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On soil bulk density and its influence to soil moisture estimation with cosmic-ray neutrons

Mandy Kasner[1], Steffen Zacharias[1], and Martin Schrön[1]

[1]UFZ – Helmholtz Centre for Environmental Research GmbH, Leipzig, Germany

Correspondence: Martin Schrön (martin.schroen@ufz.de)

Abstract. Cosmic-ray neutron sensing (CRNS) is a non-invasive technique that is used to quantify soil moisture in a representative footprint of 10–20 ha and 15–80 cm depth. In a stationary mode, CRNS is widely employed to monitor the moisture dynamics on agricultural land, which may undergo active changes of the soil compartments, e.g. due to plowing. On mobile platforms, CRNS measurements aim at mapping the spatial soil moisture distribution across various types of soil and land use.

To date, the potential effect of variable soil bulk density on the neutron measurements has not been investigated in detail. In fact, most sensors are calibrated only once on site-specific soil properties. Therefore we hypothesize that unaccounted spatiotemporal changes of soil bulk density may have impact on the quality of CRNS soil moisture products.

In this study, we quantify the effect of the soil density on the neutron response by neutron transport simulations and a dedicated lab experiment. The results indicate a significant dependency of neutrons on soil bulk density, which also depends on the soil moisture state. For the hypothetical cases with constant ratio between soil density and water content, the neutron intensity remains unaffected.

Correction functions are proposed to improve the performance of two widely used approaches to convert neutrons to soil moisture (Desilets et al. 2010, and Köhli et al. 2021). The latter approach together with the proposed correction can be recommended for practical use, as it accurately represented the simulated neutron response to soil moisture and soil bulk density with a constant – and potentially universal – calibration parameter.

1 Introduction

Soil moisture is a key variable for informing hydrological and meteorological models to provide essential predictions of land-surface fluxes, plant water availability, water scarcity, and weather events (Vereecken et al., 2008; Tramblay et al., 2020). It is affected by both seasonal and daily variations depending on various factors such as prevailing climate, soil type, location in relief, vegetation, etc. The multitude of influencing factors results in high spatial and temporal variability of soil moisture, such that observing a representative record of root-zone soil moisture beyond the point scale remains a technological challenge (Robinson et al., 2008).

The method of Cosmic-Ray Neutron Sensing (CRNS) is a non-invasive measurement technique to estimate field-scale soil moisture by averaging over most point-scale variability (Zreda et al., 2012; Franz et al., 2013). The integral measurement value is characterized by a radial footprint of 130–240 m and a penetration depth of 15—80 cm (Köhli et al., 2015). The technique is based on a passive measurement of neutrons which are generated by the omnipresent cosmic radiation in the atmosphere and the soil.

in the soil, neutrons mainly interact, i.e. scatter, with all atomic nucleii of the local material. Since neutron the interaction with hydrogen leads to an extraordinary energy loss, the neutron intensity above the ground is particularly sensitive to water near the Earth's surface and in the soil. Thus, there is an inverse relationship between the abundance of the nearby hydrogen atoms and the neutron intensity, which makes it possible to estimate the soil moisture in the footprint.

In the past, the analytical approach from Desilets et al. (2010) has been widely used to convert neutrons to soil moisture, with a few adaptions on including soil property information suggested by Villarreyes et al. (2011) and Bogena et al. (2013). Recently, Köhli et al. (2021) revisited this approach with state-of-the-art neutron transport simulations and proposed a revised relationship which performs better particularly under dry conditions.

Both approaches provide a free calibration parameter, which can be estimated using additional soil moisture measurements and may end up being specific to the local site conditions (Zreda et al., 2012; Schrön et al., 2017). However, these site conditions may be subject to change, e.g., during farming activities (plowing), while stationary sensor are usually not recalibrated more than a few times (Villarreyes et al., 2011; Iwema et al., 2015; Bogena et al., 2022). Site-specific calibration is also not feasible for mobile CRNS platforms, where various sites with different land use and soil conditions are probed (Dong et al., 2014; Schrön et al., 2018; McJannet et al., 2017; Jakobi et al., 2020). Hence, a constant sensor calibration combined with correction approaches for potential site-specific changes is key for reliable CRNS data in stationary and mobile mode.

While most relevant site-specific changes can be translated to a change of water-equivalent (such as lattice water or organic water equivalent), solid soil material undergo different interaction processes with the neutrons and needs to be considered separately. Both the two mentioned conversion approaches from neutrons to soil moisture implicitly assume that the influence of the soil bulk density on the neutron counts is negligible, as long as it is used in the traditional way to convert gravimetric to volumetric soil moisture. However, a systematic investigation of the influence of soil bulk density on the neutron's interaction physics and implications for resulting CRNS soil moisture product has never been conducted.

This study aims at exploring the influence of the soil bulk density on the cosmic-ray neutron signal and at quantifying possible implications on the soil moisture estimation. Based on the hitherto common knowledge, we start with the hypothesis that above-ground neutron intensity is invariant against the change of soil bulk density. If the hypothesis has to be rejected, we aim at quantifying the remaining effect on the neutron counts and its implications on the performance of the two available approaches to convert neutrons to soil moisture.

The hypothesis will be challenged using neutron transport simulations with varying soil bulk density and various soil moisture conditions. The results will be analysed and compared with two laboratory experiments to estimate the quality of the simulated results for near-natural conditions. The magnitude of the bulk density effect will be quantified and examined using practical examples.

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2 Theory and Methods

2.1 Neutron interactions in the soil medium

The basic principle of soil moisture estimation by epithermal neutrons relies on the fact that the neutron intensity above ground scales inversely with the water content in the ground. The concept behind this relationship is the nature of the elastic neutron scattering on atoms in a medium (Zreda et al., 2012; Köhli et al., 2015). The hydrogen atom is particularly effective in reducing the energy of epithermal neutrons ($> 0.5\,\mathrm{eV}$) during a scattering event. As a consequence, only a low number of collisions are required to thermalize a neutron, i.e., to remove it from the detectable energy domain (which is approx. 0.5–100 keV, see e.g., Zreda et al., 2012; Köhli et al., 2018). Hence, the number of measurable neutrons, N, mainly depends on the efficiency of the medium to reduce a neutron's energy per collision, expressed as ξ, by following the relationship presented in Köhli et al. (2021):

$$N \propto 1/\xi = \frac{\sum_i \sigma_i}{\sum_i \sigma_i \xi_i}. \tag{1}$$

In a complex medium that consists of various materials, the effective value of ξ depends on each atom's prescribed energy loss per collision, ξ_i, weighted by the probability of such a collision, expressed as the atom's elastic cross section, σ_i (Dobrzynski and Blinowski, 1994). The expression can be condensed to the main involved material compositions by defining their macroscopic cross sections,

$$\Sigma_i = \varrho_i \cdot \sigma_i\,, \tag{2}$$

where ϱ_i is the material's density and σ_i its atomic cross section.

A fixed volume of soil in the field typical consists of a volumetric fraction s of solid components (with Σ_s and ξ_s), such as soil minerals and organic matter, a fraction w of water (Σ_w, ξ_w), and a fraction a of air (Σ_a, ξ_a) filling the remaining pore such that $s + w + a = 1$. The neutron intensity over ground material then is:

$$N \propto \frac{s\,\Sigma_\mathrm{s} + w\,\Sigma_\mathrm{w} + a\,\Sigma_\mathrm{a}}{s\,\Sigma_\mathrm{s}\xi_\mathrm{s} + w\,\Sigma_\mathrm{w}\xi_\mathrm{w} + a\,\Sigma_\mathrm{a}\xi_\mathrm{a}} \approx \frac{s\,\Sigma_\mathrm{s} + w\,\Sigma_\mathrm{w}}{s\,\Sigma_\mathrm{s}\xi_\mathrm{s} + w\,\Sigma_\mathrm{w}\xi_\mathrm{w}} \tag{3}$$

The method of cosmic-ray neutron sensing is built on the extraordinary sensitivity of neutrons to hydrogen nuclei. In Eq. 3 water constitutes the dominant term since both, σ_w and ξ_w are by a factor ~ 10 higher than for the solid components (see values in, e.g., Zreda et al., 2012; Köhli et al., 2021). In strong contrast, air comes with σ_a and ξ_a comparable to the solid compounds, but with lower densities by factor $\sim 10^{-3}$. Hence, for typical ground conditions the term for the air-filled pores can be neglected.

