Technical note: Towards a paradigm change in observing soil water content via cosmic-ray neutron sensing

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Abstract. Observing soil moisture via cosmic-ray neutron sensing has seen a rapid methodological development and expansion during the last decade. However, to foster its application some change in perspective may be useful. We reformulate the most common calibration equation used when working with CRNS data, the *Desilets* equation, and provide a simple and insightful form. This leads us also to a new option for calibration of CRNS time series without any local

10 sampling of soil moisture, and also without knowledge on CRNS detector sensitivity. At the same time it delivers the basis for a quantitative expression on how heterogeneities in the footprint contribute to the CRNS-derived soil moisture as well as why statistical errors in practice may be larger than assumed usually. Finally, we suggest to also define the area (and volume) represented by the CNRS observation in a more pragmatic way and complement it by indicating needs for better standardization.

15 1 Introduction

Cosmic-ray neutron sensing (CRNS) is a method that can fill spatial and temporal gaps in observing soil moisture i.e. soil water content compared to other non-invasive methods such as remote sensing (Oswald et al., 2024). After its invention (Zreda et al., 2008) soon further studies investigated how the measured neutron count rates could be converted into a mean soil moisture value for the area (Desilets et al., 2010), what part of the soil is contributing (Franz et al., 2013a), what is the

20 horizontal extent of integrating soil moisture (Desilets and Zreda, 2013) or how it performs in actual field applications (Desilets et al., 2010; Rivera Villarreyes et al., 2011; Franz et al., 2012). Important components of the further progress were Monte Carlos simulations of neutron scattering (Desilets and Zreda, 2013; Franz et al., 2013b; Köhli et al., 2015; Schrön et al., 2017; Francke et al., 2024), development of corrections for other variable factors than water influencing neutron count rates (Zreda et al., 2012; Rosolem et al., 2013; Hawdon et al., 2014; Franz et al., 2013c; Baatz et al., 2015) and setting up

25 CRNS networks at national or regional scale (Zreda et al., 2012; Hawdon et al., 2014; Cooper et al., 2021; Altdorff et al., 2024). Recent developments in respect to stationary applications of CRNS have, for example, been related to improving the incoming correction by providing local estimates of neutron monitor signals (McJannet and Desilets, 2023; Heistermann et al., 2024) or measuring muons locally as proxies (Gianessi et al., 2024), but also use modified approaches to describe how soil moisture relates to the measured neutron counts (e.g. Köhli et al., 2021) that potentially could replace the original or

30 modified Desilets approach (Desilets et al., 2010; Dong et al., 2014; Hawdon et al., 2014; Power et al., 2021). Furthermore, it has been explored if CRNS detectors modified by shielding could give a directional information on soil moisture in angular sectors (Francke et al., 2022). Finally, Heistermann et al. (2024) highlighted the option to perform a calibration for a CRNS station by accounting for its detector specific sensitivity, spatial variation of incoming neutrons by geomagnetic location and altitude, bulk density and possibly local amounts of lattice water, soil organic carbon and biomass, but without

35 local soil moisture sampling needed. At the end this is a valuable alternative and could be interpreted as the developments having reached a level of understanding of how the epithermal signal in CRNS is constituted to finally get along without local calibration to adjust the absolute level in soil moisture to the CRNS location.

We will present a mathematical reformulation of the *Desilets* equation (Desilets et al., 2010) that allows to develop an approach with another perspective that can complement high-end approaches with dedicated numerical neutron transport simulations (of CRNS locations) or at highly-investigated field sites. This includes (i) a rather astonishingly simple calibration alternative not requiring anything else than a long CRNS time series to obtain an estimate for gravimetric soil moisture as time series; (ii) an explanation why the observed signal-to-noise in CRNS time series is rather worse than to be expected by just accounting for the mere Poisson statistics of the neutron count rates; and (iii) an analytical formula to describe how the CRNS-derived value of soil moisture results from a heterogenous soil moisture distribution. This is supplemented by a number of considerations to operate and use CRNS in a pragmatic way that could help to foster a more widespread application, interpretation and integration of CRNS to derive soil moisture.

2 Turning the head to the missing neutrons

The detection of a neutron signal in CRNS is achieved by specific neutron probes that are sensitive enough to detect the intensity of the natural background of neutrons and its changes, in the epithermal or sometimes also the thermal energy range,. This set-up has led to the theoretical developments for CRNS, including its simulation, based on the variations occurring over time of the neutrons detected, including their cumulative count numbers in a time interval to be the basis for estimating its statistical uncertainty. Clearly, CRNS is not per se interested in the actual neutron intensity, nor its absolute changes, but in a rather virtual quantity, that is the neutron intensity as it would be *without* variations of intensity of the incoming cosmic-ray showers, *without* variations due to air pressure changes and *without* variations due to air humidity changes. That is why for each time interval of a CRNS measurement corrections based on fluctuations of these three quantities are required, at least at some stage, resulting in a so-called corrected neutron count rate N_C (t) that represents this virtual quantity. In the following it will be shown, that this current procedure may be seen only as a first step and that moving on a further step can contribute to achieve an even more useful perspective on CRNS. For this the *Desilets* equation will be used as a starting point (Desilets et al., 2010), as this is the predominantly applied procedure to convert neutron count rates into soil moisture values. Notwithstanding, other approaches exist and might be used alternatively, that is especially the UTS function (Köhli et al., 2021) that potentially could be more accurate for some situations.

2.1 Theoretical development

As the aim is to detect a soil water content, the corrected neutron count rate for each time interval is converted into a volumetric or gravimetric soil moisture. And if the Desilets equation (Desilets et al., 2010) is used as is often done (Bogena et al., 2022), the nominal soil moisture derived by CRNS, either as gravimetric soil moisture θ_{grav} (mass of water per dry mass of soil) or θ_{vol} (volume of water per bulk volume of soil), is related to the corrected neutron counts N_C via

$$\theta_{grav} = \theta_{vol} \frac{\rho_w}{\rho_b} = \frac{a_0}{N_C/N_0 - a_1} - a_2 \tag{1a}$$

where ρ_b (g cm⁻³) and ρ_w (1 g cm⁻³) are the soil bulk density and the density of water, respectively, and $a_0 = 0.0808$, $a_1 = 0.372$ and $a_2 = 0.115$. These three parameters are usually treated as constants though a few studies have also explored modifying them (Dimitrova-Petrova et al., 2021; Rivera Villarreyes et al., 2011). This includes additional hydrogen pools (AHP) that shall be subtracted from CRNS-derived nominal soil moisture to obtain the real gravimetric or volumetric soil moisture; however, for simplicity of the development we will address just the CRNS-derived nominal soil moisture in the mathematical development.

