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Investigating temporal field sampling strategies for site-specific calibration of three soil moisture – neutron intensity parameterisation methods

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Abstract

The Cosmic-Ray Neutron Sensor (CRNS) can provide soil moisture information at scales relevant to hydrometeorological modeling applications. Site-specific calibration is needed to translate CRNS neutron intensities into sensor footprint average soil moisture contents. We investigated temporal sampling strategies for calibration of three CRNS parameterisations (modified N_0, HMF, and COSMIC) by assessing the effects of the number of sampling days and soil wetness conditions on the performance of the calibration results, for three sites with distinct climate and land use: a semi-arid site, a temperate grassland and a temperate forest. When calibrated with a year of data, COSMIC performed relatively good at all three sites, and the modified N_0 method performed best at the two humid sites. It is advisable to collect soil moisture samples on more than a single day regardless of which parameterisation is used. In any case, sampling on more than ten days would, despite the strong increase in work effort, improve calibration results only little. COSMIC needed the least number of days at each site. At the semi-arid site, the $N_{0\mathrm{mod}}$ method was calibrated better under average wetness conditions, whereas HMF and COSMIC were calibrated better under drier conditions. Average soil wetness condition gave better calibration results at the two humid sites. The calibration results for the HMF method were better when calibrated with combinations of days with similar soil wetness conditions, opposed to $N_{0\mathrm{mod}}$ and COSMIC, which profited from using days with distinct wetness conditions. The outcomes of this study can be used by researchers as a CRNS calibration strategy guideline.

1 Introduction

Soil moisture is an important state variable in land-atmosphere interaction processes (Robinson et al., 2008), ecosystem structure, function, and diversity (especially in drylands, Rodriguez-Iturbe and Porporato, 2004), and a key factor in agriculture (Siebert et al., 2005; Robinson et al., 2008; Seneviratne et al., 2010). Traditionally, soil moisture content has been measured mainly with point-scale sensors (~ 2 dm) (Topp and Ferré, 2002) or satellite sensors (e.g. Soil Moisture and Ocean Salinity (SMOS), Kerr et al., 2001) (2500–25 000 km^2), leaving a gap at intermediate scales (~ 1 km, Wood et al., 2011) relevant to hydrometeorological modeling and applications, and small watershed scale studies (0.1–80 km^2) (Robinson et al., 2008; Vereecken et al., 2008).

A novel technology that may help fill this scale gap, is the Cosmic-Ray Neutron Sensor (CRNS) (Zreda et al., 2008, 2012). The CRNS detects fast neutrons, which are produced from attenuated high-energy neutrons of cosmic origin and are attenuated further as they travel through the soil (Hess et al., 1961; Desilets and Zreda, 2001; Zreda et al., 2008). Because of the high attenuation power of hydrogen for these cosmic-ray neutrons, fast neutron intensity decreases with increasing hydrogen amount within the sensor footprint (Zreda et al., 2008). Through this inverse relationship with hydrogen prevalence, fast neutron intensity is non-linearly related with soil moisture content (Kodama et al., 1985; Zreda et al., 2008). The sensor footprint has a horizontal diameter of about 600 m at sea level (Desilets and Zreda, 2013) and a measurement depth that varies between about 12 (wet conditions) and 76 cm (dry conditions) (Desilets et al., 2010).

Site-specific neutron intensity – soil moisture relationships should be determined to derive soil moisture values, i.e. the CRNS needs site-specific calibration. The fully empirical N_0 formula (Desilets et al., 2010) is usually deployed for this calibration (Zreda et al., 2012). However, not only soil moisture content affects the fast neutron intensity (Franz et al., 2013c). All other hydrogen pools, (e.g. biomass, snow) affect the signal, complicating the finding of a unique relationship between neutron intensity and soil moisture content for a variety of sites and conditions (Zreda et al., 2012). Therefore a universal calibration function, the Hydrogen Molar Fraction method (HMF), was developed, which assumes a relationship between hydrogen prevalence and neutron intensity (Franz et al., 2013b). While N_0 and HMF both calculate an integrated, depth-weighted profile average soil moisture content, the COsmic-ray Soil Moisture Interaction Code (COSMIC) computes neutron intensities from soil moisture profiles (Shuttleworth et al., 2013) and can be directly applied in the context of hydrometeorological data assimilation (Rosolem et al., 2014).