An important consequence of Eq. 3 is that the neutron intensity is pre-dominantly a function of the ratio between the proportions of water and mineral components:

$$N \propto \frac{s\,\Sigma_\mathrm{s} + w\,\Sigma_\mathrm{w}}{s\,\Sigma_\mathrm{s}\xi_\mathrm{s} + w\,\Sigma_\mathrm{w}\xi_\mathrm{w}} = \frac{\Sigma_\mathrm{s} + \frac{w}{s}\,\Sigma_\mathrm{w}}{\Sigma_\mathrm{s}\xi_\mathrm{s} + \frac{w}{s}\,\Sigma_\mathrm{w}\xi_\mathrm{w}} \tag{4}$$

$$\Rightarrow \quad N \approx \mathrm{const.} \quad \forall \quad \frac{w}{s} = \mathrm{const.}$$

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This analysis shows that the neutron response is not unique for changing water content w. It is rather ambiguous if both, w and s undergo changes, e.g., due to alteration of soil porosity within the support volume of the CRNS. Such a change could be expressed as a change in soil bulk density, ϱ_s, which scales the macroscopic cross section of the soil Σ_s and thereby contributes non-linearly to the resulting neutron intensity.

2.2 Conversion between neutrons and soil moisture

The relationship in Eq. 3 is the basis for the hitherto accepted conversion functions from soil moisture to neutrons. The first approach, here referred as *Des. function*, has been suggested by Desilets et al. (2010), where the soil water content θ resembles the above-mentioned fraction of volume, w, filled with water:

$$\text{Des. function:}\quad N(\theta) = N_0\left(\frac{p_0}{\theta+p_1}+p_2\right) = N_\mathrm{max}\cdot\frac{p_2+p_3\,\theta}{p_2+\theta}\,, \tag{5}$$

where $p_{0\ldots3} = (0.0808, 0.115, 0.372, 0.346)$ and $N_\mathrm{max} = 1.075\,N_0$ are detector-specific scaling parameters. The relationship has been recently extended by Köhli et al. (2021) to account for changes of air humidity, h, while the fundamental hyperbolic dependency on θ is still preserved (Eqs. 3–5):

$$\text{Koe. function:}\quad N(\theta,h) = N_0\Bigg(\frac{p_4+p_5\,\theta}{p_4+\theta}\cdot\left(p_6+p_7\,h+p_8\,h^2\right) + e^{-p_9\,\theta}\left(p_{10}+p_{11}\,h\right)\Bigg), \tag{6}$$

where $p_{4\ldots11}$ =(0.0226, 0.207, 1.024, -0.0093, 0.000074, 1.625, 0.235, -0.0029) is the parameterset "URANOS drf" from Köhli et al. (2021) and N_0 is a scaling parameter similar to N_max. This revised formulation, here referred as *Koe. function*, also better represents arid conditions with soil moisture $\theta < 5\,\%$ where Eq. 5 usually fails.

In both equations, neutron intensity has been derived from Monte Carlo simulations based on a fixed bulk density, ϱ_s. This is why both authors suggested to rescale the actual volumetric soil water content, θ_vol before it can be applied to the equations:

$$\text{Des. function:}\quad \theta_\mathrm{Des} = \theta_\mathrm{vol}/\varrho_\mathrm{s}\,, \tag{7}$$

$$\text{Koe. function:}\quad \theta_\mathrm{Koe} = \theta_\mathrm{vol}/\varrho_\mathrm{s}\cdot 1.43\,\mathrm{g/cm^3}. \tag{8}$$

These scaling concepts have been also considered as a conversion from volumetric to gravimetric soil moisture and will be re-investigated in this study.

2.3 URANOS Simulations

The complex transport and interactions of neutrons at the micro-scale interface between soil, air, and water can only be captured with Monte Carlo simulations. Therefore the Ultra Rapid Adaptable Neutron-Only Simulation is used for this study (URANOS,

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see e.g., Köhli et al., 2015). The code (version URANOS v0.99ω23) considers all relevant interactions between neutrons and atomic nuclei with energies that are relevant for CRNS (Köhli et al., 2018), and allows to simulate cosmic-ray neutrons in a complex environment with various options for soil material, density, and water content (Köhli et al., 2021).

The implemented simulations are following the recommendations from Köhli et al. (2015) and Köhli et al. (2021), e.g., domain dimension of 1000×1000 m in order to track 99.9 % of the relevant above-ground flux. The neutron source intensity for the simulations is set to 12×10^6 neutrons to reach a reasonable trade-off between computational effort and a low statistical error. The composition of the air medium in URANOS is defined as 78 vol% nitrogen, 21 vol% oxygen and 1 vol% argon. The air pressure (1020 mbar), humidity (10 g/m³) and the cut off rigidity (10 GV) are constant for all simulations. The detector layer records neutrons in a horizontally infinite layer of 0.5 m thickness and a ground surface distance of 2 m. The neutrons are crossing the detector layer which ends in URANOS as a map with spatial field information of neutron densities. The solid unit of the soil is composed of 75 vol% SiO_2 and 25 vol% Al_2O_3 at a compound density of 2.86 g/cm³. The parameterization of the soil's density in URANOS is based on the specification of the soil porosity. Therefore it's necessary to convert the soil bulk density desired for the simulation into porosity and vise versa.

2.4 Experimental concept

Dedicated experiments have been conducted to support the theoretical results. Near-natural soil conditions with loose and dense bulk densities have been reconstructed in two adjacent Intermediate Bulk Containers (Ibc). The tank volume of 2×1000 liters has been filled with $\sim$2.5 tons sand for the first study and $\sim$3 tons of topsoil (sand, clay and silt mixture) for the second one.

In the first experiment the tanks were compacted as dense as possible with fine quartz sand. For this, the sand was manually added into the tank in 10–15 cm thick layers (approx. 125 kg). Then, the sand was tamped step-wise by a human body weight followed by a steel drop hammer (steel tube with bottom plate). This procedure has been repeated until the tank was filled up to the top. The surface was marked inside the tanks to insure the similarity of distance between the sensor and the surface among the individual experiments. From each tank soil samples were taken in three different heights (bottom, middle and top or in distance from detector: $\sim$45 cm, $\sim$75 cm, $\sim$84 cm) to analyze the dry bulk density and the soil water content. Four wooden laths secure the centre position of the CRNS detector on the top. The mean record period of the detector has been set to 60 minutes per experiment.

For each experiment the material volume was measured and the tanks were weighted using a truck scale. Once the experiment is done, the tanks were emptied and manually refilled as loose as possible using spades. The samples for the dense experiment were taken in two different heights (distance from detector: $\sim$40 cm; $\sim$65 cm) per tank.

The same process was done with the second material, the topsoil. To avoid any risk of damaging the tank or struggle in time by emptying and refilling, the second experiment started with the low bulk density approach for practical reasons. After filling, collecting soil samples (distance from detector: $\sim$40 cm; $\sim$65 cm) and the placement of the sensor on top of the tank, the neutrons were recorded for one hour. Like in the first experiment the tanks were emptied and refilled with the topsoil, after the record period, as dense as possible using a steel drop hammer. Again soil samples were taken in three different heights (distance from the detector: $\sim$35 cm; $\sim$60 cm and $\sim$75 cm) to analyze the water content and to identify the dry bulk density.

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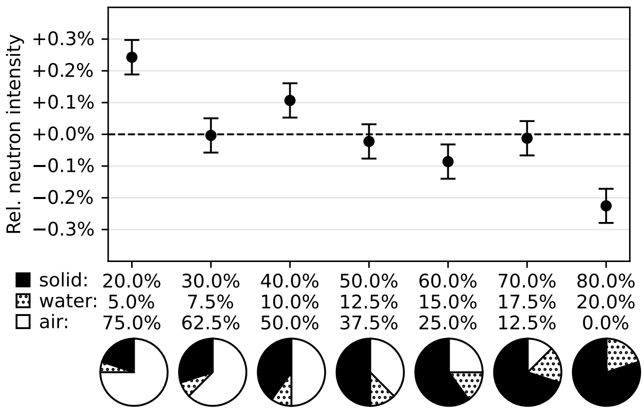

Figure 1. Simulated neutron response to soil for various combinations of solid material and water with an exemplary ratio of 4:1. The neutron intensities are displayed as relative deviations from their mean (dashed line).