The *Desilets* equation (1a) is equivalent to the following formula (Köhli et al., 2021)

$$\theta_{grav} = -a_2 \frac{1 - N_C/N_{max}}{a^* - N_C/N_{max}} = a_2 \frac{1 - N_C/N_{max}}{N_C/N_{max} - a^*} \tag{1b}$$

where $N_{max} = N_0 \cdot (a_0 + a_1 a_2)/a_2 = N_0 \cdot a_1/a^*$ and $a^* = a_1 a_2/(a_1 a_2 + a_0) = 1/(1 + a_0/a_1 a_2)$. While in Köhli et al. (2021) the latter was named $\tilde{a}_1$ we prefer this different naming (a*) as this parameter will play an important role in our development. And also we do not redefine $\tilde{a}_0 = -a_2$ as in Köhli et al. (2021) because for clarity we want to stick to the original definitions when reasonable. As a^* and N_{max} can be calculated from the original parameters of the "N_0-equation", and taking the default values of a_0, a_1 and a_2 as listed above, gives a*=0.34617 and $N_{max} = 1.07461\, N_0$; and this does not include any assumptions. If there are substantial pools of hydrogen equivalents being present in soil as lattice water or soil organic matter this could be accounted for by changing to the original a_2 value plus lattice water plus water equivalent of soil organic carbon (both in g g⁻¹) (Baroni and Oswald, 2015; Power et al., 2021). As this is site dependent, we do not explicitly account for that in the following and readers should be aware that values given will change otherwise.

That Eq. (1b) now contains only two parameters reflects that the *Desilets* equation with three parameters a_0, a_1 and a_2 (and N_0) can be reduced to contain two such parameters only (and a N_0 variant, which here is now N_{max}), as has been shown by Köhli et al. (2021) and indirectly already by Rivera Villarreyes et al. (2011). These two in the following will be a_2 and a^*, accompanied by N_{max} as the transformed calibration parameter N_0. It may be worth noting that in the literature the difference between N_0 and N_{max} was not always precisely distinguished, as N_0 was sometimes described as being the neutron count rate for very dry conditions, but which correctly is the more than 7% larger N_{max}. We will prefer formulations in the following without N_0 as this should be more instructive and useful.

One advantage of using this equation instead of the original formulation of the *Desilets* equation could be that the reduced parameters allow unique solutions either when a single site-specific parameter (so far N_0) is calibrated or when optimizing with fitting the a_i (e.g. Rivera Villarreyes et al., 2014; Dimitrova-Petrova et al., 2021). Another advantage is that N_{max}, other than N_0, represents the absolute upper bound of the site-specific (corrected) neutron count rate, and N_C reaching N_{max} would occur only for zero CRNS soil moisture. Furthermore, as in practice N_C is staying above $a^* \cdot N_{max} = a_1 \cdot N_0$, the denominator stays always larger than 0; this argument analogously applies to, and strictly speaking is required for, the original *Desilets* equation. And we now define this value as a background level of the neutron count rate, and all corrected neutron count rates will be (somewhat) larger than that

$$N_{bg} = a^* \cdot N_{max} = 1/(1 + a_0/a_1 a_2) \cdot N_{max} = 0.34617 \cdot N_{max} \tag{2a}$$

leading to

$$\theta_{grav} = \theta_{vol}\frac{\rho_w}{\rho_b} = \frac{a_2}{a^*} \cdot \frac{1 - N_C/N_{max}}{N_C/N_{bg} - 1} = \frac{a_2}{a^* \cdot N_{max}} \cdot \frac{N_{max} - N_C}{N_C/N_{bg} - 1} = \frac{a_2}{a^*} \cdot \frac{N_{bg}}{N_{max}} \cdot \frac{N_{max} - N_C}{N_C - N_{bg}} = a_2 \frac{N_{max} - N_C}{N_C - N_{bg}} \tag{2b}$$

for the soil moisture.

And furthermore, which will be useful later, the difference between maximum and background neutron count rate is

$$N_{max} - N_{bg} = (1 - a^*) \cdot N_{max} = (1 - a^*) \cdot a_1 /a^* \cdot N_0 = \frac{a_0}{a_2} \cdot N_0 = 0.70261 \cdot N_0$$

$$= \left(\frac{1}{a^*} - 1\right) \cdot N_{bg} = \frac{a_0}{a_1 a_2} \cdot N_{bg} = 1.88873\, N_{bg} \tag{2c}$$

and as well their ratio can be specified as

$$N_{max} = 1/a^* \cdot N_{bg} = 2.88873\, N_{bg} \qquad . \tag{2d}$$

We can note that additional to a_2 and a^* there is only one free calibration parameter, which is either N_{max} or N_{bg} or N_{max} - N_{bg}, and they can easily be inferred from each other based on the equations specified above. Just for being able to calculate the conversion factors as precisely as possible we also specify the expressions with the original a_0, a_1, a_2-parameters. We also keep both N_{max} and N_{bg} in the following, just for clarity of the development, but keeping in mind that they just differ by a factor a^* (eqs. (2a) and (2d) for converting).

If we name

$$N_{missing} = N_{max} - N_C \tag{3a}$$

$$N_{above-bg} = N_C - N_{bg} \tag{3b}$$

120   we receive a very simple form of the *Desilets* equation that will show to be illustrative and insightful.

$$\theta_{grav} = \theta_{vol}\frac{\rho_w}{\rho_b} = a_2 \frac{N_{missing}}{N_{above-bg}} \tag{3c}$$

The soil moisture as determined via CRNS results from the number of neutrons that did not make it to the detector because being hold back by soil water (and additional hydrogen pools) as well as the number of neutrons detected, more precisely the number detected above a background value. *CRNS-derived soil moisture results directly as ratio of the missing neutrons*

125   *relative to the ones detected beyond a background level* (and then multiplied by a_2).

In case of lattice water (LW) or soil organic carbon water equivalents (WSOC) to be accounted for this modifies to

$$\theta_{grav} = \theta_{vol}\frac{\rho_w}{\rho_b} = (a_2 + LW + WSOC)\frac{N_{missing}}{N_{above-bg}} = a_{2,AHP}\frac{N_{missing}}{N_{above-bg}} \tag{3d}$$

One now could switch to background corrected neutron count rates

$$\widehat{N}_{max} = N_{max} - N_{bg} \tag{4a}$$

130    $$\widehat{N}_C = N_C - N_{bg} \tag{4b}$$

$$\widehat{N}_{missing} = \widehat{N}_{max} - \widehat{N}_C = N_{missing} \tag{4c}$$

which would make corrected neutron count rates to start at the lower end. The formulation for soil moisture stays analogous to above as

$$\theta_{grav} = \theta_{vol}\frac{\rho_w}{\rho_b} = a_2\frac{\widehat{N}_{max}-\widehat{N}_C}{\widehat{N}_C} = a_2\frac{\widehat{N}_{missing}}{\widehat{N}_C} = a_2\left(\frac{\widehat{N}_{max}}{\widehat{N}_C}-1\right) = a_2\left(\frac{\widehat{N}_C}{\widehat{N}_{max}-\widehat{N}_C}\right)^{-1} \tag{4d}$$

135   It is also possible to get one step further and work with a normalized corrected neutron count rate, which will always be within 0 and 1, somewhat similar to the definition of an effective saturation in soil science compared to a water content.

$$N_{C,norm} = \frac{N_C - N_{bg}}{N_{max}-N_{bg}} = \frac{\widehat{N}_C}{\widehat{N}_{max}} \tag{5a}$$

This could be useful to fully compare CRNS neutron count rates independent of the sensitivity of the individual CRNS device and other factors on the absolute level of neutron count rates such as altitude or geomagnetic location.