It is usually assumed that only one parameter of N_0 needs to be calibrated, and that this can be achieved by using a single calibration point constructed from soil moisture profiles measured on a single day (Zreda et al., 2012), whereas for HMF estimations of additional hydrogen sources are also needed (Franz et al., 2013b). Originally, COSMIC was site-calibrated against neutron particle transport model Monte Carlo N-Particle eXtended (MCNPX, Pelowitz, 2005), using 22 hypothetical profiles covering a range of possible soil moisture profiles, but weighted towards the more probable profiles at each considered site (Shuttleworth et al., 2013).

Although a number of investigations have used single calibration points from measured soil moisture profiles for each of the three methods (Rivera Villarreyes et al., 2011; Zreda et al., 2012; Franz et al., 2013c; Bogena et al., 2013; Baatz et al., 2014), to our record, there has been no previous study on whether this is feasible for each of these three methods at distinct sites. The fact that hydrogen pools (e.g. biomass, litter layer water) vary differently over time than soil moisture content profiles, and that not all these hydrogen pools can always be monitored completely and accurately (Bogena et al., 2013; Rivera Villarreyes et al., 2011), could be a complicating factor. Therefore we posed the following research questions:

- What are the benefits and limitations of the three different soil moisture – neutron intensity parameterisation methods (N_0, HMF and COSMIC) across sites with distinct climates and land cover types?

- How often should soil moisture profiles be sampled in order to reliably calibrate the three soil moisture – neutron intensity parameterisation methods?

- Under what type of wetness conditions or combinations of wetness conditions should soil moisture profiles be sampled in order to reliably calibrate the three soil moisture – neutron intensity parameterisation methods?

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In order to answer these questions, we calibrated the three parameterisation methods for three sites with distinct types of land cover and climate: a semi-arid, sparsely vegetated site, a humid grassland, and a humid spruce forest. We used data from 2012 to evaluate whether different days or different combinations of days would lead to different calibration results and to investigate our hypothesis that a single calibration day is not always sufficient. We used depth-weighted average soil moisture content to see whether wetness conditions affect calibration results, and whether combinations of days with different wetness conditions would yield different calibration results.

2 Materials and methods

2.1 Methodology

We calibrated the three methods with different numbers of sampling days: 1, 2, 4, 6, 10, and 16. The one day sampling strategy (1DAY) corresponds to using a single, randomly selected day within the time series to calibrate each method; the two days strategy (2DAY) is based on a pair of days randomly selected from the time series, and so on. We compared these temporal sampling strategies (see Table 1 for all abbreviations) with a reference strategy in which all available days from the year 2012 were used to calibrate the three methods. As a proxy for soil moisture samples, we used data from in-situ soil moisture sensor networks, because no year long series with daily soil moisture samples is usually available. Despite having slightly different uncertainties compared to gravimetric/volumetric soil samples obtained in the field, in-situ sensors have been already successfully used in previous studies for comparison of CRNS and smaller-scale soil moisture sensors (Franz et al., 2012; Bogena et al., 2013; Baatz et al., 2014).

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2.2 Site and data description

2.2.1 Santa Rita Creosote (SR)

Santa Rita Creosote (Table 2 and Fig. 1), hereinafter referred to as SR, is a semi-arid site in Arizona, USA (Scott et al., 1990), which is sparsely vegetated (~ 24 % of surface area) with Creosote bush (~ 14 % of surface area) and other species of bushes, grasses and cacti (Cavanaugh et al., 2011). Daytime temperatures above 35 °C in Summer and above 15 °C in Winter are common, and precipitation falls mostly in Summer and Winter (Scott et al., 1990; Franz et al., 2012). The soil texture can be characterised as sandy loam with 5 to 15 % gravel (Cavanaugh et al., 2011). At SR 18 paired in-situ sensor profiles, with sensors at 5, 10, 20, 30, 50 and 70 cm depth, were installed with the spatial distribution as described by Franz et al. (2012), with all equal horizontal weights. We computed a simple mean horizontal soil moisture content for each sensor layer on every day. In 2012, there were 362 days with available data.