The collected soil samples from each experiment were analyzed as described in the DIN 18 125 T1 and T2 to obtain the dry bulk density and the soil water content. Therefore the collected soil samples were dried by 105 °C for at least 22 h in a muffle furnace. Now the bulk density ϱ_s can be estimated by the mass m_solid of oven-dry soil per the volume V_soil of soil material (Arnold, 1986).

$$\text{Bulk Density:} \quad \varrho_\mathrm{s} = \frac{m_\mathrm{solid}}{V_\mathrm{soil}}. \tag{9}$$

Considering the fact that quartz is the most important and abundant solid component of soils, the density of quartz (2.65 g/cm³) can be generally assumed to equal to the particle density, $\varrho_\mathrm{particle}$, of the vast majority of soils. From this perspective, the calculation of porosity, Θ, can be simplified as follows:

$$\text{Porosity} \quad \Theta = 1 - \frac{\varrho_\mathrm{s}}{\varrho_\mathrm{particle}} \approx 1 - \varrho_\mathrm{s}/2.65\,. \tag{10}$$

3 Results

3.1 Constant soil-water ratio

The first simulation experiment investigates the neutron response to a constant ratio between solid soil and water content in the soil medium. As explained in the section 2.1, basic theoretical considerations suggest that the neutron count rate remains constant for changing soil bulk density only if the water content changes in the same way.

As an example, seven simulations has been conducted with a constant ratio of 4 units of water per 1 unit of solid soil (ratio 1:4). In the simulation setup, saturated soil was represented by 80 vol% solid soil (equal 20 vol%) and a soil water content

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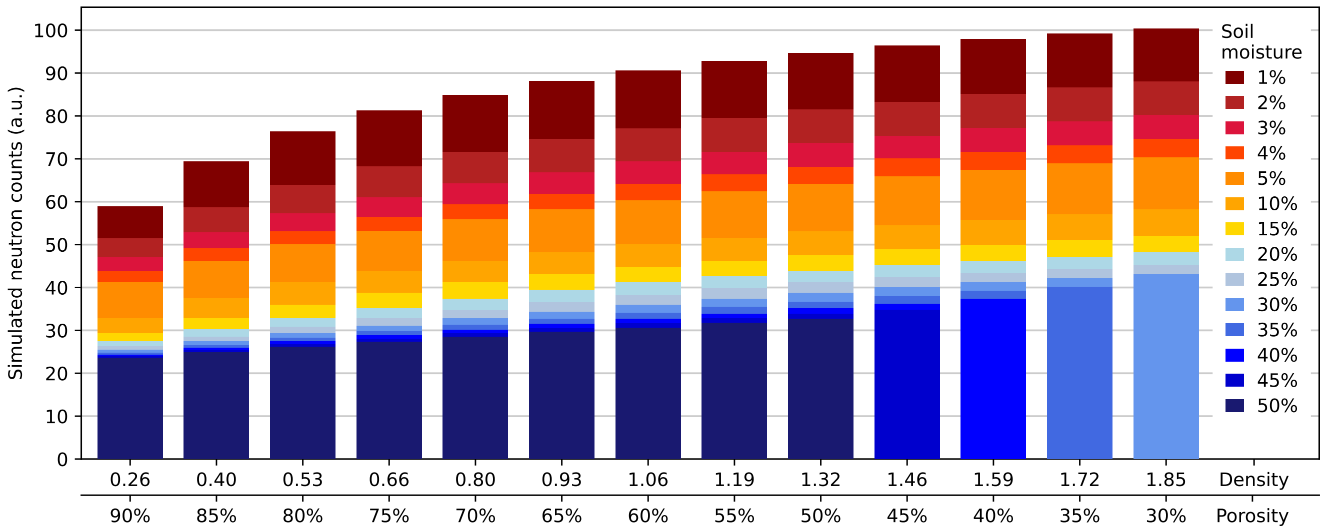

Figure 2. Quantitative influence of the soil bulk density (in g/m³) resp. porosity (in %) on the simulated neutron signal for various soil moisture states (colors).

of 20 vol%. Another example is a soil that consists of 50 vol% solid soil (equal 50 vol% porosity) and a soil water content of 12.5 vol%.

The results of this study are shown in Figure 1. With the exception of the two extreme end points of the simulation, the deviations from the mean value were in the range of ± 0.1 %. Only in the range of the extreme values (dry and saturated), where the approximation of Eq. 3 may no longer be completely valid, a slightly larger deviation was observed, but still below typical detection limits (± 0.25 %).

3.2 Variable soil moisture and bulk density

To identify the influence of soil bulk density on the neutron signal, the simulations were set with a fixed soil water content and a variable porosity, starting with $\Theta_i =$2,3,4,5 vol% and then in steps of 5 % up to 90 vol% porosity. The simulations have been repeated for soil moisture values of $\theta_i =$1,2,3,4,5 vol% and then in steps of 5 % up to 50 vol% soil moisture.

The bar chart in Fig. 2 illustrates the influence on the neutron signal at various bulk densities and porosities. The highest neutron intensity can be achieved for very dry and dense soils, while it decreases with increasing soil bulk density (or decreasing porosity). Figure 3 shows the same data, but normalized to the maximum neutron intensity. This allows to identify the percentage effect of the variables (density and soil moisture) independently of the total number simulated (or detectable) neutrons. Different behaviour in three main sections can be identified in this data: i) dry conditions from 1–5 vol% soil moisture, ii) moderate moisture from 5–35 vol% and iii) wet conditions from >35 vol% soil moisture.

For soils under wet conditions (blue coloured curves in Fig. 3) the decrease of the neutron counts is almost linear, whereas the dry soil shows a parabolic behaviour. In the beginning the slope is flat but becomes steeper if it's dry and highly porous. A

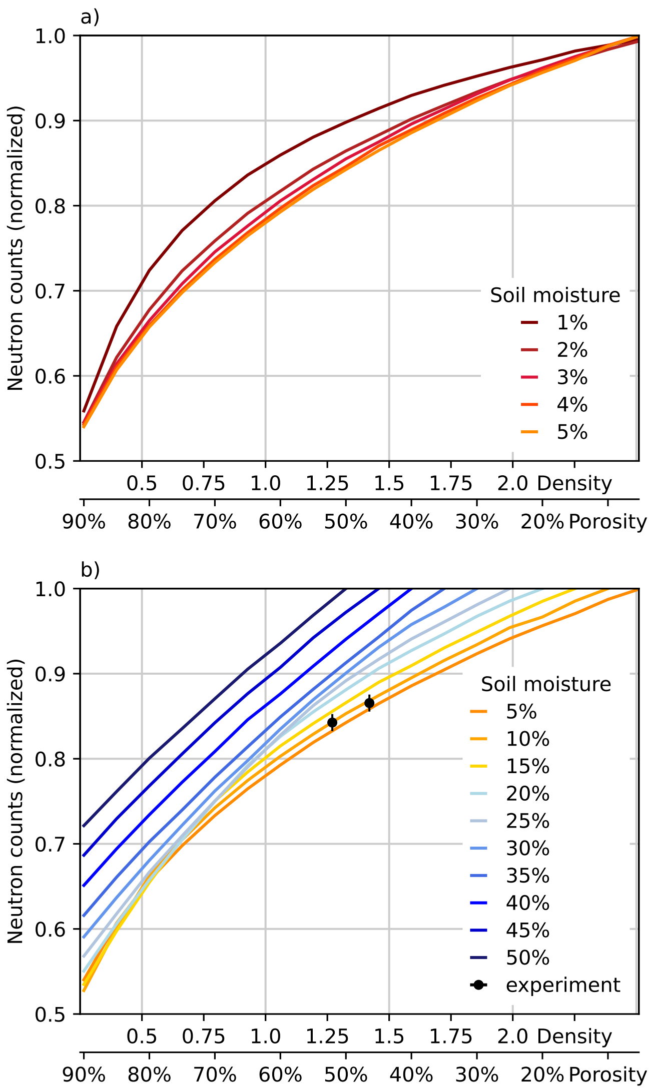

Figure 3. Quantitative influence of the soil bulk density (in g/m³) resp. porosity (in %) on the simulated neutrons. In contrast to Fig. 2, neutron intensities are normalized the their mutual maximum. The curves show different thrust for different soil moisture regimes, such that the Figure is separated into panels (a) very dry soil (≤ 5 vol%) and (b) dry to wet soil (≥ 5 vol%). The results from the box experiments with quartz sand are indicated as black points.

similar progression is evident for the curves between 5–35 vol% of soil moisture. Particularly noteworthy is the range between the moisture of 1 and 5 vol% . This section shows a significant deviation in the character of the curves. Exceedingly the dark red coloured curve (1 vol%) remains flat up to bulk densities of 1.6 g/cm³ (equal to porosity 40 vol%) and then drops sharply at densities < 1 g/cm³ (porosity > 65 vol%).