140    $$\theta_{grav} = \theta_{vol}\frac{\rho_w}{\rho_b} = a_2\left(\frac{1}{N_{C,norm}}-1\right) = a_2\frac{1-N_{C,norm}}{N_{C,norm}} \tag{5b}$$

Soil moisture results in all these three variants (eqs. (3c), (4d), (5b)) as the ratio of how much the neutron count rate differs from a maximum one divided by a neutron count rate.

2.2 Changes in interpretation

It is possible to switch easily from existing N_0 formulations and applications of the *Desilets* equation to an N_{max} or an N_{bg}

145   based formulation (or even using $N_{max} - N_{bg}$ only), without loss of accuracy, by applying

$$N_{max} = (a_0 + a_1 a_2)/a_2 \cdot N_0 = a_1/a^* \cdot N_0 = 1.07461 \cdot N_0 \tag{6a}$$

$$N_{bg} = a_1 \cdot N_0 = 0.372 \cdot N_0 \tag{6b}$$

$$N_{max} - N_{bg} = (1 - a^*) \cdot a_1/a^* \cdot N_0 = \frac{a_0}{a_2} \cdot N_0 = 0.70261 \cdot N_0 \tag{6c}$$

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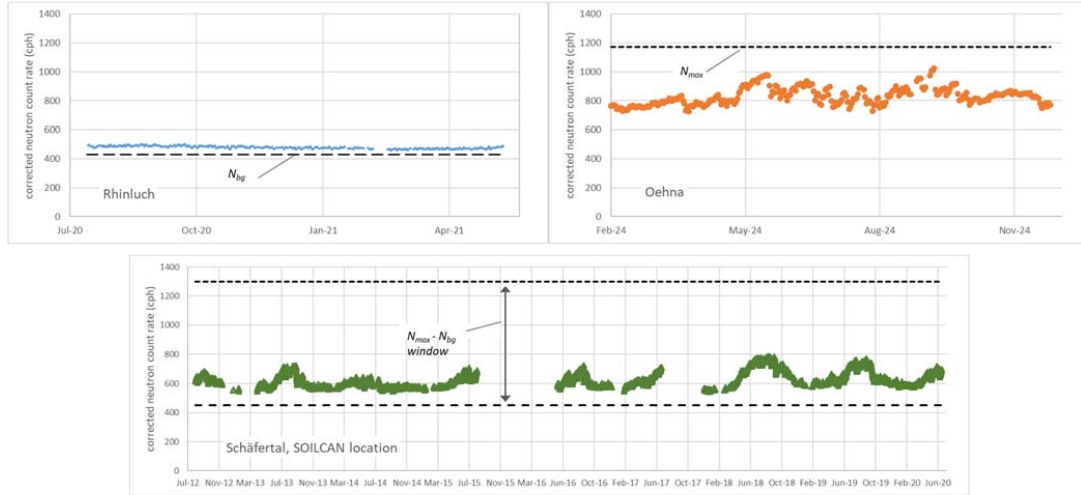where values are rounded to the fifth digit after the decimal in Eq. (6a) and Eq. (6c).

150 When working with these new formulations we should be clear about the physical-hydrological meaning of N_{max} and N_{bg} to fully exploit it in our understanding. N_{bg} is not identical to the minimal count rate for a site (at fully saturated conditions), but is somewhat lower than that; and this may also depend on the type of corrections applied to calculate N_C. For any site the actual minimum of the neutron count rates (for very wet conditions) would be even lower if the porosity would be even higher, and thus the full saturation corresponding to a larger maximum soil moisture. In our formulations of the *Desilets*

155 equation we can directly see that corrected neutron counts reaching N_{bg} is an extreme, asymptotic case, and conclude that N_{bg} is the corrected neutron count rate for a pure water column ($\rho_b \rightarrow 0$; N_C-$N_{bg} \rightarrow 0$; $\theta_{grav} \rightarrow \infty$; but θ_{vol} --> 1 cm^{-3}; see for example Eq. (3c)), at this site for this CRNS device. Situations with ponding water or snow packs could shift corrected neutron count rates further towards N_{bg}, in case of snow packs potentially even somewhat below; and as long as this is not clear periods with substantial snow water equivalent should rather be avoided in such an analysis.

160 Taking the second one, N_{max} is somewhat higher than a maximum corrected neutron count rate in completely dry soil (that is at residual water content as occurring under environmental conditions), because the neutron count rate may be reduced by scattering of neutrons in AHPs and biomass (and depending potentially also on geometrical structure of the vegetation), air humidity (and water vapor in soil pores) or the presence of rare elements in soil such as boron or gadolinium. If such effects have been part of the correction procedure, then corrected neutron count rates can be expected to come close to N_{max} for very

165 dry conditions. Below ground biomass could contribute to such a difference, as it is not only variable, but constitutes a water pool that occupies (pore) space that is not accessible any more to soil moisture and comes on top of the residual water content.

2.3 Implications for use in respect to a simple calibration procedure for CRNS time series

Instead of N_0, now N_{max} can be used (directly) as calibration parameter; or N_{bg} could be used as calibration parameter (and

170 then N_{max} calculated as N_{bg}/a^*). This could be done using the neutron count rates at a particular time and obtaining soil moisture values within the footprint ("local calibration") and determining N_{bg} or N_{max}, e.g. using eqs. (2a) and (2b).

However, the development offers also a new calibration option, ~~different to a local calibration~~, exploiting long CRNS time-series and the physical-hydrological meaning of these new calibration parameters. *This calibration option does not require local soil moisture information,* neither does it require a known sensitivity of the CRNS detector applied (relative to a

175 standard) as in the general calibration recently suggested (Heistermann et al., 2024); these sensitivities can vary by an order of magnitude between devices (e.g. Heistermann et al., 2023). N_{max} could be derived directly from a neutron count rate time series, if it includes times of very dry conditions. N_{bg} could be derived, if the CRNS time series includes times of very wet conditions. A combined window (N_{max} - N_{bg} = a^* N_{max}) could be derived by fitting to a neutron count rate time series when including both, dry and wet conditions. This N_{max} - N_{bg} window approach can also be applied to CRNS time series that do not

180 cover extremer conditions, however, the uncertainties in the inferred values of the calibration parameter will be larger.