2.2.2 Rollesbroich (RB)

Rollesbroich (Table 2 and Fig. 1), located in Germany and hereinafter referred to as RB, is a humid grassland site, dominated by rye grass and smooth meadow grass (Baatz et al., 2014). The seasonality in precipitation is small with on average 540 mm in Winter and 610 mm in Summer (DWD, 2014). Average temperatures are 4.9 °C in Winter and 10.9 °C in Summer (DWD, 2014). The soil contains mainly silt (~ 61 %) and some sand (~ 20 %) and clay (~ 18 %) (Qu et al., 2014). The in-situ sensor network (SoilNet, Qu et al., 2013, 2014) consisted of 83 profiles with soil moisture sensors installed at 5, 20, and 50 cm depth. While the sensor profiles at SR were positioned such that all had equal weights, this was not the case at RB, where we calculated horizontal average daily soil moisture contents by assigning weights to the sensor profiles representing their distance to the CRS, as described in Bogena et al. (2013). In 2012, there were 310 days with available data.

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2.2.3 Wüstebach (WB)

Wüstebach (Table 2 and Fig. 1), hereinafter referred to as WB, is a humid Norway Spruce (90 % of surface area) forest test site in Germany, with little undergrowth (Etmann, 2009; Baatz et al., 2014). The seasonality in precipitation is small with on average 550 mm in Winter and 650 mm in Summer (DWD, 2014). Average temperatures are 4.5 °C in Winter and 10.5 °C in Summer (DWD, 2014). The most prevalent soil texture is silty clay loam containing a substantial amount of course material in the deeper parts and a litter layer of variable depth (0.5 to 14 cm) (Bogena et al., 2014). 150 profiles with in-situ soil moisture sensors (SoilNet, Rosenbaum et al., 2012) at 5, 20, and 50 cm depth were installed. Horizontal averaging was done with the same distance-weighting method as for RB. Because snow layers complicate the interpretation of CRNS soil moisture estimates (Zreda et al., 2012), days with snow cover were omitted for both German sites, RB and WB (Baatz et al., 2014), while at SR no snow cover was recorded. In 2012, there were 280 days with available data.

2.2.4 CRNS and in-situ soil moisture data preprocessing

We corrected the CRNS observed neutron intensities at each site for variation in high-energy neutron intensity, atmospheric pressure and atmospheric water vapour content (Rosolem et al., 2013), following the suggestions of Zreda et al. (2012) and Baatz et al. (2014). To simulate a single day soil sampling campaign, we used daily average soil moisture contents from each in-situ soil moisture sensor layer and daily average neutron intensities (Fig. 2).

2.3 Soil moisture – cosmic-ray neutron parameterisations

2.3.1 Modified N_0 method

The N_0 method was originally developed by Desilets et al. (2010), using MCNPX. Bogena et al. (2013) introduced some changes to the N_0 method by taking into consider-

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ation dry soil bulk density to calculate the volumetric water content, and adding lattice water and soil organic matter water equivalent (Eq. 1):

$$\theta = \frac{a_0 \cdot \rho_s}{N_{pih}/N_0 - a_1} - a_2 \cdot \rho_s - \mathrm{lw} - w_{SOM}, \tag{1}$$

where the parameter values $a_0 = 0.0808\,(\mathrm{cm^3\,g^{-1}})$, $a_1 = 0.372\,(-)$, $a_2 = 0.115\,(\mathrm{cm^3\,g^{-1}})$, and N_0 (cph) is a site dependent normalisation parameter. Parameters lw and w_{SOM} are the CRNS-footprint average volumetric lattice water content and soil organic matter equivalent water content ($\mathrm{cm^3\,cm^{-3}}$) respectively, and ρ_s ($\mathrm{g\,cm^{-3}}$) is the dry soil bulk density, usually determined from soil samples. N_{pih} is corrected fast neutron intensity and θ is CRNS-footprint average volumetric soil moisture content ($\mathrm{cm^3}$ water $\mathrm{cm^{-3}}$ soil).