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3.3 Evidence in the sand box experiment

Sampling of the filled boxes showed an average dry bulk density for the fine quartz sand of 1.27 g/cm³ for the loose condition and 1.42 g/cm³ for the compact soil. For the loose and the dense experiment the soil water content were about 4.85 vol% (±0.3) and 5.75 vol% (±0.8), respectively. Comparing the measured average neutron response from the experiment with the two different bulk densities the counts increased significantly by 3 % after soil compression, while the stochastical error is about 1 %. Due to the fact that the same volume is compared to each other, the amount of solid soil components raised by 6 %, as shown in Tab. 1. The soil water content was almost constant (within 1 % uncertainty) so it can be assumed that the experiment could be represented by the simulated 5 vol% soil moisture curve (Fig. 3). The simulated effect of variable densities show good agreements with the neutron response detected during the lab experiment, using fine quartz sand. In the second experiment, an even larger variance in bulk density (1.07 g/cm³ and 1.42 g/cm³) was obtained by using topsoil. However the soil moisture between the loose and the dense experiment has also a larger dispersion (3 %) compared to the first experiment using sand (<1 %).

In addition, no significant difference between the loose and the compact soil could be identified in the neutron signal. Tab. 1 lists all results from the soil samples and the detected neutron counts, as well as the deviation between the loose and dense soil conditions. Another potential influencing property that also needs to be considered is the ratio between soil water and solid soil components. In the first experiment (material: sand) the ratio deviation between low and high bulk densities is about 0.51 . In contrast, the topsoil experiment shows only a ratio deviation of 0.2 . Despite the differences in soil moisture and densities, the neutron count rate remains almost the same for all experimental setups, which is explained by the ratio effect (as shown in the previous section).

3.4 Performance of the two conversion functions

As explained in section 2.2, the bulk density is used as a conversion factor between the gravimetric and the volumetric soil moisture derived from neutron counts (Eq. 8).

Figure 4 shows the derived soil moisture from simulated neutrons using (a) the Des. function and (b) the Koe. function. The dotted lines represent the water content as set in the URANOS simulations. The dashed lines shows the result when soil bulk density is not taken into account during the conversion (or left constant, here: $\varrho_\mathrm{s} = 1.46\,\mathrm{g/cm^3}$). The solid line represents the approach with direct consideration of the current storage density, as is traditionally done with the cross-conversion of gravimetric and volumetric soil moisture. (Eqs. 5 and 6)

If bulk density changes are unknown or not taken into account (dashed lines), both the Koe. and the Des. function show a similar physical progression. For that a rapid increase in soil moisture overestimation at lower densities ($\varrho_\mathrm{s} < 1.46\,\mathrm{g/cm^3}$) and a increase in soil moisture underestimation at high densities ($\varrho_\mathrm{s} > 1.46\,\mathrm{g/cm^3}$) occurs. Clearly changed courses of the estimated soil water contents appear when the actual bulk density is taken into account in the Des. and Koe. functions (solid line). The Des. function shows a similar progression as with a constant bulk density value and results in improved results for the estimated soil moisture. Despite this improvement, there are still large deviations compared to the simulated soil moisture. The

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Table 1. Comparison of parameters from the conceptional experiment for two soil substrates.

Quartz sand	loose soil	dense soil	differential
dry bulk density (g/cm³)	1.27	1.42	0.15
porosity (%)	52	46	6
soil moisture (%)	4.85	5.75	0.9
solid soil (%)	48	54	6
ratio	9.9	9.39	0.51
neutron counts	9950	10248	3%
topsoil			
dry bulk density (g/cm³)	1.07	1.42	0.35
porosity (%)	59	46	13
soil moisture (%)	12	14.9	2.9
solid soil (%)	41	54	13
ratio	3.42	3.62	0.2
neutron counts	10889	10943	0.4%

application of the Des. function in practice, requires a site-specific calibration of the sensor before a conversion of the neutrons can take place. Thereby the detector- and site-specific parameter N_0 has to be determined once. Depending on the analyzed hydrological condition (dry, moderate or wet), in which the sensor is calibrated, the resulting N_0 can at least approximate the real moisture in the actual range while considering the actual site-specific bulk density. Outside of the range of calibration (soil moisture and bulk density), the results are subject to higher uncertainty.

If the actual bulk density is taken into account in the Koe. function, there are more significant improvements compared to the Des. function, independent from N_0. Only above a soil moisture $\theta > 30\,\%$, noteworthy deviations are visible. However, at soil moisture contents above $\theta > 30\,\%$ and a bulk density less then $\varrho_\mathrm{s} < 1.0\,\mathrm{g/cm^3}$, the deviation increases sharply. For example, at a density of $\varrho_\mathrm{s} = 0.75\,\mathrm{g/cm^3}$ and a prevailing soil water content $\theta = 50\,\%$, the real moisture would be underestimated by 5 %, and at a density with $\varrho_\mathrm{s} = 0.5\,\mathrm{g/cm^3}$ it is assumed to be 10 % lower as the real moisture.

4 Discussion

4.1 Constant soil-water ratio

As shown in section 3.1, the neutron rate is an invariant property when the ratio between solid soil and soil water is constant (Fig. 1). This persistence of the neutron intensity above soils with different soil texture may have several causes. On the one hand, more solid soil contains more heavy atomic nucleii and thus increase the epithermal neutron production from high-energy cosmic rays in the ground (Zreda et al., 2008). At the same time, it also adds additional scattering partners for the

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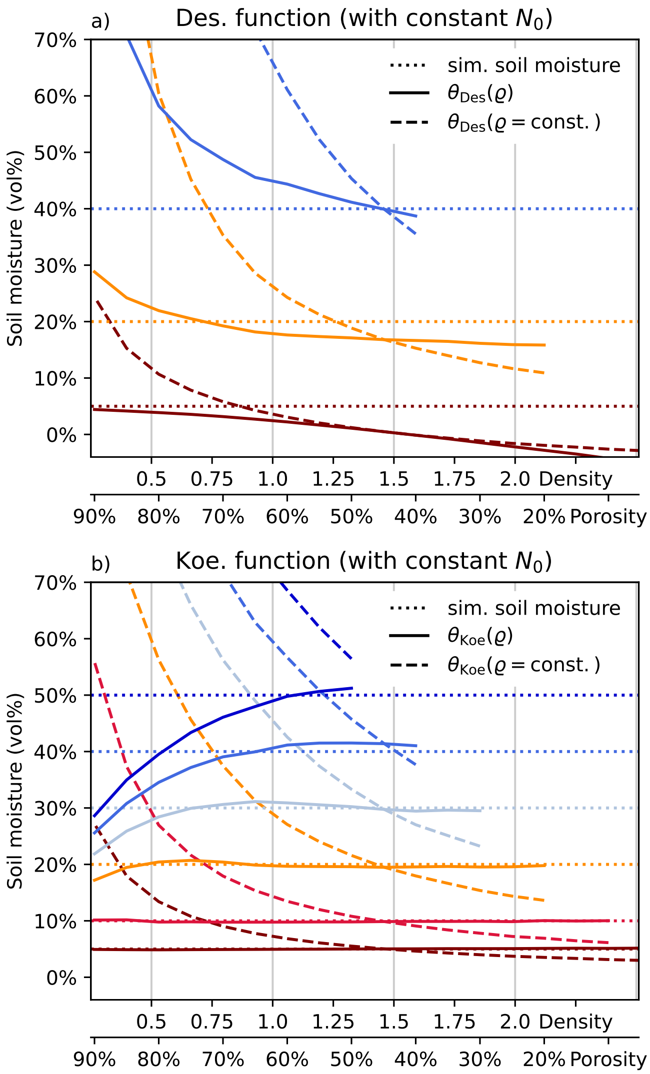

