Reviewer #3:

We thank reviewer #3 for taking the time to review our manuscript and the helpful comments which will improve the quality of the manuscript. In the following section we will reply to all comments of reviewer #3 by numbering reviewer comments starting with R3-1 (i.e. reviewer 3, comment 1) and our response with A3-1 (i.e. author response to R3-1).

R3-1: In the introduction (Chapter 1), the publication by Kodama et al. (1985, https://journals.lww.com/soilsci/Abstract/1985/10000/APPLICATION_OF_ATMOSPHERIC_NEUTRONS_TO_SOIL.1.aspx) should be mentioned.

This publication is about a passive below-ground neutron sensor and therefore it is needed to briefly mention how the current manuscripts relates to this work from the 1980's.

A3-1: We are glad about this suggestion and agree that it should be mentioned in the introduction of our manuscript. Kodama et al. (1985) measure both, above-ground and below-ground cosmic-ray neutrons and describe the change of observed neutron intensity with varying soil moisture. The below-ground measurements of Kodama's study cover the shallow subsurface with depths down to 40 cm, using moderated detectors.

In these shallow depths, the maximum intensity of cosmic-ray neutrons can be expected, making it suitable for soil moisture estimation with comparatively high statistical accuracy. On the other hand, this shallow sub-surface monitoring depth largely corresponds to the vertical measurement depth of above-ground cosmic-ray neutron sensing. In the scope of the present study, we explicitly explore the potential of CRNS beyond the measurement depths of classical above-ground CRNS. We also emphasize that placing detectors in shallow depths leads to the contribution of neutrons which previously interacted with the atmosphere and which originate from larger horizontal distances to the detector location. This makes it difficult to interpret the neutron signal and its response to nearby soil moisture changes in the depth of the below-ground neutron detector. For this reason, the equations presented in this study are valid for shielding depths greater 75 g cm^{-2}. For example, a measurement depth of 40 cm with an average soil bulk density of 1.43 g cm^{-3} would lead to a shielding depth of only 57 g cm^{-2} for a completely dry soil.

In order to mention Kodama et al. (1985), we will add the following sentence in line 65:

Original:

"… as well as the typically non-continuous nature of snapshot measurement campaigns with active neutron probes. Against this background, we investigate the possibility of using CRNS-related sensors in a passive downhole technique
(d-CRNS) to estimate soil moisture in different depths of the root zone and deeper unsaturated zone. "

Adjustment:

"… as well as the typically non-continuous nature of snapshot measurement campaigns with active neutron probes. Kodama et al. (1985) observed the response of cosmic-ray neutrons to changes in soil moisture in depths down to 40 cm., largely covering the sensitive measurement depth of above-ground CRNS.
Against this background, we investigate the possibility of using CRNS variants in a passive downhole technique (d-CRNS) to estimate soil moisture in different depths below 40 cm, also including the deeper unsaturated zone. "

R3-2: Chapter 2 Material and Methods, Section 2.4, page 9, lines 196-204: The HESS-reader could be helped by explaining a bit more how the roles protons, muons, and neutrons play, differ and how much different processes dominate in relative terms (moderation and in-soil neutron production)

Please, if explained in the manuscript text, keep this very brief.

A3-2: In order to give a brief example, we will add the following sentence in line 200:

Original:

"Although simulating only neutrons and not e.g. protons and muons as well might be sufficient at the soil-atmosphere interface with a detector placed above the surface, the simulation of the neutron flux in different depths of the

soil requires the inclusion of several other types of particles that induce neutron production in the soil volume itself. That is
because the atmospheric neutron flux is attenuated strongly within the soil volume and in-soil neutron production dominates
the thermal neutron flux below several decimetres soil depth."

