generation within CRNS as it lacks the spatial neutron transport, which CRNS claims to use as a unique feature compared to other methods.

Thank you for your comment. According toa decent number of published and widely accepted literature, COSMIC is able to adequately mimic the neutron generation from soil moisture profiles Shuttleworth et al. (2013); Rosolem et al.

(2014) Baatz et al. (2014), Iwema et al. (2015), Han et al. (2015), Han et al. (2016), Brunetti et al. (2019), Mwangi et al. (2020), Patil et al. (2021)). Of course, a mathematical model can never represent the full range of physical processes involved, however, as the authors from Shuttleworth et al. argue, it aims at representing the main processes in the vertical dimension (such as signal attenuation and neutron production/evaporation based on soil composition). This dimension is most relevant for large-scale models (500–4000 m). Spatial neutron transport at typical scales of 1–300 m might be necessary for detailed and complex terrain, as was shown by, e.g. Schattan et al., (2019), Schrön et al. (2023), and Köhli et al. (2023). But on average the typical mHM pixel size is at least one order of magnitude larger than the scale of lateral neutron transport, while the chosen sites exhibit homogeneous land use. Hence, we consider the 1D model assumptions adequate for the target application.

[(11):] (11) is missing

Thank you for pointing this out. This is a layout issue and will be resolved in the revision.

[l241:] explain the term "geometric integral"

We are here referring to equation 8 as mentioned in the text. As was explained, it resembles an integral of the vertical neutron transport, geometrically projected to the vertical axis. See also Schuttleworth et al. (2013).

[l275:] What are "COSMOS models"?

We will correct it to "COSMIC model".

[l293:] "COSMIC is physically based, a loss of the physical meaning of the parameters in question would be very critical." - as described above COSMIC takes an incomplete subset of physical processes in order to justify its model. In this sentence the authors echo the critics which have been mentioned with respect to this model. Without the representation of neutron transport, for example, any possible source-only model can hardly justify itself to be correct.

As stated above and as has been demonstrated in plenty of respective literature, the COSMIC model represents the vertical neutron transport in a 1D soil column in a physically consistent manner. Based on several confirming studies in the literature (see above), we consider it as a reasonable approach to be implemented within mesoscale hydrological models, in which horizontal resolution is orders of magnitude larger than the scale of lateral neutron transport. For detailed small-scale processes, snowpack quantification, and heterogeneous terrain, we would agree that COSMIC could be improved, but this is out of the scope of this study and probably even unnecessary given the large spatial scales on which typical hydrological and land-surface models operate. During the revision of the manuscript, we will reflect on these parts to make them clearer.

[Fig. 4:] Why is the depiction of the histograms so coarse? Please enlarge the scale to the relevant range.

The plots already show the full range of the 100 000 data for the prior range and 10 data points taken from the objective function which is the posterior range in the x-axis. The main message of the plots is to show how the posterior distribution was constrained compared to the respective prior distribution. That is why we plot both distributions along with their full ranges.

[Fig. 4:] As many columns have the same height, the reviewer questions the representativeness of the results. The exact same height could mean that either the model provides on the basis of the 100 000 data sets the same values or most of the results were discarded and the authors want to draw conclusions from just a few values.

The reviewer seems to misinterpret the Figure and we would be happy to sharpen the corresponding explanations in the revised manuscript. The sample size for all sites is fixed at N = 100 000 as the prior range, and the iterations are conducted within the N_0 range of 600-1500 along with another 28 parameters for Desilets method and 30 parameters for the COSMIC method for each site. Consequently, when utilizing the prior sample range, it appears identical for all sites due to this uniform setup.

[l323:] Given the fact that the authors chose to represent the soil in very coarse layers, the "crowding cows" in the otherwise very wet catchment, seem to be a distracting and out of scope reasoning by the authors and at that point do not strengthen the scientific quality of the material presented.

Evidence for the influence of crowding cows at this site has been mentioned in Schrön et al. (2017) and may introduce additional uncertainty to the data in specific periods (Aug to Sept). We agree that this is not a major issue particularly since there are no cows for the major part of the year. We further demonstrated that the choice of vertical layers is adequate, as explained above, and will add this to the revised manuscript.

[Fig. 5 and Fig. 6.:] Both are plotted in such a tiny way, that it is hard to identify the different lines from each other and blur the relevant deviations.

Thank you for the feedback, we will replot the data to improve visibility and make it easier to distinguish the lines and relevant deviations.

[l379+:] citep missing. "which are typically 5–60 cm and sensitive to shallow soil moisture" the reference tells that CRNS actually measures deeper than that and for that reason the choice of only simulating up to 60 cm seems wrong or incomplete.

Thank you for your feedback. We will add the citation with the citep command. Our calculation was based on the formulas given in the citation and specific to the investigated sites. In the revised manuscript, we will mention that the theoretical measurement depth for the cosmic-ray probe varies, ranging from 12 cm in wet soils to 76 cm in dry soils (Zreda et al., 2008, 2012; Rosolem et al., 2013). For the sites in our study, we typically do not see measurement depths beyond 60 cm (Bogena et a. 2022).

[l445:] "Overall, the three methods (NDes,U, NDes,W, and NCOSMIC) in mHM were able to consistently simulate the neutron count" - the results were inconsistent and the variability was only partially covered.

Thank you for your comment. In the paragraph, the statement is that "Overall, the three methods ($N_{\mathrm{Des,U}}$, $N_{\mathrm{Des,W}}$, and N_{COSMIC}) in mHM were able to consistently simulate the neutron count variability throughout the available data period." Here the consistency in simulating neutron count variability means that mHM has the capability of capturing the general trend and pattern of the simulated data, as illustrated in (Figs. 5 and 6). The light grey color shows the top 1% of the model run with the best $KGE_{\alpha\beta}$ values. Furthermore, we have provided a comprehensive discussion of the performance and variability of neutron count simulations with the three methods at each site, from lines 405-455.

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