Figure 4. Soil moisture simulated in URANOS (dotted lines), derived from the simulated neutrons by the conversion functions (Eqs. 8) using variable bulk density (solid lines), and constant bulk density (dashed lines). Panel (a) uses the Des. function (Eq. 5), panel (b) uses the Koe. function (Eq. 6), while both approaches were calibrated once, using a single N_0 value for all combinations of soil moisture and bulk density.

neutron and thereby increases its probability to hit a hydrogen atom on the way. In turn, the additional water reduces the number of epithermal neutrons equally, such that the resulting neutron intensity remained constant. Moreover, higher bulk density also means lower penetration depth for the neutrons, as described by the inverse relationship from Köhli et al. (2015) and Schrön et al. (2017). For example, if the dry bulk density is 1.59 g/cm³ (i.e., 40 % porosity) and the soil moisture is 10 vol%, the neutrons penetrate twice as deep into the soil as in soils with a dry bulk density of 0.53 g/cm³ (i.e., 80 % porosity) and a soil moisture of 20 vol%.

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While the situations of constant soil-water ratio will most likely not remain for long in real places, this theoretical concept still highlights the ambiguous nature of the neutron response and their non-unique relationship to soil moisture and density.

4.2 Variable soil moisture and bulk density

The true and complex nature of neutron interactions in the soil medium emerges as soon as the ratio between soil moisture and soil density changes variably. This is particularly evident for very dry soils, where every single hydrogen or oxygen atom can make a huge difference (Zreda et al., 2012; Köhli et al., 2021).

The strong parabolic shape of the curves in Fig. 3) with up to 5 vol% soil moisture is due to the strongly non-linear neutron response in this very dry regime. If the soil is particularly dry, the neutrons react especially sensitively on each additionally hydrogen atom. On account of the small number of hydrogen atoms, there is now an increased relative influence of the oxygen atoms (Zreda et al., 2012). For soils with 1 vol% soil moisture the total influence of oxygen atoms is almost equal to the impact of a hydrogen atom, an effect which can be also observed for porosities > 70 vol%. This effect is visualized in the diagram (Fig.3) by the strong negative slope and the coincidence of the curves up to 25 vol% soil moisture. It is consistent with the analysis of Zreda et al. (2012), where the dynamics of the neutron count rate depends on the surrounding water and oxygen atoms. The error on the neutron signal increases for all approaches with decreasing bulk density. In the most relevant regime of $1.2 < \varrho_s < 1.7\,\mathrm{g/cm^3}$ the error is small but under certain circumstances relevant to consider.

4.3 Relevance for CRNS sites, roving, and farming

The investigated range of bulk density is actually relevant for the variety of environmental research sites. In general, soil bulk density can be categorized into loose ($\varrho_s < 1.4\,\mathrm{g/cm^3}$), medium dense ($\varrho < 1.6$–$1.8\,\mathrm{g/cm^3}$) and compact soils ($\varrho > 2.0\,\mathrm{g/cm^3}$). For the neutron transport simulations, a range of bulk densities from 0.265 to $2.60\,\mathrm{g/cm^3}$ was investigated, which covered the majority of the bulk densities occuring in natural soils. For example, in the distribution of the bulk density of more then 750 soils from the UNSODA database V2.0 (Unsaturated Soil Hydraulic Database) (Nemes et al., 2001), the range extends from 0.17 g/cm³ to 2.1 g/cm³ and shows a mean bulk density of 1.44 g/cm³ and a standard deviation of 0,25 g/cm³).

The data collection of European CRNS sites (Bogena et al., 2022) supplies soil moisture data from 65 Cosmic-Ray neutron in Europe, covering a wide range of climate zones and various land use types. Besides the soil moisture it provides information about the bulk density. Numerous soils indicate bulk densities below $\varrho_s = 1\,\mathrm{g/cm^3}$, so that the simulation analyses were extended for the whole range of soil conditions. Within the simulations, only mineral soils without any organic parts are considered. Soils with $\varrho_s = 1\,\mathrm{g/cm^3}$ have low abundance and commonly include a high organic carbon content which introduces an additional effect to θ.

Some sites also show extreme values of soil density, such as the CRNS site in Northern Germany, where Rasche et al. (2021) reported up to 89 % porosity. In contrast, minimal porosity can be found in rocky terrain, where plants are mainly fed by rock moisture (Rempe and Dietrich, 2018).

Even if those sites would not undergo substantial density changes over time, regional mapping of soil moisture using mobile CRNS has to take into account this impressive variability. Numerous scientific studies also investigated the influence of different

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land uses on the soil bulk density (e.g. Lal et al., 1994; Sorokina and Thomas, 1996; Unger, 1995; Younesi Alamouti and Navabzadeh, 2008). For the mobile application of cosmic ray, therefore, more attention should be given to the land use and the corresponding bulk density when studies are performed on a regional scale. For instance, the same soil type can be used as a cattle pasture, or is used as a meadow. Animals or farming vehicles cause soil compaction (Chyba et al., 2014), whereas the influence is completely absent in the case of the meadow. This leads, compared to the grazing cattle, to a lower bulk density.

In case of stationary sensors, it is essential to consider the bulk density influence if they are located on agriculturally used areas. Due to the soil tillage, there is an annual bulk density change of the topsoil of approx. $0.16\,\mathrm{g/cm^3}$, investigated by Younesi Alamouti and Navabzadeh (2008).

Figure 6 shows a reduction in density from 1.6 g/cm³ to an average mean value of 1.46 g/cm³ in between the first 30 cm of the ground, caused by plowing. Converted into porosity values used in the URANOS simulations it's equal to 37 vol% and 45 vol%. As the theoretical results shown above have demonstrated, neglecting to account for these porosity changes can lead to relevant errors in the derivation of soil moisture.

Figure 5 illustrates a derivation of the soil moisture without considering the influence of the bulk density on the neutron signal. For example the detected neutron counting rate is about 22.5 counts/hour and the analysed porosity is about 40 vol%. According to the traditional conversion function by Desilets et al. (2010) (see equation 5), the estimated soil moisture is about 10 vol% and can be seen in the diagram 5. Assuming that a rain event occurs, the counting rate drops to 21 counts/hour and results in an estimated soil moisture of 25 vol%. Now, consider a change in porosity caused by soil tillage from 40 to 60 %. If this event is neglected, the sensor will significantly overestimate the actual soil moisture from this moment on (red solid line). In order to estimate the real soil moisture, it is necessary to work with the curve that represents the actual soil condition (here: green solid line). This effect even intensifies with increasing moisture and densities deviations.

The decrease in the neutron count rate due to the heavy tillage of the topsoil is also evident in the diagram (6). Here, soil layers of different thicknesses are simulated with various bulk densities typical for tillages. The upper soil layer has a porosity of 45 vol% and the bottom layer has 35 vol%. The simulations show the reduction of the neutron response as a function of the thickness of the modified soil layer, where the upper soil is looser than the deeper one. In most cases, a change in the soil densities is obtained to a depth of 30 cm, which leads to a reduction in the neutron response of 2.5–4.5 vol% depending on the soil moisture.

4.4 Performance of the two conversion functions

The results from section 3.4 in Fig. 4 illustrate the importance of the prevailing bulk density near the CRNS sensor concerning the conversion of neutrons to volumetric soil water content. If the bulk density is not taken into account, massive deviations occur by estimating the real soil moisture, especially when using the Des. function (Eqs. 5). For stationary CRNS sensors, a N_0 value appropriate for the environment under investigation can be calibrated. Thereby, the bulk density near the sensor is commonly measured and already considered during the calibration of the sensors. If the bulk density remains constant, useful soil moisture results can be achieved. However, if the density of the subsoil changes, a realistic soil moisture interpretation may fail.