We demonstrate this simple procedure in the following by exemplary sketches based on real CRNS time series obtained all via a CRS 1000 (Hydroinnova), which is the most frequently applied CRNS detector so far, at sites in Northern Germany at low to medium altitude (Fig. 1). At a site with very wet conditions at least in parts of the year the corrected neutron count rates come close to the N_{bg} level, though not reaching it completely (as this would be the case for a pure water column only).

185 In the example of *Rhinluch* (Fig. 1 top left, peatland site with very low bulk density (about 0.3 g cm^{-3}) and typically saturated conditions for winter and spring) corrected neutron count rates can be assumed to be close to the background value and used for fitting N_{bg}, accounting for that at the wet end neutron count rates vary much less with soil moisture than for medium conditions. In the example of *Oehna* (Fig. 1 top right, cropped field with occasional pivot irrigation in summer when soil can become very dry, even despite some irrigation) the setting could be used for fitting N_{max}. It should be

190 accounted for that at the dry end neutron count rates vary more strongly with soil moisture and thus small remaining amounts

of soil moisture will contribute to not reaching N_{max} level completely; and this is similar for amounts of AHPs at the site that to some degree also reduce neutron count rates.

Figure 1. Exemplary sketch of procedure for three CRNS time series (corrected neutron counts as moving 24 h average or daily value) and N_{bg} value, N_{max} value or N_{max} - N_{bg} window plotted as horizontal lines. Top left: wet peatland with agricultural use at Rhinluch, North-West of Berlin, Germany (Dobkowitz, S. and Oswald, S., 2022), fitted N_{bg}. Top right: cropped field with occasional pivot irrigation during summer, Oehna, Southern Brandenburg, Germany (Altdorff et al., 2024), fitted N_{max}; Bottom: mix of cropped field, meadow with a small creek and some pieces of forest at Schäfertal, Harz, Germany (SOILCan station at 51.655041° N, 11.052505° E, data set SCC004 (starting from 17 Aug 2012) provided by Bogena et al. (2022) fitted N_{max} - N_{bg} window. Periods with presumed snow conditions, outliers and singular data points have been excluded.

If a site is not coming close to really wet or dry conditions, during the period of CRNS observation or in general, it is better to go for the N_{max} - N_{bg} – window when fitting a calibration parameter. In the example CRNS time series from Schäfertal (Fig. 1 bottom, *SOILCan* location; see Fig. 2 in Schrön et al. (2023) for location details) there is a mixed land use and vegetation around the CRNS station, and it is located rather at the bottom of a hillslope not far from a small creek. Thus, this site has heterogenous soil moisture contributions, and neither extreme high neutron count rates (due to remaining wetter conditions around the creek) nor extreme low count rates (due to hillslope character and not low bulk density) can be expected for the CRNS-derived soil moisture average. But via fitting a N_{max} - N_{bg} – window it is still possible to do a calibration, best with accounting for some gaps remaining on both ends, though uncertainties may be higher than in the previous examples. If desired, also the N_0 parameter can be calculated from the newly obtained calibration parameter such as N_0=2,68873 N_{bg} etc. (see Eq. (6a-6c)), e.g. for comparison with former calibrations.

2.4 Implications for statistical treatment of corrected neutron count rates

As background-subtracted neutron count rates are lower than original ones (about half or 1/3 of N_C), the absolute statistical error may be lower, if taken as $\sqrt{N_C}$, but the relative one will be higher that is worse than $1/\sqrt{N_C}$. If we address this based on Eq. (2b) and using a statistical deviation from the neutron mean count rates σ_{N_C} we get

$$
\begin{aligned}
\theta_{grav}(N_C + \sigma_{N_C}) \quad &= a_2 \frac{N_{max} - (N_C + \sigma_{N_C})}{N_C + \sigma_{N_C} - N_{bg}} \\
&= a_2 \frac{N_{max} - N_C}{N_C - N_{bg}} - a_2 \frac{N_{max} - N_{bg}}{(N_C - N_{bg})^2} \sigma_{N_C} + \sigma(\sigma_{N_C}^2) \\
&= \theta_{grav}(N_C) - a_2 \frac{N_{max} - N_{bg}}{N_C - N_{bg}} \frac{\sigma_{N_C}}{N_C - N_{bg}} \\
&= \theta_{grav}(N_C) - \frac{a_2}{N_{c,norm}} \frac{\sigma_{N_C}}{N_C - N_{bg}}
\end{aligned}
\tag{7}
$$

220   by using the Taylor expansion of $f(x)=(a-x)/(x-b) = -a/b+(b-a)/b^2 \cdot x$, and neglecting higher order terms. Thus, we see that the deviation in soil moisture by the statistical error in the corrected neutron count rates is different to taking N_C only. And in general, it becomes the larger the closer N_C is to N_{bg}.

However, is the number of neutrons in cosmic-ray neutron sensing given by a simple Poisson distribution, or is it a result of a multiplicative series of two Poisson type processes (one for the number of primary particles hitting the atmosphere above

225   the site and creating a particle shower, and the second one the number of neutrons finally generated in the shower caused by this individual event)? In the latter case the relative uncertainty may be (much) higher, as the statistical variation in the incoming particle numbers are much higher (relatively), given the much lower number of events, but this will depend on how frequent the primary events will occur within the integration time interval chosen for the CRNS observation.

Furthermore, high statistical noise in CRNS signal may result not only from statistics in presence of cosmic-ray neutrons, but

230   also from the random exploration of soil moisture in the footprint, if the soil moisture distribution is not homogeneous; and inhomogeneity of soil moisture is the reason for applying field-scale integration methods such as CRNS in the first place. The neutrons counted as well as the neutrons missing have sampled soil in the footprint at particular locations (one or potentially a few), and each one does represent a single, binary event only (stopped or not stopped) at that location, say patch, with its particular soil moisture value. A number of such events is needed for that patch, or patches with the same soil moisture

235   to represent its soil moisture value in the CRNS detection. As a simple example, let us say we want to quantify soil moisture in the range between 1% and 50%, then 50 events (e.g. 37 neutrons out of 50 have been detected, 13 are missing) on top of the background would be needed to provide that in about 1% soil moisture step, that is 50 categories; though, actual steps would not be equal in size due to the non-linear character of the *Desilets* equation. If we take a corrected neutron count rate for a CRNS of 1000 cph then 20 patches within the footprint could be sampled by 50 neutrons each within one

240   hour. However, if we want to obtain soil moisture in 0.1% steps, in our example the neutron count rate would be sufficient for sampling two patches only within one hour. Clearly, sampling two values from a realistic distribution of soil moisture values in the footprint could take us far from the true average; and even 20 samples still have to expect some statistical deviation. For a quantification, a spatial distribution of soil moisture has to be assumed, with a spatial correlation length of patches and distribution of values within the patches, which will be site specific and temporally varying.