However, our preliminary results indicated that the N_0 method failed to accurately estimate the soil moisture measurements consistent to the sites (especially at SR; results not shown). The likely reason was the fixed coefficients defined in the equation, which was also found by Rivera Villarreyes et al. (2011). We therefore modified Eq. (1), giving Eq. (2).

$$N_{pih} = \frac{b_0 \cdot \rho_s}{\theta + \mathrm{lw} + w_{SOM} + b_2 \cdot \rho_s - b_1} \tag{2}$$

This equation contains parameters b_0 ($\mathrm{cph\,cm^3\,g^{-1}}$), b_1 (cph), and b_2 ($\mathrm{cm^3\,g^{-1}}$), which all need site-specific calibration. We hereinafter refer to this equation as the modified N_0 method (N_{0mod}). Also notice that, in order to better compare the results with the HMF and COSMIC methods, we have rearranged terms in the N_{0mod} formulation, so that neutron counts are calculated based on given soil moisture. We calculated depth-weighted profile average soil moisture contents with the methods proposed by Bogena et al. (2013).

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2.3.2 HMF method

The HMF method was first developed to avoid site-specific calibration of the CRNS where soil sampling is difficult and also to facilitate the application of the mobile cosmic-ray soil moisture sensors (i.e. rover applications) (Franz et al., 2013b). In such cases soil moisture could be calculated provided neutron intensity and other hydrogen sources are known. However, for sites for which reliable soil moisture samples can be obtained, the HMF method can also be used for site-specific calibration of the CRNS. In the HMF method, the fast neutron intensity is calculated with Eq. (3):

$$N_{\mathrm{pih}} = N_{\mathrm{s}} \cdot \{4.486 e^{(-48.1 \cdot \mathrm{hmf})} + 4.195 e^{(-6.181 \cdot \mathrm{hmf})}\}, \tag{3}$$

where hmf is $\sum(\mathrm{H})/\sum(E_{\mathrm{all}})$ is total hydrogen molar fraction (mol H/total mol). $\sum(\mathrm{H})$ is the sum of all hydrogen (mol), including hydrogen in above ground biomass, lattice water hydrogen, hydrogen in and bound to soil organic matter, and soil water hydrogen; and $\sum(E_{\mathrm{all}})$ (mol) is the sum of all elements: atmospheric N and O, soil solids (quartz), lattice water, soil organic matter water equivalent, soil water, above ground biomass (cellulose) and above ground biomass water. N_{s} (cph) is a normalisation parameter which needs to be site-calibrated.

We employed HMF following the same approach as done by Franz et al. (2013b), and calculated average profile soil moisture contents with the same depth weighting method used for the $N_{0\mathrm{mod}}$ method. We neglected root biomass, and litter layers. To calculate total amounts of chemical elements, we used a horizontal footprint radius of 335 m for all three sites (Franz et al., 2013b). We calculated measurement depths with the method from Bogena et al. (2013).

2.3.3 COSMIC

COSMIC was developed as a data assimilation forward operator, and is a simpler, computationally less expensive fast neutron transport model than MCNPX (Shuttleworth et al., 2013; Rosolem et al., 2014). COSMIC considers three processes: (1) exponential decay of high-energy neutron intensity with depth, (2) creation of fast neutrons as a consequence of collisions with soil and water particles and (3) exponential decay of fast neutrons while they travel upward from the place where they were created. COSMIC can be written as a single formula (Eq. 4):

$$N_{\mathrm{pih}} = N \int_0^{\infty} \left[e^{\left(-\left[\frac{m_{\mathrm{s}}(z)}{L_1} + \frac{m_{\mathrm{w}}(t,z)}{L_2}\right]\right)} \cdot \left[\alpha \rho_{\mathrm{s}} + \theta(t,z) + \mathrm{lw} + w_{\mathrm{SOM}}\right] \cdot \frac{2}{\pi} \cdot \int_0^{\frac{\pi}{2}} e^{\left(\frac{-1}{\cos(\beta)}\right) \cdot \left[\frac{m_{\mathrm{s}}(z)}{L_3} + \frac{m_{\mathrm{w}}(t,z)}{L_4}\right]} \mathrm{d}\beta \right] \mathrm{d}z, \tag{4}$$