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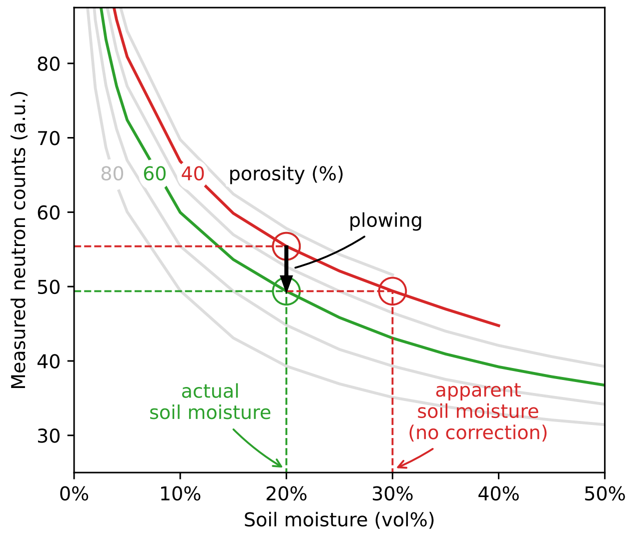

Figure 5. Neutron counts over soil moisture for various soil porosities (solid lines). The example illustrates the effect of porosity changes before (red) and after (green) tillage (black arrow). Without bulk density correction, the dropped count rate could be misinterpreted as a soil moisture change (red dashed lines).

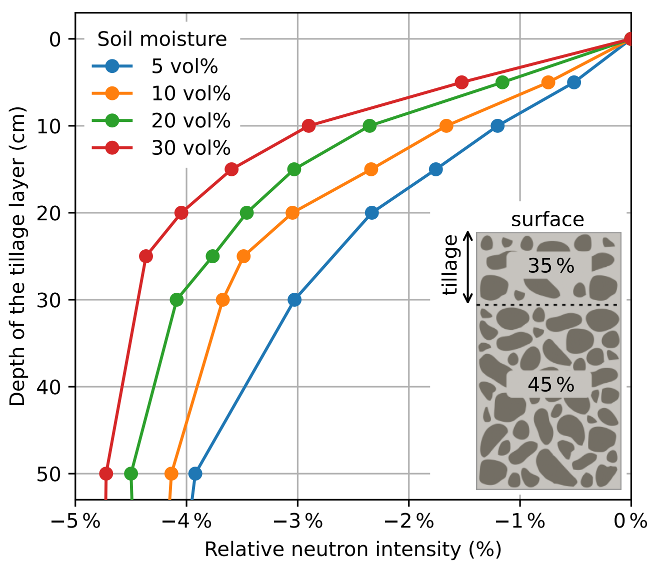

Figure 6. Percentage decrease of the neutron count rate with increasing thickness of the tillage layer. The porosity of the upper modified horizon is 45 vol% and the lower denser layer has 35 vol%.

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Mobile CRNS detectors can survey areas on a regional scale with heterogeneous soils, which is why a frequently adjustment of N_0 would be impractical and unfeasible, so in practice a constant N_0 is normally used for the duration of the measurement (Fersch et al., 2018; Schrön et al., 2021). Regarding the changing bulk densities in the subsurface that occur during large-scale mobile CRNS surveys, a large uncertainty without adjustment of N_0 and the bulk density seems inevitable. Comparing the results with a constant N_0 and by use of the conversion function from Köhli et al. (2021) (Eq. 6, a clearly improvement can be seen. Through the improved integration of N_0 into the Koe. function itself, an impressive improvement of the mobile CRNS measurement accuracies could be achieved.

In cases of unknown soil densities, it is common to assume an average soil bulk density for further calculations. The error that occurs in the conversion under this assumption is shown in section 4.2 and Fig. 4 (dashed lines).

Based on the findings of this study, a correction approach for the bulk density dependence is needed to obtain an accurate understanding and interpretation of the signal, especially for the mobile use of CRNS sensors. Because of the strong N_0 dependency in the Des. conversion function, the this study will focus the bulk density correction on the Koe. function. However, since the Des. function is still widely and successfully used in many places until today, an correction approach for the Des. function is also be proposed in the appendix.

It should be noted at this point that the Koe. function was developed using the same model assumptions as the simulation results shown here. Therefore, the good agreement of the Koe. function with the model results was partly expected. However, URANOS and the model assumptions used here have been successfully validated in various studies in recent years (Köhli et al., 2015; Jakobi et al., 2020; Weimar et al., 2020; Rasche et al., 2021; Köhli et al., 2021, among others).

4.5 The correction approach

We introduce a new correction factor for the solid soil bulk density, C_s, which can be applied as a correction to the actual observed neutron counts N, such that the conversion function $\theta_\mathrm{Koe}(N)$ from Köhli et al. (2021) matches the actual soil moisture θ_real:

$$\theta_\mathrm{Koe}(N_\mathrm{sim} \cdot C_\mathrm{s}^{-1}) = \theta_\mathrm{real}. \tag{11}$$

$$\Rightarrow \quad C_\mathrm{s}^{-1} = \frac{N_\mathrm{Koe}(\theta_\mathrm{real})}{N_\mathrm{sim}}, \tag{12}$$

where $N_\mathrm{Koe}(\theta)$ is the inverse function of $\theta_\mathrm{Koe}(N)$, calculated by Schrön (2021). Note: The problem could also be considered the other way round, where C_s is used to correct the estimated neutron count rate to better match reality:

$$N_\mathrm{sim} = N_\mathrm{Koe}(\theta_\mathrm{real}) \cdot C_\mathrm{s}, \tag{13}$$

which goes in line with the traditional correction factors for atmospheric changes, road effect, and vegetation, as presented e.g. in Fersch et al. (2018) or Bogena et al. (2022).

The approach for this correction function has been based on the presented theoretical dependency of the neutron counts on ratio between water content and bulk density (see section 2.2, Eq. 4). In this process, a polynomial function is fitted on these

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Table 2. Comparison of parameters and performance of the different approaches for the correction function $C_\mathrm{s}(\varrho_\mathrm{s},\theta)$ and the uncertainty of the fit (range of relative deviations) for the conversion-function in Köhli et al. (2021).

Approach for C_s	valid range $(\mathrm{m}^3/\mathrm{m}^3)$	a	b	c	d	R^2
$a+b\left(1/\varrho_\mathrm{s}\right)+c\left(1/\varrho_\mathrm{s}\right)^2+d\left(1/\varrho_\mathrm{s}\right)^3$	$0.35\leq\theta\leq0.50$	1.15943	−0.25085	0.08571	0.00465	0.943
$\left(a+b\exp\left(c\,\varrho_\mathrm{s}\right)\right)^{-1}$	$0.35\leq\theta\leq0.50$	1.02038	−0.19976	−2.12401		0.918
$a+b\left(\theta/\varrho_\mathrm{s}\right)+c\left(\theta/\varrho_\mathrm{s}\right)^2+d\left(\theta/\varrho_\mathrm{s}\right)^3$	$0.20\leq\theta\leq0.50$	1.01776	−0.16509	0.35565	−0.13413	0.944
$\left(a+b\exp\left(c\,\varrho_\mathrm{s}/\theta\right)\right)^{-1}$	$0.20\leq\theta\leq0.50$	1.00451	−0.23026	−1.28373		0.896

quotient:

$$C_\mathrm{s}(\varrho_\mathrm{s},\theta)=a+b\left(\theta/\varrho_\mathrm{s}\right)+c\left(\theta/\varrho_\mathrm{s}\right)^2+d\left(\theta/\varrho_\mathrm{s}\right)^3 \tag{14}$$

As the Koe. function leads to excellent results over the whole range of bulk densities and up to soil moisture contents $\theta<20\,\mathrm{vol\%}$, a correction is not recommended for the soil moisture range from 0 to 20 vol%. Only beyond this range a model deviation from the real soil moisture is evident and increases with increasing soil moisture, especially in loose soils. For bulk densities above $\varrho_\mathrm{s}=1.0\,\mathrm{g/cm^3}$, the error remains relatively small. For example, the deviation for soil moisture of $\theta=40\,\mathrm{vol\%}$ is approximately 2 vol%.