245   Overall, we have to expect that the statistical deviation in the CRNS signal (neutrons detected and neutrons missing), is larger than the mere $\sqrt{N_C}$, as it will have additional contributions from $N_C - N_{bg} < N_C$, from N_C resulting from a twofold Poisson process, and from the statistical sampling of a soil moisture being distributed within the footprint.

2.5 Quantitative signal interpretation for non-uniform soil moisture conditions

For n circular sectors of equal size covered by the CRNS, we will show how the CRNS-derived soil moisture depends on the

250   gravimetric soil moisture values in the sectors ($\theta_1, ..., \theta_n$). The treatment as of equal size is not a real limitation, because adjacent sectors could have the same soil moisture value and could be combined to any sizes, thus implicitly also the case of different sizes is included. Also, the radial differences in signal weighting could be accounted for by working with sections within an annulus, for which a particular but known radial weighting factor needs to be applied.

First, we determine how the corrected neutron count rate contribution (in absolute terms) $N_{C,i}$ for each sector is resulting

255   from the $\theta_1, ..., \theta_n$. Then how the CRNS-derived soil moisture depends on them. Finally, an illustrative example for $n=2$.

If the corrected neutron count rate originating from the sector i is named $N_{C,i}$ (θ_i) we can deduct how its value depends on θ_i if we start from a situation where the whole area has a gravimetric soil moisture θ_i everywhere, and the neutron count rate is therefore the n-fold of the corrected neutron count rate from the individual sector i,

$$\theta_i = a_2 \frac{N_{max} - N_C}{N_C - N_{bg}} = a_2 \frac{N_{max} - n \cdot N_{C,i}}{n \cdot N_{C,i} - a^* \cdot N_{max}} \tag{8}$$

$$\Rightarrow N_{C,i}(\theta_i) = \frac{N_{max}}{n} \frac{a_2 + a^* \cdot \theta_i}{a_2 + \theta_i} \tag{9}$$

Then the corrected neutron count rate N_C for the heterogenous case with different sectors, which depends on all the individual soil moisture values θ_i in the sectors, results as

$$N_C(\theta_1, \cdots, \theta_n) = \frac{N_{max}}{n} \sum_i^n \frac{a_2 + a^* \cdot \theta_i}{a_2 + \theta_i} = \frac{N_{bg}}{n \cdot a^*} \sum_i^n \frac{a_2 + a^* \cdot \theta_i}{a_2 + \theta_i} \tag{10}$$

And we can constitute the CRNS-derived soil moisture as

$$\theta_{grav}(\theta_1, \cdots, \theta_n) = a_2 \frac{N_{max} - N_C(\theta_1, \cdots, \theta_n)}{N_C(\theta_1, \cdots, \theta_n) - a^* \cdot N_{max}} = a_2 \frac{n - \sum_i^n \frac{a_2 + a^* \cdot \theta_i}{a_2 + \theta_i}}{\sum_i^n \frac{a_2 + a^* \cdot \theta_i}{a_2 + \theta_i} - n \cdot a^*} = a_2 \frac{1 - \frac{1}{n} \sum_i^n \frac{a_2 + a^* \cdot \theta_i}{a_2 + \theta_i}}{\frac{1}{n} \sum_i^n \frac{a_2 + a^* \cdot \theta_i}{a_2 + \theta_i} - a^*} \tag{11a}$$

By the way, this is independent of the calibration parameter and thus not only independent of its value but also which one is chosen.

When dividing the sectors into k annular segments at different radial distance of equal contribution to the CRNS signal, and thus having $n \cdot k$ basic areal elements contributing together to the CRNS-derived soil moisture, this would change to

$$\theta_{grav}(\theta_1, \cdots, \theta_n) = a_2 \frac{N_{max} - \frac{N_{max}}{n \, k} \sum_j^k \sum_i^n \frac{a_2 + a^* \cdot \theta_{i,j}}{a_2 + \theta_{i,j}}}{\frac{N_{max}}{n \, k} \sum_j^k \sum_i^n \frac{a_2 + a^* \cdot \theta_{i,j}}{a_2 + \theta_{i,j}} - a^* \cdot N_{max}} = a_2 \frac{n \cdot k - \sum_j^k \sum_i^n \frac{a_2 + a^* \cdot \theta_{i,j}}{a_2 + \theta_{i,j}}}{\sum_j^k \sum_i^n \frac{a_2 + a^* \cdot \theta_{i,j}}{a_2 + \theta_{i,j}} - n \cdot k \cdot a^*} \quad . \tag{11b}$$

The design of the annular segments will depend on the radial weighting of CRNS, as known for example from Schrön et al. (2017), and could be based on the mean soil moisture as long as they can be assumed not to depend substantially itself on the soil moisture patterns occurring. This allows us to tell how a CRNS-derived soil moisture is composed by the soil moisture values, even for quite heterogenous distribution patterns, which could be approximated by $n \cdot k$ annular segments in the sectors, with the appropriate number and spatial resolution needed for that.

For the simple case of a circular footprint being split into two sectors only ($n=2$)

$$\theta_{grav}(\theta_1, \theta_2) = a_2 \frac{2 - \left(\frac{a_2 + a^* \cdot \theta_1}{a_2 + \theta_1} + \frac{a_2 + a^* \cdot \theta_2}{a_2 + \theta_2} \right)}{\left(\frac{a_2 + a^* \cdot \theta_1}{a_2 + \theta_1} + \frac{a_2 + a^* \cdot \theta_2}{a_2 + \theta_2} \right) - 2 \cdot a^*} = a_2 \frac{2 - 2 N_C(\theta_1, \theta_2)/N_{max}}{2 N_C(\theta_1, \theta_2)/N_{max} - 2 \cdot a^*} \tag{12}$$

we address the CRNS-derived soil moisture as being constituted from the different soil moisture levels in the two sectors
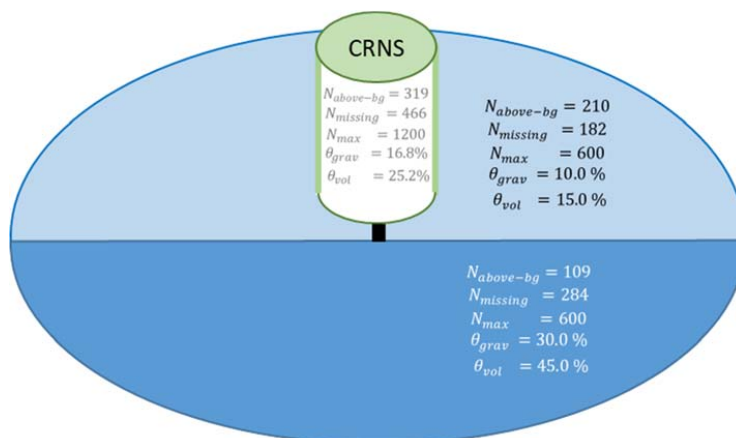
$$\theta_{grav}(\theta_1, \theta_2) = \gamma_1 \theta_1 + (1 - \gamma_1) \theta_2 \tag{13a}$$