where $\beta\,(-)$, $L_1 = 162.0\,(\mathrm{g\,cm^{-2}})$, $L_2 = 129.1\,(\mathrm{g\,cm^{-2}})$, and $L_4 = 3.16\,(\mathrm{g\,cm^{-2}})$ are universal parameter values, and $L_3\,(\mathrm{g\,cm^{-2}})$, N (cph), and $\alpha\,(-)$ are site dependent parameters. The parameters m_{w} and m_{s} are the integrated mass per unit area $(\mathrm{g\,cm^{-2}})$ of dry soil and water respectively and ρ_{s} and ρ_{w} are the dry soil bulk density and soil water density $(\mathrm{g\,cm^{-3}})$. In the original model, the soil water included soil moisture and lattice water (Shuttleworth et al., 2013), while Baatz et al. (2014) added soil organic matter water equivalent to this. We used an empirical relation with a high correlation ($r^2 = 0.995\,(-)$) between parameter L_3 and soil bulk density (ρ_{s}) (see Fig. 3) to derive values for L_3 at the three sites. Hence, we calibrated only parameters N and α in this study.

2.4 Calibration methodology

To investigate the first research question (What are the benefits and limitations of the three parameterisations across distinct climates and land cover types?), we introduced a reference temporal strategy: for each site, we calibrated each parameterisation using all available days of the year 2012. This yielded nine best solutions (one parameter set for each site/parameterisation combination), against which we compared the results from the six lower order temporal strategies (Table 1). We calibrated the parameterisations, for the 1DAY strategy, for each site, for each day of the year, resulting in as many calibration solutions as there were days with data (e.g. 362 for SR). While we could calibrate the parameterisations for the 2DAY temporal strategy for all possible combinations of different days (e.g. 65 000 for SR), for the higher order strategies this would, in theory, have resulted in an impractical number of combinations and consequently be highly expensive computationally (Table 1). Therefore, we drew random samples of day combinations, equal in size to the total number of combinations of the 2DAY strategy (e.g. 65 000 for SR), from the populations of possible combinations. To investigate whether the chosen sample sizes were sufficiently large, we drew for each parameterisation and each site, for the 4DAY and 16DAY strategies, four extra random samples of the same size. Additionally, we drew samples with different numbers of day combinations (500, 5 000, 50 000, 200 000, 1 000 000) for each parameterisation at each site. The results of both tests (not shown) indicated that using a sample of sizes 65 000, 47 895, and 39 060 for respectively SR, RB, and WB was sufficient for our analyses.

To determine parameter calibration ranges for the $N_{0\text{mod}}$ method, we first applied relatively wide ranges (b_0: 25–1000, b_1: 10–3000, and b_2: 0.01–1.0) based on the original values of parameters a_0, a_1, and a_2 and values of N_0 from the COsmic-ray Soil Moisture Observing System (COSMOS) (Zreda et al., 2012; data available at http://cosmos.hwr.arizona.edu/) and Baatz et al. (2014). Using the initial ranges, we calibrated the $N_{0\text{mod}}$ method against soil moisture content – neutron intensity combinations obtained from COSMIC simulations for each of these sites. We used a range ($\theta = 0.00 : 0.01 : 0.50\,\text{cm}^3\,\text{cm}^{-3}$) of homogeneous soil moisture profiles as input for COSMIC to calculate the neutron intensities for COSMOS sites from Shuttleworth et al. (2013) (except two volcanic Hawaïan sites) and the two German sites used in this study. We used COSMIC parameter values from calibration against MCNPX (Shuttleworth et al., 2013) for this purpose, and added the two German sites with parameter values from Baatz et al. (2014) because these showed, in contrast with the COSMOS sites,

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neutron intensities below 750 (cph). The resulting parameter ranges were smaller than the initial ranges and we created safe margins around them for use in our analyses (Table 3). We constructed a calibration range for HMF parameter N_s (Table 3) with safe margins around values reported by Franz et al. (2013b) and Baatz et al. (2014), and we based the parameter calibration ranges for COSMIC (Table 3) on the values found by Shuttleworth et al. (2013) and Baatz et al. (2014).