In this context, a performant solution for the bulk density correction, is presented in the range for $20\leq\theta\leq50\,\mathrm{vol\%}$ and leads to $R^2=0.944$. Therefore, the optimal parameters are $a=1.01776\pm0.00323$, $b=-0.16509\pm0.01764$, $c=0.35565\pm0.02482$, and $d=-0.13413\pm0.00937$.

Another exponential approach, $C_\mathrm{s}=a+b\exp\left(c\,\varrho_\mathrm{s}/\theta\right)$ is tested, which has the advantage to converge against 1 for $\varrho_\mathrm{s}>1$, thereby sustaining the already good match of the conversion function in this regime. The exponential approach, however, led to slightly lower performance $R^2=0.896$ throughout $20\leq\theta\leq50\,\mathrm{vol\%}$ and is thus not the optimal solution for the correction approach.

The soil moisture θ often is the quantity of interest in typical CRNS applications and therefore it's usually not known *a priori*. Hence, the parameters are also optimized based another variant of this function, that is only depend on soil bulk density and is independent of the soil moisture (i.e., Eq. 14 without the θ terms). As already explained, the neutron count rate depends on the ratio between the water content and the bulk density. Consequently, the performance of this approach for $20\leq\theta\leq50\,vol\%$ is much lower, $R^2=0.765$. For this reason, the use of this function is recommended only for soil moisture contents $\theta>35\,\mathrm{vol\%}$, where the performance is $R^2=0.943$. The optimal parameters for the solution, independent from soil moistures are: $a=1.15943\pm0.01468$, $b=-0.25085\pm0.05656$, $c=0.08571\pm0.06399$, and $d=0.00465\pm0.02195$.

Fig. 7 demonstrates the positive effect of the correction factor C_s on the performance of the Koe. function. The already good progressions in the dry and humid domain is evident, as well as the improvement obtained in the wet domain. The factor $C_\mathrm{s}(\theta/\varrho_\mathrm{s})$ can be used over a wide range of moisture, $\theta>20\,\%$, and is particularly useful in very loose soils $\varrho_\mathrm{s}<1.0\,\mathrm{g/cm^3}$. The RMSE between the simulated and the derived corrected soil moisture steadily decreases and can be reduced by up to one

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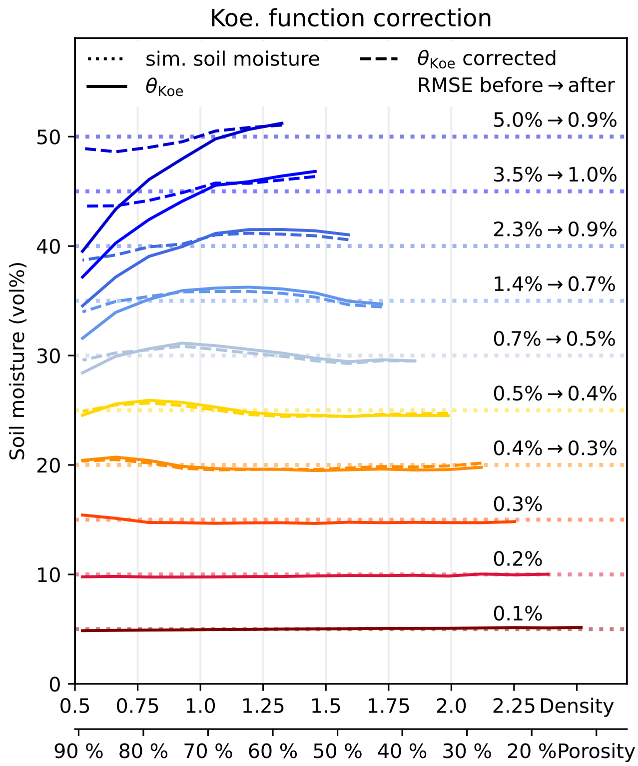

Figure 7. Soil moisture simulated in URANOS (dotted lines), derived from the simulated neutrons by the Koe. function (Eq. 6), and corrected for bulk density using the cubic $C_\mathrm{s}(\varrho_\mathrm{s},\theta)$ (Eq. 14) for $\theta \geq 20\,\mathrm{vol\%}$. The RMSE (in vol%) indicates the performance before and after the correction.

fifth in wet soils. Slightly lower and more unreliable performance can be achieved by the correction variant $C_\mathrm{s}(\varrho_\mathrm{s})$, i.e., without the dependency on θ (not shown), where RMSEs can be reduced by up to one fourth.

All in all, it is possible to proceed as follows in combination with the correction function C_s and the parameters from Tab. 2 in combination with the function from Köhli et al. (2021):

1. **The soil is dry** ($\theta < 20\,\%$) then it's not necessary to use an an additional bulk density correction with C_s.

2. **The soil moisture is unknown:** then option a) determine the soil moisture according to Köhli et al. (2021) and subsequently correct with the resulted soil moisture according to Eq. 14, or b) if the soil seems to be very wet ($\theta > 35\,\%$) it's useful to follow the Eq. 14 without the θ terms.

3. **The soil moisture can be estimated** with, e.g. independent measurements like TDR and the moisture is above $\theta > 20\,\%$, the correction can be done as with the Eq. 14.

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Since the Des. function is the most used one up to now, the development of a practicable bulk density correction approach for this function might be requested, too. However, the role of the determined N_0 for the calculated soil moisture according to Desilets et al. (2010) plays an exceedingly important role, in comparison to Köhli et al. (2021). The definition of an universal N_0 in wet as well as in dry areas leads to strong deviations in the opposite case. Therefore, N_0 needs to be calculated and used according to the prevailing soil moisture regime as well as according to the prevailing bulk density. This is not practicable for the use of mobile CRNS measurements. Hence, two calibration approaches for wet and dry conditions were investigated and are further described in Appendix A. Using this correction approach for the Des. function, a significant improvement over the entire range can be achieved, while the optimizer also tries to fix the general mismatch of the Des. function to the simulations independent of soil bulk density. In general, a calibration under moist conditions might be more advantageous, but compared with the Koe. function there are still substantial deficits. Especially for applications of mobile CRNS sensors, where local calibration is not feasible, the Koe. function together with a proper C_s-correction might be able to provide more robust resuls.

5 Summary and Conclusions

This study identified a significant influence of soil bulk density on cosmic-ray neutrons. The finding is based on theoretical considerations, neutron transport simulations, and experimental evidence, and has the following implications:

1. The neutron intensity mainly depends on the ratio between solid soil fraction and water. This implies that neutrons perceive different soil textures in a non-unique way when the ratio of dry matter to soil water is equal. In the investigated example (Fig. 1), the neutron count rate changes by less than 0.3 % for bulk densities varying within $0.5 < \varrho_\mathrm{s} < 2.1\,\mathrm{g/cm^3}$ and water content varying between 5 % and 20 %, provided that their ratio remains at 4:1.

2. The neutron-water relationship revealed a significant dependency on soil bulk density. On average, neutron count rates decrease by $-1\,\%$ for every $+10\,\%$ increase in porosity. This effect may become much more enhanced in porous soil ($\Theta > 70\,\mathrm{vol\%}$) and under dry conditions ($\theta < 10\,\mathrm{vol\%}$). Neglection of bulk density changes may introduce substantial deviations between the actual and the apparent soil moisture (Fig. 5).

3. The conversion function from Köhli et al. (2021) is more robust than the one from Desilets et al. (2010) in terms of sensitivity to N_0 and bulk density changes. If the correct bulk density used, the Koe. function shows excellent results for up to $20\,\mathrm{vol\%}$ soil moisture. For wetter soils, the preformance weakens especially for small low bulk densities ($\varrho_\mathrm{s} < 1.0\,\mathrm{g/cm^3}$). For denser soils, the accuracy of the method is better than $2\,\mathrm{vol\%}$. In contrast, the Des. function demonstrated low overall performance and strong dependency on the point of the N_0 calibration.

