Reviewer #3

We thank reviewer #3 for taking the time to review our manuscript and their valuable suggestions regarding our manuscript. We are certain that these comments greatly improve our manuscript and they will be incorporated in a revised version of the manuscript. In the following section we will reply to all comments of reviewer #3 with R3-1 (i.e. reviewer 3, comment 1) and A3-1 (i.e. author response to R3-1), respectively.

R3-1: Fig 6a: Why is there so little change in the R86 footprints in this figure (as measured by first soil contact) compared to Fig 3a? In the case of simulation set 3 (dashed lines Fig 6a) far field soil moisture drops from 0.7 to 0.2 which is very similar to the drop from 0.7 to 0.1 in Fig 3, but in Fig 6 we also have that the near field soil moisture is decreasing. Surely there should therefore be a larger change in the various footprints in Fig 6? In fact R86 actually decreases slightly in simulation set 2 between scenario 1 (wettest) and scenario 6 (driest)! Is there a mistake? Have missed something important?

A3-1: Thank you for this comment! We checked the postprocessing procedure of the simulation data of all simulation scenarios conducted and found a mistake in the code. Fixing the code leads to different absolute simulated neutron intensities and radial footprints. For instance, the average footprint radius of epithermal neutrons in simulation set 1 decreases from 134 to 121 m as we now also use the detector boundary instead of the detector centre for calculating the distances to the point of origin of each neutron. Although the absolute values are different, in relative terms, the results are very similar to those already in the manuscript and thus, fixing the code does not lead to a different interpretation of the simulation results. This also confirms the low sensitivity of our results to the site-specific footprint size. Nevertheless, we apologize for this mistake and will update all values throughout the manuscript and update all figures. The updated figures are shown below.

In respect to Figure 6, correcting the code does not have a major effect. First of all, simulating a relatively small virtual detector in a large model domain leads to a limited number of simulated neutrons actually reaching the neutron detector compared to e.g. measuring the total number of neutrons in a certain energy range are reflected from the soil in the entire model domain which cannot be done under heterogeneous soil moisture conditions. Consequently, a certain degree of statistical variations has to be considered. This is also displayed in Figure 4 and can explain certain variations visible also in the figures showing the calculated R_{86} and D_{86}. This is likely to be the most important reason for the slight decrease and variations visible for the R_{86} in fig. 6a for epithermal neutrons.

The footprint change of epithermal neutrons differs between the simulation set 1 and those of simulation set 2 and 3. This can also be related to the fact of the footprint change becomes smaller with more water (i.e. hydrogen) being in the model domain. Due to this non-linearity, the largest footprint changes can be expected under rather dry conditions from e.g. 0-0.15 m^3 m^{-3}. As a consequence, one reason for the small differences in footprint changes can be related to the high soil moisture contents simulated and adds to the statistical uncertainty of the Monte-Carlo simulations mentioned before which has a higher impact if the footprint change with changing soil moisture is smaller.

When more water is located close to the detector, where it is most sensitive, fewer neutrons reach the detector and the statistical noise increases. However, simulating a discrete virtual neutron detector requires a very high number of source neutrons to be simulated and is computationally intensive. This study is a first investigation of the influence of soil moisture patterns on the radial footprint sizes and thus, a full and general analysis of the measurement footprint of thermal and epithermal neutrons is beyond the scope of this study, but underway for thermal neutrons in a recent preprint of some of the authors. Despite the limitations regarding the accuracy of the simulation results compared to the real-world site, they still allow valuable conclusions within the scope of this study, that e.g. thermal neutrons have a smaller footprint radius, that far-field soil moisture variations still have an influence on the thermal neutron count rate and thus, that the definition of the origin for calculating the footprint radius (e.g. point of thermalization or point of first soil contact) needs to be investigated further – especially under heterogeneous distributions of soil water in the model domain. Lastly, the influence of the geometry and spatial distribution of hydrogen (-variations) in respect to the detector location remains largely unknown and could also be a reason for the partly inconclusive behaviour of calculated radial measurement footprints for the simulations with an equal decrease of soil moisture. The anisotropy of CRNS footprints was already described in Schattan et al. (2019).