A total of 100 000 parameter sets were sampled from the parameter space of the N_{0mod} method, 5000 for the HMF-method and 200 000 for COSMIC, using Latin Hypercube Sampling (LHS). We ran the parameterisations with these generated parameter sets for each day, and simulated the neutron intensity. We calculated the Absolute Error (AE) for the 1DAY strategy, and the Mean Absolute Error (MAE) for the multiple day strategies. The best solution for each day was found by selecting the parameter set which gave the lowest AE or MAE. To compare the overall performance throughout the whole year of a given calibrated parameterisation, we computed the MAE over all available days (with respect to simulated and observed neutron intensities) of 2012, for each best solution, hereinafter referred to as $\mathrm{MAE}_{\mathrm{val}}$.

3 Results and discussion

3.1 Identification of strengths and weaknesses of the three parameterisations when calibrated against all available data

Figure 4 shows calibration results using all three parameterisations, at the three sites. The simulated neutron intensities closely matched the observed neutron intensities with relative errors ($\mathrm{MAE}_{\mathrm{val}}$ divided by mean neutron intensity) between 1.1 % (N_{0mod} at WB) and 1.9 % (HMF at SR). However, at SR, observed neutron intensities were systematically overestimated (by 20 to 160 cph) by all three parameterisations during the monsoon (mid July–mid September) and underestimated between mid November and mid December (by 40 to 170 cph). Additionally, from early January till half March

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COSMIC matched the observed fast neutron intensities well, while the two other parameterisations underestimated fast neutron intensity (by up to 80 cph for $N_{0\mathrm{mod}}$ and 105 cph for HMF). At RB $N_{0\mathrm{mod}}$ seemed to have yielded the best calibration result, while HMF, and to a lesser extend COSMIC, showed some periods of both over- and underestimation with absolute errors up to 35 cph. Finally, at WB the calibration solution for HMF seemed to have had most difficulty simulating the observed neutron intensities, and showed larger neutron intensity variation than the other two parameterisations (SD of 10.8 cph compared to 9.2 cph for the observations 7.2 cph for $N_{0\mathrm{mod}}$, and 7.7 cph for COSMIC). Although at SR more daily neutron intensity estimations were outside the observed uncertainty bounds (e.g. 67 % for HMF at SR and 9 % at WB), we note that this is due to the relatively lower uncertainty caused by the higher observed neutron intensities (Zreda et al., 2008). Overall $N_{0\mathrm{mod}}$ performed best at the two temperate sites, HMF showed poorest results at all three sites, and COSMIC performed best at the semi-arid site and the humid forest site, and average at the humid grassland site.

The periods of over/underestimation for all parameterisations at SR could be related to either the used data, or to deficiencies common to all three parameterisations. Insufficient corrections of the neutron intensities (e.g. water vapour correction) due to measurement errors in the data used (e.g. atmospheric states), or due to deficiencies of the used correction methods, could have yielded observed neutron intensities that could not be matched by any of the parameterisations. Errors or inaccuracies in the in-situ soil moisture data (e.g. failure of certain sensors), which would result in incorrect simulated neutron intensities, are also a possible cause. Instead of measurement errors, temporal variations in hydrogen pools, like biomass, intercepted water and temporally ponding water; which have not been taken into account, could be involved. The fact we did not find similar phenomena for RB and WB could possibly be due to the larger variation in wetness conditions caused by the limited vegetation cover, and higher variability in precipitation and temperature at SR.