4. A new correction factor for soil bulk density has been introduced, $C_\mathrm{s}(\varrho_\mathrm{s}, \theta)$, which may improve the conversion function from Köhli et al. (2021). For wet soil ($\theta > 35\,\mathrm{vol\%}$) the factor only depends on ϱ_s, for intermediate soil the factor depends on $\varrho_\mathrm{s}/\theta$ and should be solved iteratively, while for dry soil ($\theta < 20\,\mathrm{vol\%}$) no correction is necessary (see Eq. 14 and Tab. 2).

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Table A1. Comparison of parameters and performance of the different approaches for the correction function $C_\mathrm{s}(\varrho_\mathrm{s},\theta)$ using Desilets et al. (2010) as the conversion.

Approach for $C_\mathrm{s}, N_0(\theta=5\%)$	valid range ($\mathrm{m}^3/\mathrm{m}^3$)	a	b	c	d	R^2
$a+b\left(1/\varrho_\mathrm{s}\right)+c\left(1/\varrho_\mathrm{s}\right)^2+d\left(1/\varrho_\mathrm{s}\right)^3$	$0.05\leq\theta\leq0.50$	1.00000	−0.48605	0.43524	−0.09921	0.276
$\left(a+b\exp\left(c\,\varrho_\mathrm{s}\right)\right)^{-1}$	$0.05\leq\theta\leq0.50$	1.00000	0.27605	−0.70737		0.532
$a+b\left(\theta/\varrho_\mathrm{s}\right)+c\left(\theta/\varrho_\mathrm{s}\right)^2+d\left(\theta/\varrho_\mathrm{s}\right)^3$	$0.05\leq\theta\leq0.50$	1.00000	−0.62937	0.64079	−0.19816	0.873
$\left(a+b\exp\left(c\,\varrho_\mathrm{s}/\theta\right)\right)^{-1}$	$0.05\leq\theta\leq0.50$	1.00000	0.24848	−0.11103		0.932
Approach for $C_\mathrm{s}, N_0(\theta=40\%)$	**valid range ($\mathrm{m}^3/\mathrm{m}^3$)**	**a**	**b**	**c**	**d**	**R^2**
$a+b\left(1/\varrho_\mathrm{s}\right)+c\left(1/\varrho_\mathrm{s}\right)^2+d\left(1/\varrho_\mathrm{s}\right)^3$	$0.05\leq\theta\leq0.50$	1.00000	−0.10655	0.12876	−0.02404	0.535
$\left(a+b\exp\left(c\,\varrho_\mathrm{s}\right)\right)^{-1}$	$0.05\leq\theta\leq0.50$	1.23006	−0.16885	0.32714		0.575
$a+b\left(\theta/\varrho_\mathrm{s}\right)+c\left(\theta/\varrho_\mathrm{s}\right)^2+d\left(\theta/\varrho_\mathrm{s}\right)^3$	$0.05\leq\theta\leq0.50$	1.13432	−0.61614	0.59802	−0.18014	0.888
$\left(a+b\exp\left(c\,\varrho_\mathrm{s}/\theta\right)\right)^{-1}$	$0.05\leq\theta\leq0.50$	1.00000	0.16715	−0.85209		0.126

The revealed sensitivity on bulk density changes is relevant for stationary sensors at highly managed sites, as soil porosity may change due to plowing or cattles. Moreover, the presented correction approaches may be particularly relevant for mobile CRNS campaigns where only a single calibration parameter is used across various land use types and soil textures. This research may also push the research on universal calibration functions and parameters to reduce the diversity of N_0 among CRNS stations worldwide and potentially also the sampling effort for their calibration.

Appendix A: Correction of the Des. function

Since the conversion function from Desilets et al. (2010) is still used in the community, this study also presents an approach optimize the sensor performance based on the actual bulk density. Due to the strong N_0 dependency of the Des. performance when compared to the simulation results, two cases were investigated: a dry calibration of N_0 on 5 vol% soil moisture, and a wet calibration of N_0 on 40 vol% soil moisture. Fig. A1 gives an impression on how the two calibration methods differ, and how a fitted correction function $C_\mathrm{s}(\varrho_\mathrm{s},\theta)$ can be used to improve the overall performance. The best performing parameters can be taken from the Tab. A1. It is evident, however, that the optimizer implicitely tried to correct also the general inability of the Des. function to match the simulation results independent of the bulk density. Hence, the function from Köhli et al. (2021) should be preferred in the future, especially for mobile CRNS investigations.

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Competing interests. The authors declare no competing insterests.

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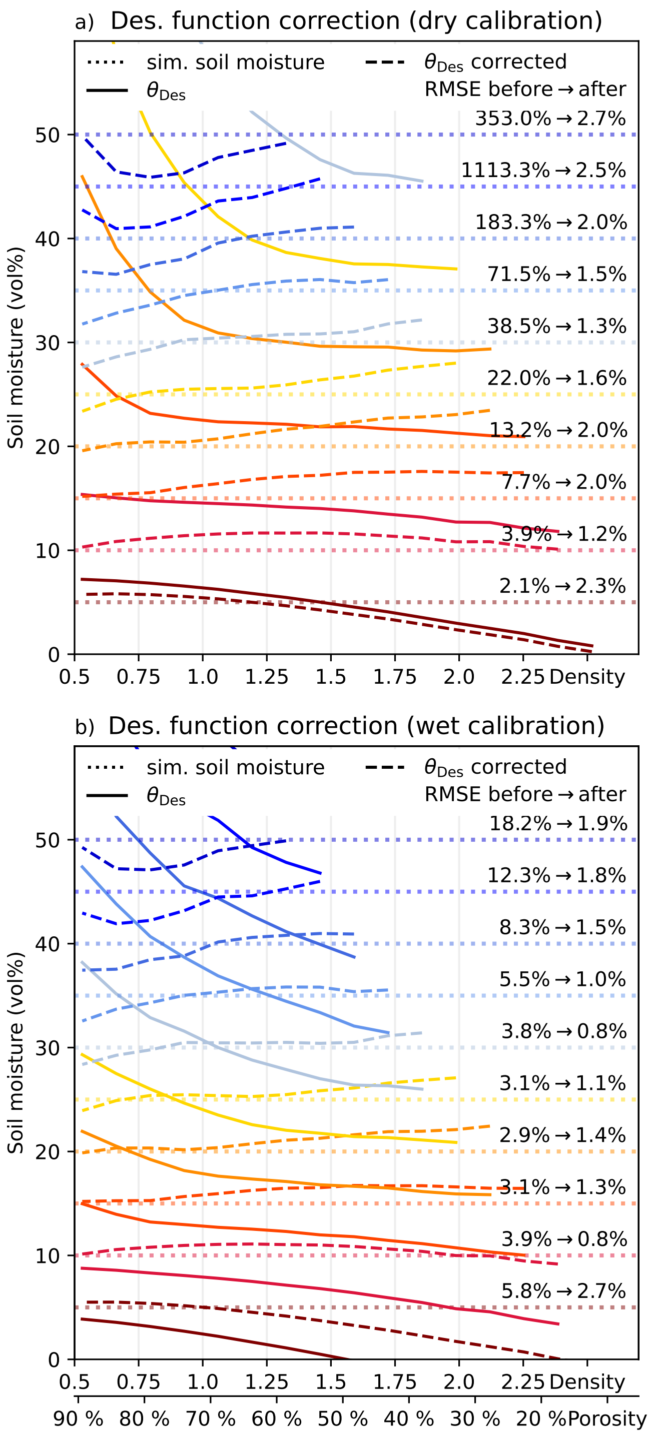

Figure A1. Soil moisture simulated in URANOS (dotted lines), derived from the simulated neutrons by the Des. function (Eq. 5), and corrected for bulk density using the cubic $C_s(\varrho_s, \theta)$ (Eq. 14). The RMSE (in vol%) indicates the performance before and after the correction. Data in panel (a) uses N_0 calibrated on $\theta = 5$ vol%, where as panel (b) uses an N_0 calibrated on $\theta = 40$ vol%., showing that the performance strongly depends on the individual calibration point.