Updated figures:

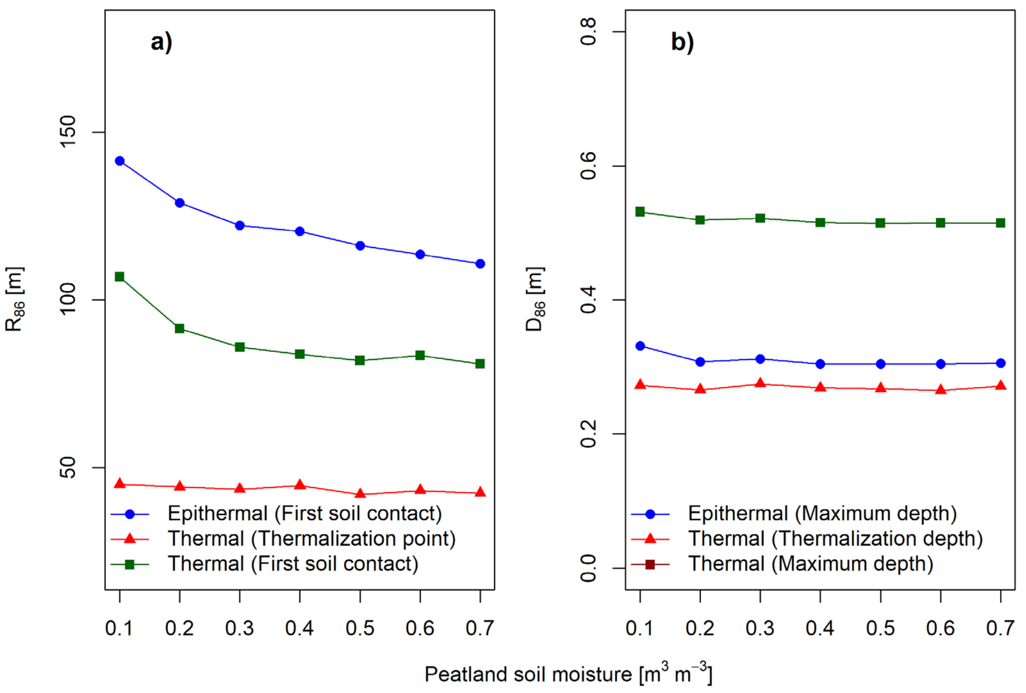

Figure 3. Simulation results for the measurement footprint radius (a) and depth (b) of detected thermal and epithermal neutrons.

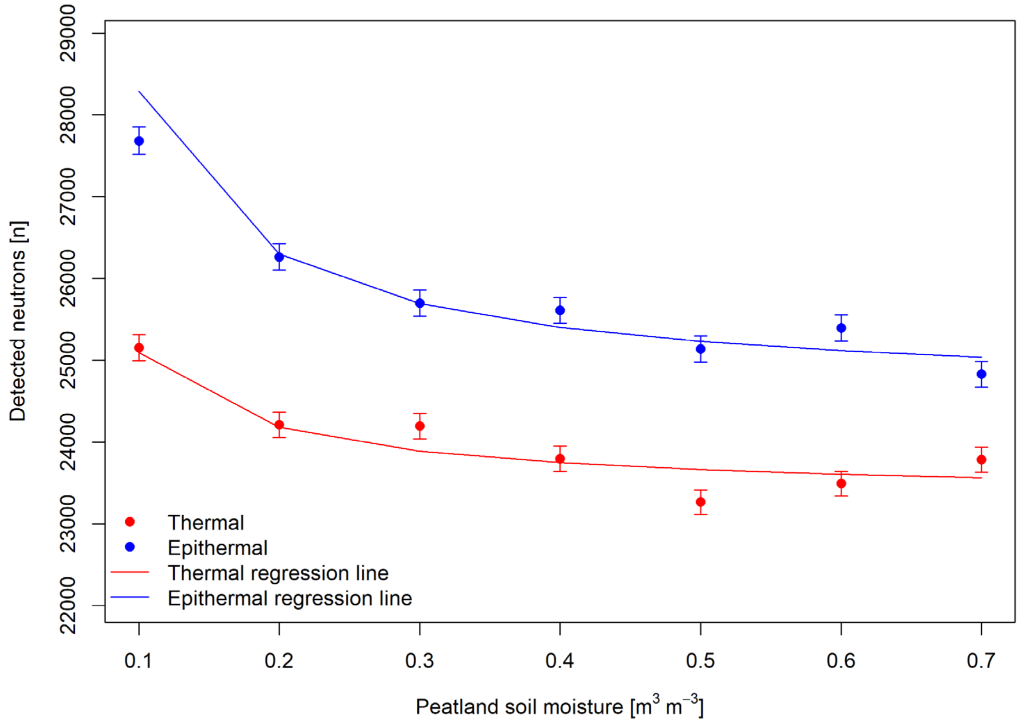

Figure 4. Total number of neutrons in the thermal and epithermal energy range observed by the virtual detector per simulated peatland soil moisture.