<u>Adjustment:</u>

"Although simulating only neutrons and not also protons and muons might be sufficient at the soil-atmosphere interface with a detector placed above the surface, the simulation of the neutron flux in different depths of the soil requires the inclusion of several other types of particles that may induce neutron production in the deeper soil volume. As the atmospheric neutron flux is attenuated strongly within the soil volume the in-soil neutron production dominates the thermal neutron flux below several decimetres soil depth. In-soil neutrons are generated by different cosmic-ray particle species depending on the soil depth. Within the first few meters the inelastic collisions of high-energy protons and neutrons with atomic nuclei lead to particle production in hadronic showers (e.g. see Mollerach and Roulet 2018). During the collision neutrons are ejected from the nucleus with energies peaking at few hundred MeV (e.g. Gudima et al. 1983). The target nucleus remains in an excited state after the impact and deexcites via the emission of lower energetic neutrons with few MeV. This process is called evaporation. The hadrogenic neutron production falls off rapidly with soil depth due to the short penetration length of high-energy neutrons and protons. Below that and down to several tens of meters, hadrogenic neutron production is significantly lower and is dominated by muons (Heusser 1996) through capture processes that releases neutrons with few MeV. "

R3-3: Chapter 3 Results, Section 3.1.3, page 7, line 362: Why from wilting point to field capacity (these are rather arbitrary soil moisture contents that, formally, relate to the plant grown) and why not to saturation?

A3-3: Section 3.1.3 describes an exemplary procedure to derive the soil moisture content in the depth of measurement from the presented equations and observed downhole neutron intensities. For the average soil moisture content in the layer between the surface and the depth of measurement, we argue that these boundaries are justified as it is unlikely that the average soil moisture content is larger than field capacity or reaches saturation over the entire depth range given the sandy soils and large groundwater table depth at the study site.

In contrast, in the depth of the d-CRNS measurements, soil water saturation may be reached and for this reason the upper limit is set to saturation in step 3 of the procedure (line 364).
However, the described approach to derive soil moisture in the depth of measurement remains an exemplary procedure and other boundaries might be used for different site conditions and may be tested in future studies. For this reason, we will change the following sentence in line 356:

Original:

"We propose an alternative, more simple approach to estimate the soil moisture time series in the depth of measurement from
the observed neutron ratios by using Eq. (5-9)."

Adjustment:

"We propose an alternative, and more simple approach to estimate the soil moisture time series in the depth of measurement from the observed neutron ratios by using Eqs. (5-9). This approach is in some way exemplary in that while reasonable for the conditions of our study site, the assumed range of soil moisture between wilting point and field capacity in Eqs. 5-9 may need to be modified for other sites. "

R3-4: In chapter 4 Discussion: The possible uncertainties introduced by vertically highly heterogeneous soils should be discussed.

These heterogeneities can affect the outcomes through both vertically variant soil bulk densities and, during certain periods, vertically heterogeneous soil moisture contents.

To what extent does not knowing the exact vertical variation matter to the outcomes and uncertainty?

To what extent would vertically heterogeneous soils affect the applicability of the methods at different sites, given more in-situ sampled data might be needed?

A3-4: We agree with the reviewer that potential uncertainties arising from vertically heterogenous distributions of bulk density and soil moisture should be mentioned.

In fact, vertically distributed soil moisture information as well as bulk density profiles are essential parameters for the presented set of equations in order to predict downhole neutron ratios. The respective bulk density information is also required to estimate soil moisture contents in the depth of measurements following the procedure in chapter 3.1.3 making it necessary to consider uncertainties in these parameters. However, an in-depth assessment of the impact of the quality and uncertainties in vertically distributed soil moisture and bulk density information on derived neutron ratios and estimated soil moisture information is beyond the scope of this proof-of-concept study.

Considering the sensitive measurement volume of the downhole neutron detector, vertically heterogenous bulk density and soil moisture distributions may also be important. Similar to above-ground CRNS e.g. soil moisture close to the detector (centre) can be expected to have a larger impact on the observed neutron signal than the soil moisture in greater (vertical and horizontal) distance to the downhole neutron detector. This point as well as the need for further research has already been mentioned in lines 482-490.

Nevertheless, potential uncertainties of vertically highly heterogeneous soil bulk density and soil moisture distributions should be briefly mentioned in chapter 4.2 and thus, we will adjust the following paragraph (line 570):

<u>Original:</u>

"As this study is restricted to a single observation site, further research is required to test both the soil hydraulic model-based approach and the approach used here under different site-specific boundary conditions, set-ups and measurement depths.
Nevertheless, these two approaches are available in order to retrieve soil moisture information from d-CRNS and hence, allowing for direct application of the methodological approach in the scope of hydrological research."