$$\theta_{vol}(\theta_{1,vol}, \theta_{2,vol}) = \gamma_1 \theta_{1,vol} + (1 - \gamma_1) \theta_{2,vol} \tag{13b}$$

where γ_1 is the fraction of θ_1 contributing to the CRNS-derived soil moisture (that is also the weight to be used when averaging). Both together set the condition that is to be fulfilled

$$\gamma_1 \theta_1 + (1 - \gamma_1) \theta_2 = a_2 \frac{2 - \left(\frac{a_2 + a^* \cdot \theta_1}{a_2 + \theta_1} + \frac{a_2 + a^* \cdot \theta_2}{a_2 + \theta_2} \right)}{\left(\frac{a_2 + a^* \cdot \theta_1}{a_2 + \theta_1} + \frac{a_2 + a^* \cdot \theta_2}{a_2 + \theta_2} \right) - 2 \cdot a^*} \tag{14}$$

$$\Rightarrow \gamma_1 = \left(a_2 \frac{2 - \left(\frac{a_2 + a^* \cdot \theta_1}{a_2 + \theta_1} + \frac{a_2 + a^* \cdot \theta_2}{a_2 + \theta_2} \right)}{\left(\frac{a_2 + a^* \cdot \theta_1}{a_2 + \theta_1} + \frac{a_2 + a^* \cdot \theta_2}{a_2 + \theta_2} \right) - 2 \cdot a^*} - \theta_2 \right) / (\theta_1 - \theta_2) \tag{15}$$

Figure 2: Perspective sketch on the contribution of a wet and dry area to the CRNS-derived soil moisture – simple example of two sectors (semicircles) with different soil moisture levels. N_{max} is taken as 1200 cph, corresponding to a value of 932.1 cph for N_{bg},

290 **and a bulk density of 1.5 g cm^{-3}. However, the result for the CRNS-derived gravimetric soil moisture value is independent of that. Values in graph are rounded.**

Now taking some values as example, and starting from volumetric soil moisture values and a bulk density of 1.5 g/cm³ we choose $\theta_{1,vol} = 15\%$ and $\theta_{2,vol} = 45\%$. This gives $\theta_1 = 10\%$ and $\theta_2 = 30\%$. Now evaluating Eq. (15) yields $\gamma_1 = 0.6587$ and $\theta_{grav}(\theta_1, \theta_2) = 16.83\%$, whereas the arithmetic mean is 20.0% (Fig. 2). In terms of volumetric soil moisture, we obtain

295 by CRNS a volumetric soil moisture $\theta_{vol} = 25.24\%$, while the arithmetic mean is 30.0% (Fig. 2). As can be seen by the γ_1 value the lower soil moisture is getting a higher weight than the higher one and the observed value is to some degree shifted to a lower value. This results from the non-linearity of the *Desilets* equation, or in other words the higher level of missing neutrons in the wetter part does not fully compensate for the higher level in neutrons above background resulting from the drier area (cf. Eq. (3c)). This is independent of the CRNS detector sensitivity or site properties others than soil moisture distribution. To

300 complete the example, for an $N_{max} = 1200$ cph there would be 466.1 cph neutrons missing ($N_{missing}$) in total, 182.5 cph and 283.6 cph from the first and the second sector, respectively; and 318.5 cph of neutrons above the background ($N_{above-bg}$), 209.8 cph and 108.7 cph from the first and the second sector, respectively (Fig. 2).

3 Flexible handling of footprint size or support volume of CRNS

3.1 Working with a representative horizonal footprint instead of a fixed general one

305 For CRNS the useful property "footprint", also called "support volume", has been defined as the area that contributes 86% to the neutrons detected, and has been taken as circular area around the CRNS detector or a half sphere above it including values for its radius or diameter as determined by neutron particle transport modeling (Desilets and Zreda, 2013; Schrön et al., 2017). This is in a way arbitrary as on one hand there is a non-negligible contribution from outside the area defined in such a way as the footprint and on the other hand the inner area contributing the majority is substantially smaller than the

310 footprint, that is about 50 m radius instead of the 150-200 m, or in area about a tenth of the footprint area only. Also, there could be taken other shapes of the footprint and thus somewhat other shapes to contribute the same amount to the CRNS measurement. And we have seen that the number of neutrons missing contribute to the CRNS-derived soil moisture as well as the neutrons detected above background.

This leads us to a more practically applicable option to handle the CRNS footprint. A user could decide about what is the

315 landscape unit to be represented by the CRNS measurement, while (i) keeping in mind that the area of the landscape unit should be between 1 and 10 ha (see values for radius as discussed above); (ii) making sure when placing the CRNS detector to have the core area (about 1 ha) to be lying completely within the unit chosen to be represented; (iii) just avoiding extreme

locations within the area when setting up the CRNS detector, such as local depressions, buildings close by or unusually dry spots within the area (e.g. indicated by vegetation); and (iv) in case of adjacent agricultural fields using the distance given in

320 Schrön et al. (2023) to decide about the minimal distance needed to an adjacent irrigated agricultural field, to avoid having a significant contribution of that field to the CRNS soil moisture measurement in the field targeted. Then it could be reasonable to associate the CRNS-derived soil moisture with the thus chosen area to be represented (Fig. 3 giving an example how this could look like). This procedure could be useful in agricultural settings, but is not limited to that and could be used analogously in other parts of the landscape.
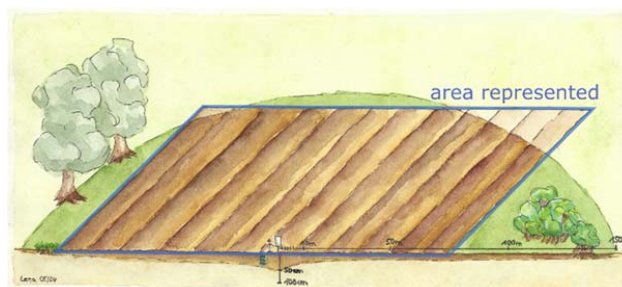
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Figure 3: Illustration of how an area could be chosen alternatively to be represented by the CRNS investigation. A schematic set-up within an agricultural field is shown, adapted from Scheiffele (2024). This area could contribute to the neutron count rates similarly to the circular standard footprint, but should be taken as a meaningful unit in the landscape to be represented, such as a
330 **managed agricultural field.**