The differences between the best solutions of the three parameterisations for certain periods, found at all three sites, might be related to differences in parameterisation complexity. Where COSMIC performed better compared to the two other methods, this indicates the benefits of explicitly resolving individual soil layers as opposed to using depth-weighted soil moisture as employed by the other two methods. The periods during which HMF performed worse compared to $N_{0\text{mod}}$ and COSMIC at RB and WB, might have been caused by insufficient estimation of the measurement depth, because HMF seems relatively sensitive to subtle changes in below-ground measurement volume.

To get a better idea of how good the best solutions from the reference strategy actually were, we compared them with calibration results obtained from previous research, see Fig. 5 and Table 4. The original N_0 solution (only parameter N_0 calibrated) for SR was taken from the COSMOS website (Zreda et al., 2012), for HMF from Franz et al. (2013a) and for COSMIC from the MCNPx calibrations from Shuttleworth et al. (2013). We took all original solutions for RB and WB from Baatz et al. (2014). Only parameter N was calibrated for COSMIC at RB and WB (Baatz et al., 2014), while parameters L_3 and α were computed with relationships from Shuttleworth et al. (2013). The original solutions matched the observed neutron intensities equally or less good compared to the best solutions from the reference strategy. The most striking difference is that N_0 at SR was not able to match the observed neutron intensities because of the shape of the neutron intensity- soil moisture relationship defined by parameters a_0, a_1, and a_2 (notice this was one of the main motivations for introducing the modified N_0 method, as discussion in Sect. 2.3.1). As mentioned in Sect. 2.3.1 for our preliminary results, this suggests that using these fixed parameter values should be avoided. At RB the original COSMIC solution was clearly worse than our reference strategy solution and at WB this occurred for HMF and COSMIC at WB.

To identify the reasons for the relatively worse performance of the original solutions of HMF and COSMIC at RB and WB, we compared these with calibration solutions for which we used the same single days, but with our model and calibration settings (in-situ soil moisture data, COSMIC with both parameters N and α calibrated). The differences between the original and reference solution of HMF seemed to have been caused by

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the chosen sampling days. The main cause for the systematic underestimations by COSMIC was that Baatz et al. (2014) calibrated only parameter N, since our solutions using the same days performed clearly better (MAE_{val} = 7.6 cph at RB; 5.0 cph at WB).

3.2 Assessing a suitable soil sampling frequency for the three methods

In Fig. 6, the 25, 50 and 75 percentiles of the MAE_{val} populations of best solutions are represented by dots, for each temporal strategy. The MAE_{val} values of the best solutions of the reference temporal strategy are indicated with coloured horizontal lines. This figure can be interpreted as such that 25 % of the best solutions of a population had an MAE_{val} equal to or smaller than the MAE_{val} of the 25 percentile, the 50 % best calibration solutions had values smaller than the 50 percentile MAE_{val}, etcetera. The MAE_{val} value of the 25 percentile hence tells us how good the better solutions were; a low value means the chance of obtaining a good solution was high. A MAE_{val} value for the 75 percentile closer to the 50 and 25 percentiles means the overall range of solutions was reduced, and hence the chance of obtaining a relatively poor performance due to calibration was relatively small.

We see that for the 1DAY strategy at SR, for all three percentiles, the MAE_{val} values of N_{0mod} were between 1.6 and 3 times higher than those of HMF and COSMIC. Subsequent increase of the used number of days, however, made the results of N_{0mod} approach those of HMF, and at 6DAY its MAE_{val} was less than 1.3 times higher than that of HMF. With increasing number of sampling days, the population range was reduced for all three parameterisations, and hence also the chance of obtaining poor solutions decreased. The differences between the temporal strategies were smallest for HMF at all three sites: between 1DAY and 16DAY MAE_{val} values of HMF got 1.5 to 1.7 times smaller while MAE_{val} values of e.g. COSMIC got 1.7 to 2.2 times smaller.

From the 75 percentiles we see that the MAE_{val} values for HMF decreased sharply (1.3 to 1.5 times lower) between the 1DAY and 4DAY strategies at SR, between 1DAY and 6DAY at RB, and between 1DAY and 10DAY at WB. The response for N_{0mod} and COSMIC flattened out around the 10DAY strategy, after between 1.4 and 2.2 times improvements in MAE_{val}. After these sharp decreases, little improvements (up to 1.2 times) were made by increasing the number of days to those of the reference solutions. From a fieldwork perspective, this means that despite the strong increase in work effort, only a small improvement in parameterisation quality will be gained. The quicker improvement (to relatively poor reference strategy solutions), and smaller differences between the temporal strategies, of HMF, could be due to the fact that HMF contains only one free parameter.