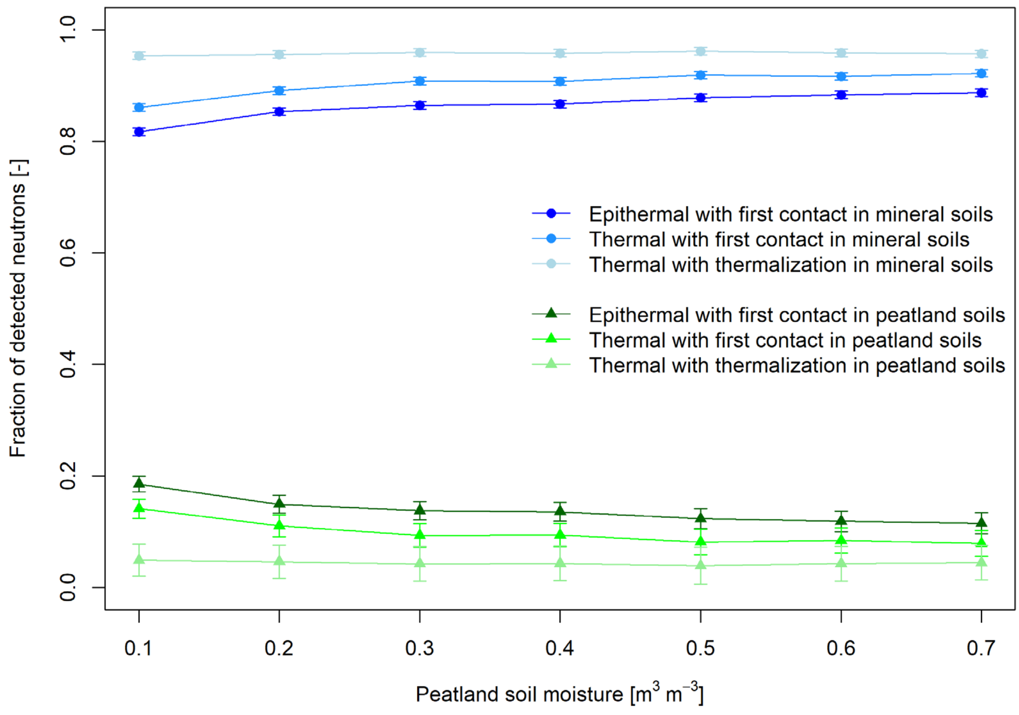

Figure 5. Fraction of detected epithermal and thermal neutrons with increasing soil moisture originating from areas covered with peatland soils and mineral soils in the model domain. For epithermal neutrons, the point of origin is defined as the point of first soil contact while for thermal neutrons both calculations, for the point of first contact and the point of thermalization are shown.