Along these lines we could also think about other applications, as one of the big potentials of CRNS is being integrated into hydrological or land surface models (Patil et al., 2021; Fatima et al., 2024) or being used as ground truthing for satellite remote sensing (Hornbuckle et al., 2012; Montzka et al., 2017; Döpper et al., 2022; Meyer et al., 2022; Oswald et al., 2024). Also, for these applications it is challenging to use a circular footprint and potentially even account for some size variation

335 for changing soil moisture levels. However, this is the case also for in-situ point measurements at a given location, often these probes are installed to represent a particular depth, e.g. at 10 cm, while the diameter of the support volume is several cm. This volume will vary between different types of probes, in size and shape, and depend on changes in bulk permittivity and the distribution of water within this, but nevertheless values on that are not specified usually (Jackisch et al., 2020). Despite this a point measurement is frequently attributed to a location and a particular depth, e.g. in cm (or even millimetre),

340 but not a particular footprint. Furthermore, in remote sensing the observational value may be extracted from a complex signal, and the pixel size retrieved could depend on background models and calibration procedures used (Chen et al., 2022) or has different contribution of areas in the pixel to the signal including that some areas may be masked out (e.g. water surfaces, forest, snow; depending on internal thresholds) when calculating the pixel value for the actual product (Gruber et al., 2020; Balenzano et al., 2021). If we treat CRNS analogously, it could be seen as a point measurement at landscape scale

345 for a predefined pixel size that the signal is assigned to. A suggestion could be to attribute it at the upper end to (i) a square of 300 m· 300 m (9 ha); or (ii) a 1/3 km · 1/3 km resolution (1/9 km²); or at the lower end to (iii) a square with edges of 0.1 meridian arc minute ('), which is about 185 m length resulting in an area of close to 3 ha, and give its position to the 0.01' (that is down to 18.5 m). This is, referring to the example above, the equivalent to provide a point probe measurement by specifying its position as 10.0 cm depth, while the measured volume actually has an extent of at least a centimeter (in the

350 vertical and lateral dimension). A reasonable size for a fixed circle, if requested alternatively, in this simple approach could be 10 ha = 0.1 km² and thus a radius of 178.4 m.

3.2 Working with a fixed vertical footprint size

With similar reasoning one could argue for using a fixed vertical footprint size, also called integration depth or penetration depth or D_{86}. It has been defined in an analogous way to the horizontal footprint definition and there is a strong weighting
355   towards the shallower depths. However, remote sensing observational products of water storage in the subsurface often are based also on a signal decaying with depth. Nevertheless, a value for a particular depth compartments is retrieved, ranging from surface soil moisture to terrestrial water storage, though this is neither precisely defined nor strictly the same everywhere. Thus, also CRNS-derived soil moisture could be attributed just to a product that could be characterized as root-zone soil moisture. As such, this represents the top decimeters of soil water storage and is an order of magnitude larger than
360   satellite remote sensing observations of surface soil moisture. Real depth information about soil moisture distribution as time series could be obtained instead by soil moisture profile measurements, though these profiles will also vary not only with time but also with location and a field-scale average is not easy to obtain, as requiring a number of profile probes, such as reported by Heistermann et al. (2023), or a soil moisture sensor network, such as reported by Bogena et al. (2010), to be installed permanently.

365   If there is such soil moisture profile information available as time series covering CRNS observation periods, this information can also be used to distort the inherently vertically weighted soil moisture derived from CRNS (Scheiffele et al., 2020, 2025). Even a single profile can be sufficient to do so, especially when close to the CRNS detector. The profile information is used to estimate a correction factor, as a time series according to the desired times of the CRNS evaluation, defined as the CRNS-weighted profile average divided be the non-weighted average (Fig. 4). This is a useful option when a
370   root-soil zone moisture product shall be derived in a simple way or if users are interested in the overall water pool present in the vertical footprint. A root-zone soil moisture product from CRNS with this correction should be more representative for this compartment as a whole than without. This should be relevant for straightforward comparison with models, for CRNS networks (Heistermann et al., 2023; Altdorff et al., 2024) or for direct individual use at a location in an applied context.
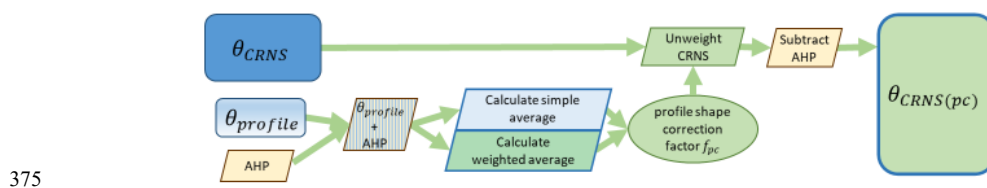

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Figure 4: Procedure to obtain a soil moisture that does not contain the inherent weighting of CNRS anymore; adapted from Scheiffele et al. (2020).

3.3 Need for standardization and other adaptations

Aiming for easing CRNS applicability there seem to be some relatively simple improvements that are listed in the following
380   i.   Standardize the way that parameters are taken for correcting neutron count rates; e.g. a reference air pressure taken as a global mean may be off for sites at higher altitude and cause correction factors to be far from 1. This could transfer into other values for calibration parameters and hinder comparability. Ideally correction factors during long time-series should vary around 1 and have a mean of close to 1.0 (with exception of the biomass correction). If we use reference parameters according to a common procedure this would improve the situation, for example taking P_0
385   in the air pressure correction (Zreda et al., 2012; Bogena et al., 2020) as the mean air pressure of the site during beginning of 2010 until end of 2019. Such a common reference period should be feasible, and the values could be taken from the weather station nearest to the site, and some gaps in the record should not be a problem.
        ii.   Standardize the definition of the correction factors as some of them have been defined in inverse forms sometimes (cf. for example Zreda et al. (2012), Hawdon et al. (2014), Andreasen et al. (2017) and McJannet and Desilets

390 (2023)). This could lead to errors in handling. Suggestions are to define all correction factors as product that has to be multiplied with the raw cosmic-ray neutron count rates to obtain the corrected ones as in some recent work (Bogena et al., 2022; McJannet and Desilets, 2023; Heistermann et al., 2024).

 iii. The formula for integration depth D_{86} (Köhli et al., 2015) seems not to be suited for low-density and/or soils with extremely high soil moisture levels (e.g. peatlands), such as in Fig. 1 (top left) and gives unrealistically large values.