<u>Adjustment:</u>

"As this study is restricted to a single observation site, further research is required to test both the soil hydraulic model-based approach and the approach used here under different site-specific boundary conditions, set-ups and measurement depths. This also includes the consideration of uncertainties arising from soils with high vertical variability in bulk density (and possibly soil moisture), their impact on predicted neutron ratios, and on the estimated soil moisture in the depth of measurement. For example, lower bulk density and lower soil water content would lead to more neutrons penetrating into greater depths, and hence, to increased count rates and footprint volumes. Nevertheless, the two mentioned approaches are available for soil moisture retrieval from d-CRNS and could be applied under different soil-hydrological conditions in future studies."

R3-5: Chapter 4 Discussion, page 23, line 466 "...may lead to different results": such as?

A3-5: This statement refers to the comparison of the R_{86}, Vc_{86} and V_{86} of a tube made of PVC and stainless steel but with equal material thickness. A detector placed in a stainless steel or PVC tube with thinner walls is likely to have a larger measurement volume as less neutrons are absorbed or scattered away from the downhole neutron detector. Vice versa, a thicker wall can be expected to reduce the measurement volume. However, the degree of difference in the measurement volume depending on wall material and material thickness remains to be assessed and was therefore not specified further. We will add the following statement (line 466):

<u>Original:</u>

"As the average difference for R86 between a stainless steel and a PVC tube is approximately 1 cm and for Vc86 as well as V86 between 8 and 5 cm, the influence of the material composition on the sphere of influence can be identified but may be regarded as negligible. However, a thinner or thicker wall of the tube may lead to different results."

<u>Adjustment:</u>

"As the average difference for R86 between a stainless steel and a PVC tube is approximately 1 cm and for Vc86 as well as V86 between 8 and 5 cm, a small effect of the material composition on the sphere of influence can be identified but may be regarded as negligible. However, a thinner or thicker wall of the tube is likely to have a stronger impact on the measurement volume. For instance, a thicker PVC wall can be expected to reduce the measurement volume."

R3-6: Chapter 5 Conclusions, page 27, lines 585-590: Please, discuss here and possibly in Chapter 4 Discussion, Section 4.2, that using soil hydraulic models could introduce further uncertainties due to assumptions made during the modelling process. In addition, applying a soil hydraulic model to obtain the results, make these less observations and more model results.

A3-6: We agree that such additional uncertainties should be briefly mentioned in the discussion chapter. We will add the following sentence in line 566:

Original:

"A first option would be the use of Eq. (5-9) as a forward operator in combination with a soil hydraulic model. Similar approaches have been conducted using e.g. the COSMIC forward operator model code (Shuttleworth et al., 2013) for above-ground CRNS applications (e.g., Brunetti et al., 2019; Barbosa et al., 2021). Although the application as a forward operator in combination with soil hydraulic modelling may produce more accurate results as the soil water transport is simulated in different depths and also allows for the retrieval of soil moisture simulated in several soil layers, a large number of input parameters is required which may not be available at all sites."

Adjustment:

"A first option would be the use of Eq. (5-9) as a forward operator in combination with a soil hydraulic model. Similar approaches have been conducted using e.g. the COSMIC forward operator model code (Shuttleworth et al., 2013) for above-ground CRNS applications (e.g., Brunetti et al., 2019; Barbosa et al., 2021). Although the application as a forward operator in combination with soil hydraulic modelling may produce more accurate results as the soil water transport is simulated in different depths and also allows for the retrieval of soil moisture simulated in several soil layers, a large number of input parameters is required which may not be available at all sites.

Furthermore, coupling the derived equations with a soil hydraulic model may introduce additional uncertainties by the model assumptions and by the propagation of uncertainties from input parameters."

Additional references:

Gudima, K. K., Mashnik, S. G., Toneev, V. D.: Cascade-exciton model of nuclear reactions, Nuclear Physics A, 401, 329-361, https://doi.org/10.1016/0375-9474(83)90532-8, 1983.

Heusser, G.: Cosmic ray interaction study with low-level Ge-spectrometry. Nuclear Instruments and Methods in Physics Research A, 369, 539-543, https://doi.org/10.1016/S0168-9002(96)80046-5, 1996.

Mollerach, A., Roulet, E.: Progress in high-energy cosmic-ray physics, Progress in Particle and Nuclear Physics, 98, 85-118, https://doi.org/10.1016/j.ppnp.2017.10.002, 2018.