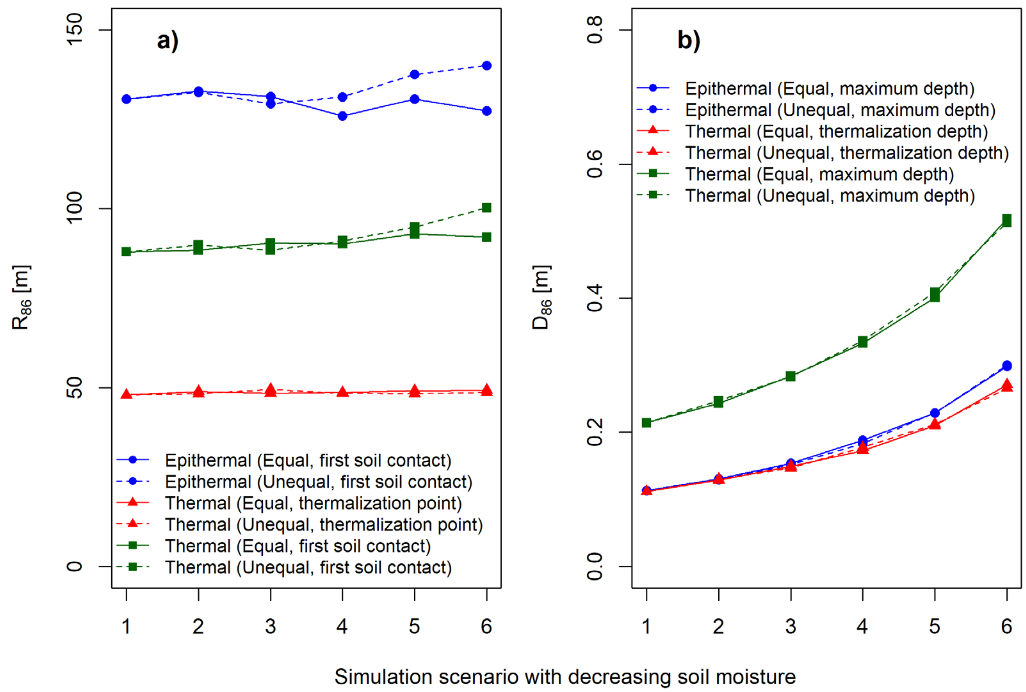

Figure 6. Simulated measurement footprint radius R86 (a) and depth D86 (b) of thermal and epithermal neutrons when soil moisture in areas with mineral and peatland soils decreases by the same amount (solid lines), and when peatland soil moisture decreases twice as much (dashed lines).

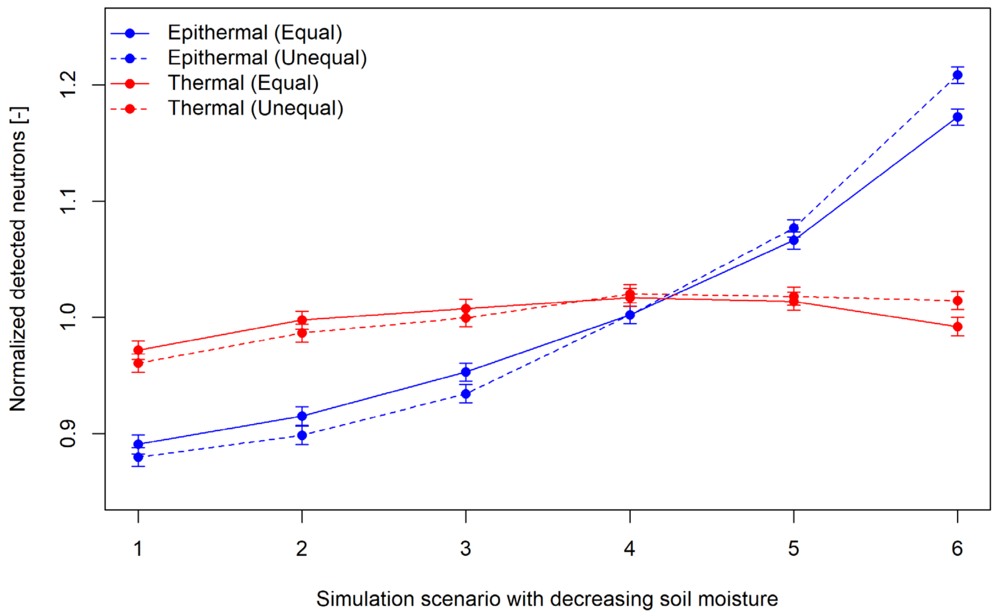

Figure 7. Simulated normalized thermal and epithermal neutron response when soil moisture in areas covered with mineral and peatland soils decreases in equal intervals (solid lines) and when peatland soil moisture decreases twice as much (dashed lines).