395 As this was derived rather for standard bulk densities an extension of different existing formulas providing a penetration depth estimate (Franz et al., 2013a; Baroni and Oswald, 2015; Köhli et al., 2015) to low bulk density (and very wet) soils and testing would be beneficial. A first step in this direction has been presented in a preprint by Kasner et al. (2022).

 iv. It could be recommended to obtain at least one profile of soil moisture measurement as time series accompanying

400 the CRNS observation, to create the basis for retrieving an unweighted soil moisture product from CRNS. Installation should be close to the CRNS detector, as the contribution to the signal will be high there, and the most practical position being not a separate obstacle for management and the option to have the data recorded to the data logger of the CRNS station. This seems to be a cost-efficient enhancement of CRNS stations compared to the costs for a basis CRNS station, even if those costs have halved in the last decade and may continue to decrease,

405 fortunately for its users and a widespread application.

4 Discussion

As the main developments presented is a reformulation of the *Desilets* equation the essential limitations and possible shortcomings are the ones of this equation itself. While there may be alternative approaches that could be more accurate in some respects at least, such as the one presented by Köhli et al. (2021), this is something that has to be demonstrated, and

410 themselves potentially could also modified to account for a clearer representation of missing neutrons and more directly meaningful calibration parameters. As long as the *Desilets* equation is used for a CRNS observation the framework presented here could be applied without additional impairment.

The simple, direct calibration approach presented could be attractive for long CRNS time series with strong dry and/or wet ends. CRNS detectors could even be placed initially at the site close to a water body for some time, or even on it as in

415 Schrön et al. (2024), to include wet end values allowing for a calibration via determining N_{bg}. At the other end, locations with long dry periods or even deserts ~~count rates,~~ are suited for this alternative calibration approach, ~~then~~ via determining N_{max}. Clearly, there will be some uncertainty in how close these calibration parameter levels shall be taken to the time series values, and site conditions should be taken into account for that, such as how high is the soil moisture during saturation for the wet end or how much AHPs (lattice water, soil organic carbon) are present to contribute to the gap at the dry end.

420 However, it is possible to do so as soft information, and the result may be better than the one from a low-key field sampling for local calibration or when CRNS detector sensitivity has to be estimated for applying the general calibration approach suggested by Heistermann et al. (2024), or this sensitivity has crossly changed due to hardware or firmware changes to the CRNS station. Notwithstanding, it is not meant as a replacement for these existing approaches, but as a pragmatic alternative if those are not feasible or necessary. For short CRNS times series and/or sites with corrected neutron count rates limited to a

425 medium range due to soil moisture conditions being overall not at extreme~~r~~ ends the N_{max} - N_{bg} window variant could still be used, but certainly will have high uncertainties and may just be better than not having a calibration at all.

If measured or estimated values for lattice or soil organic matter water equivalents are available, they can be included instead of implicitly accounting for them in fitting N_{max} by using the modified a_2 parameter to obtain a more accurate absolute soil moisture value (cf. Eq. (3d)). For conversion into volumetric soil moisture values inherently there is the need to measure (or

430 estimate) local bulk density, for all three named calibration methods, but for the calibration approach presented here it may

be the only one, except the information of the CRNS time series itself as having explored soil moisture ranges at the particular site.

For incorporating statistical uncertainties of corrected neutron count rates in improved form further work and accounting for local conditions will be needed. The presence of strong soil moisture heterogeneities can contribute to the statistical

435 uncertainty in the signal and thus the variability of corrected neutron count rates besides the variability of the incoming showers. Its relative contribution can also be reduced by longer time periods of integrating or higher sensitivity CRNS detectors, both implying more neutrons having explored soil moisture and either being stopped (and missing) or making it into the detector. Whatsoever, for the mean signal we can quantify the resulting apparent soil moisture derived from CRNS for such heterogenous conditions by equations (11a) or (11b), and the latter should allow to approximate any given (or

440 desired) soil moisture distribution. However, the contribution of each soil moisture patch to this CRNS-derived soil moisture cannot be quantified directly for larger numbers of different soil moisture patches. For that a linearization of these equations would be needed or numerical neutron transport simulations for a particular site as in Schrön et al. (2023).

The concepts presented for defining the horizontal and vertical footprint of CRNS are meant as basis for further discussion towards enabling also more pragmatic handling of CRNS observations. Notwithstanding they could be used right away, for

445 example an agricultural research institute or farming cooperative could install a CRNS station inside a field of fitting size, taking some care on choosing an appropriate spot, and then associate the resulting soil moisture values with the water storage in the upper part of the soil down to the plough layer of the cropped field as such. This would be a pragmatic way not too different from how soil moisture point sensors are installed in a particular depth, making some compromise on the location, e.g. choosing another spot when a thick root or stone are hindering installation, or estimating what is the depth of that spot

450 when the soil surface is not really smooth. Possibly a soil moisture profile observation could be added to the CRNS station, and the results should be interesting, for example if the field is irrigated some times, and could also be used to unweight the CRNS-derived soil moisture. Clearly, other applications that need a more detailed understanding of mixed land use or terrain effects or deriving vertical fluxes from CRNS observations may well require more detailed interpretation and use of the CRNS data than taking a fixed size or representative area and a fixed integration depth. However, also those could benefit

455 from improvements in standardization of correction procedures and formulas for bulk density influence as suggested above.

5 Conclusions

With the developed reformulation of the *Desilets* equation and the simple calibration approach described a pragmatic procedure is available to perform long-term CRNS observation without much additional information needed, besides a local bulk density (if volumetric soil moisture is desired). This will not match more accurate calibration procedures but could be

460 useful if the compromise between effort and accuracy is towards minimizing the effort. And for periods in the CRNS time series after changes in the CRNS detector, its firmware or even a replacement of the type of sensor, which could invalidate an existing calibration, the calibration approach presented could be applied individually in these periods, if they are long enough to explore drier and/or wetter conditions.

Together with the concepts to associate the CRNS-derived soil moisture to a root-zone soil moisture product in the

465 represented area, may it be a land use unit or a pixel or grid cell, this could enhance the practical application of CRNS observations. Furthermore, a need for standardization in handling CRNS data was addressed exemplarily, which is a timely task for the CRNS community to take care of. This should be beneficial also when providing software tools (e.g. Power et al., 2021) that could open doors for a broader, more efficient and better reproducible correction of CRNS raw data, their calibration and use in research as well as applications by authorities or stakeholders. Given the considerations on statistical

470 deviations a conclusion could be to usually work with daily values if standard CRNS detectors such as the CRS 1000 are used for observations of soil moisture. Also, in respect to CRNS networks to be established and the link to modelling or

remote sensing the pragmatic definitions of the support volume and calibration could be at least a starting point before higher-level procedures, with higher effort needed, could be deployed.

Data availability

475 No experimental data have been retrieved within this mathematical and conceptual study. Data used to exemplify concepts are publicly available, at least as raw data, or upon considerate request to the author.

Competing interests

The author declares that he has no conflict of interest.

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