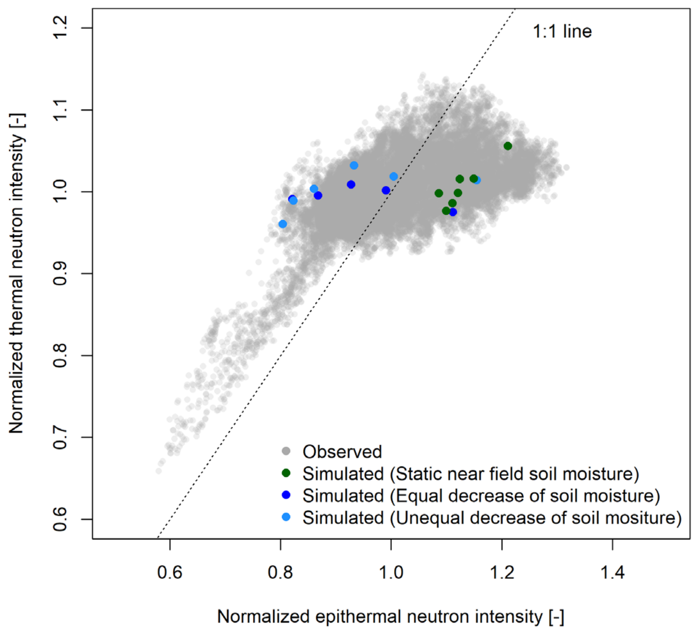

Figure 9. Relationship between normalized thermal and epithermal neutron intensities for in-situ observations and relationship between the normalized detected epithermal and thermal neutrons for simulated data. The simulated values refer to the simulation set and scenarios summarised in Table 1. Simulated neutrons are normalized by the average number of detected neutrons of all simulations in the respective energy range.

R3-2: Footprints: One question that remains in my mind is the practical relevance of simulated R_{86} and D_{86} footprints. This is especially the case for the thermal neutrons where the authors explicitly consider different definitions for the distance travelled by an individual neutron. But even for an epithermal neutron a choice is made to measure distance from the first interaction with the soil, rather than for example some weighted average of the distances from all interactions with the soil. This isn't a criticism particular to this manuscript - it is a general practice when simulating R_{86} for epithermal energies.

One might hope that the R_{86} footprint would approximately have something like the following property,

$$N = 0.86*(p1*N1 + (1-p1)*N2) + 0.14*(p2*N1 + (1-p2)*N2)$$

where N is the counts detected at the detector, N1 and N2 are the counts that would be detected if the entire area was mineral soil or peat soil respectively (with their own VWC), and p1 and p2 are the proportion of the landscape from within or outside of the R86 distance respectively that is mineral soil. This kind of reasoning is already alluded to around lines 425. But perhaps this can be quantified maybe using something like the equation above? Perhaps p1 and p2 could be estimated? N1 and N1 could be added to Fig 4? Would similar hold for the both thermal and epithermal footprints? One could even envisage using the above equation as a definition for a footprint radius if a simplified circular geometry (p1=1, p2=0) was employed for the mineral soil. In any case extra discussion would be helpful.

A3-2: Thank you for this interesting comment and like the idea of the proposed equation. Parameters p1 and p2 in the proposed equation would change with soil moisture content which requires them to be estimated for each combination of soil water contents in mineral and peatland soils. More importantly, we consider the radial measurement footprint in our study but the real footprint is likely to be rather anisotropic at study sites with distinct different soil moisture patterns. This was already mentioned by Schattan et al. (2019) for partly snow-covered conditions. This does not falsify the equation above but complicates its application and the estimation of the parameters p1 and p2 for different site conditions. Additionally, we did not conduct simulations with the porosity and soil moisture for either mineral or peatland soils in the entire model domain. Performing further simulations with these set ups and several moisture contents is beyond the scope of this study. Nevertheless, we agree, that this requires further investigation and should be addressed in future studies. This is pointed out by the reviewer when mentioning that different definitions of the neutron origin or the R_{86} might be considered. The definition of the origin of a neutron in the model domain remains under debate and different definitions might even be more suitable. In the scope of dedicated footprint studies the above described equation could be tested when the most suitable footprint definition has been found. This also leads to irrigation experiments using centre pivots mentioned by reviewer #1 which could assist in evaluating results from neutron transport simulations.

R3-3: Fig 3: Perhaps a comment on why R86 for thermal neutrons as measured from the first soil contact isn't in fact larger than R86 for the epithermal neutrons. I could imagine that as an epithermal neutron undergoes further collisions it will eventually reach thermal energies and will had further opportunity to travel from its initial soil contact – although I appreciate the picture is not be as simple as this.

A3-3: Thank you for this comment. We think that, when the point of first soil contact is used, the smaller footprint of thermal neutrons compared to epithermal neutrons might also be linked to the deeper integration depth. A secondary neutron generated from a high energy neutron in the soil via nuclear evaporation it is more likely to escape the soil as a neutron with less energy when it was generated in deeper layers due to more scatterings in the soil. When leaving the soil, the travel distance is then limited due to its lower energy. However, we agree that this is only one possible explanation and cannot be fully assessed within the scope of this manuscript. This again illustrates the need for more dedicated future footprint experiments either by simulations or in the field.

R3-4: Equation 6: This is an equally weighted normalised average of NT and NE. But its not clear at this point why this is done. It is explained that this combination makes the response have a "shallower slope" than NT, but one normally expects reduced sensitivity to be a bad thing! Perhaps the actual reason is a compromise between having a footprint more representative of the location in which the soil moisture sensors are installed (NT), and the better sensitivity of NE? There is additional explanation around line 545. Also, when using this "alternative approach 2" perhaps one needs to recalibrate the parameters a0, a1, a2, as I believe the original choice of these was made for the epithermal neutrons?

A3-4: Reviewer #2 made a similar comment (see also R2-15 and A2-15). The rescaled signal based on equation 6 is more similar to the theoretical epithermal intensity occurring if the entire footprint would have the soil moisture conditions of the near-field of the sensor and thus, better matching the shape of the functional relationship of the standard transfer function developed for epithermal neutrons.

One reason for is the smaller footprint of thermal neutrons more likely to less influenced by far-field soil moisture variations but then requires the better sensitivity of epithermal neutrons as pointed out by reviewer #3.

A more important reason for the improvement is the generally smaller decrease of thermal neutrons with increasing soil moisture. As a consequence, we can make use of thermal neutrons as proxy for a different signal response better matching the response which would occur if the soil moisture conditions of the near-field would cover the entire footprint at our site.

As described in the responses to reviewer #1 and #2, this approach may not be directly transferable to sites with different spatial patterns of soil moisture and different dynamics. However, the more general approach by adjusting the transfer function instead of adjusting the neutron signal could be used instead. This will be more strongly emphasized in the revised version of our manuscript.

R3-5: Fig 3b: There's a problem with the legend.

A3-5: Thank you, we will correct this in the revised version of the manuscript.

R3-6: Lines 16 and 84: "spatial discretization" is supposed to be "spatial disaggregation"? Also line 84 could be clearer.

A3-6: We will replace "spatial discretization" with "spatial disaggregation" as suggested.

R3-7: Section 2.2.1: Some of the details in this section are general to all simulations (e.g. the detector radius, the energies of the thermal/epithermal neutrons) and would therefore be better in section 2.2.

A3-7: This was already mentioned by reviewer #2. We will shift lines 166-183 to section 2.2, insert them after line 149 and make it a bit clearer.

R3-8: Fig 5: I can't really see the reason to show both the blue lines and the green lines – they sum to 1.

A3-8: Yes, the lines sum to 1. We think it makes it easier to see how many neutrons originate from either region (peatland or mineral soils) when both lines are shown.

R3-9: Fig 6: Could be more easily understood if x-axis labelled by near field soil rather than scenario. This is especially because when reading the x-axis left to right it becomes drier which is the opposite way around compared to Fig3.

A3-9: We agree with the reviewer on the improvements on this figure. Using the simulated soil moisture in the near-field instead of the scenario number does help interpreting the figures. We will modify figures 6 and 7 accordingly.

R3-10: Fig 9: I can understand the authors might be pleased with this figure but why not simply add the simulation points to Fig 8a instead.

A3-10: We decided to use a separate figure because we find that merging the information with Figure 8a would make the latter difficult to read and visually separate the data points based on the neutron simulations. We would also prefer to keep Figure 8 purely measurement based instead of mixing in simulations here.

R3-11: Line 433: Add reference to the Figure.

A3-11: We will add the reference to figure 4.

R3-12: Line 272: I think the bandwidth should have time/frequency units? Partly I ask because, I think that if the smoothing is too intense your residual "noise" will actually contain some of the soil moisture signal. I therefore want a rough idea how much smoothing occurred. Not that I think excess noise causes a problem, given the result stated on line 512. And I never doubted that the different approaches where significantly different.

A3-12: The smoothing bandwidth of 1,000 in the Nadaraya–Watson kernel smoother does indeed lead to an intense smoothing effect. It keeps the seasonal variations of soil moisture and does also remove some of the soil moisture dynamics in order to generate large residuals for subsequently generating random value distributions per time step which can be compared between the different approaches. We do agree that the selection of the bandwidth is somewhat speculative and an inherent limitation of this time series comparison. We will add this information to the methods section in the manuscript.

References

Schattan, P., Köhli, M., Schrön, M., Baroni, G., and Oswald, S. E.: Sensing Area-Average SnowWater Equivalent with Cosmic-Ray Neutrons: The Influence of Fractional Snow Cover, Water Resources Research, 55, 10 796–10 812, https://doi.org/10.1029/2019wr025647, 2019.