To get a better idea of how many sampling days were needed to obtain a sufficiently good calibration result for each parameterisation at each site, we compared with mean values (indicated with horizontal black lines in Fig. 6) of the reference and original solutions for each site. We used this approach to acknowledge the best possible solutions obtained when sampling up to the maximal available calibration days of a year, as well as previously used calibration results (Shuttleworth et al., 2013; Franz et al., 2013b; Baatz et al., 2014). If we look, for example, at the 75 percentile (hence assuming a 75 % chance of obtaining a calibration result equal to, or better than the threshold sufficiently reduces the uncertainty), at SR between ten and sixteen days would be needed for $N_{0\text{mod}}$, between six and ten for HMF and between two and four for COSMIC. $N_{0\text{mod}}$ and COSMIC needed between six and ten days at RB, while HMF could not meet the threshold because of its relatively poor reference strategy solution. $N_{0\text{mod}}$ and HMF needed between six and ten days at WB, while COSMIC needed between four and six days. COSMIC hence needed the least number of days at each site. These results mean that for COSMIC fewer soil moisture profiles (sampling days) are needed than the 22 MCNPX simulations used by Shuttleworth et al. (2013). While $N_{0\text{mod}}$ and HMF are often calibrated using a single calibration day only (Desilets et al., 2010; Zreda et al., 2012; Baatz et al., 2014), our results indicate this is insufficient. Visual inspection of simulated neutron series compared to observed neutron intensity uncertainty bounds (not shown) indicated that the thresholds used were relatively strict, especially at RB and WB.

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The distributions of the parameter values are shown in Figs. 7 and 8. The 75 percentile ranges of b_0 and b_1 were for all three sites, with increasing numbers of days, reduced in size by to two to four times, and approached the parameter values of the solutions of the reference strategy (Table 4). Instead, the range of b_2 at RB and WB did not change substantially, while it did at SR. This could mean this parameter relates to variation in wetness conditions and soil profile shapes, which were more extreme at SR. The 75 percentile parameter ranges of HMF and COSMIC converged towards the parameter values from the reference temporal strategy for all three sites.

In addition to the MAE_{val}, we evaluated the Coefficient of Determination (r^2; results not shown), and the mean bias (results not shown) with respect to the observed and simulated neutron intensities of all days of 2012. While the mean bias improved (decreased) clearly with increasing numbers of sampling day, for all sites and methods (up to twenty times smaller for reference solutions compared to 1DAY), r^2 remained nearly constant. These findings indicate that parameterisation dynamics, which are reflected in r^2, are more strongly conditioned by the input data whereas systematic biases can be caused by poor parameter selection. The found improvement of the MAE_{val} with increasing number of sampling days was hence due to reduced systematic biases. This is important, because systematic biases in soil moisture may hinder modeling applications (e.g. data assimilation, Dee, 2005).

Based on our results we do not reject our hypothesis that calibrating with individual days or combinations of days would lead to the different outcomes than when all days would be used. Calibrating with a single day is likely insufficient to guarantee accurate/acceptable parameterisation performance. That HMF showed least differences between few and many sampling days was probably caused by the fact that it has only one parameter that needs calibration. Moreover the reference strategy yielded relatively poor calibration results for HMF anyway. If the periods of systematic mismatch between HMF and the observed neutron intensities were caused by measurement errors, then HMF would require fewer days than our results indicate.

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The results for the reference strategy and the other sampling strategies indicate that N_{0mod} is more easily calibrated for sites with relatively low seasonality in temperature and precipitation. While the reference solutions of HMF were relatively poor, less days seemed needed to approach these. COSMIC performed relatively similar for sites with different vegetation cover, and precipitation and temperature variability.

3.3 Evaluating preferred wetness conditions for calibration

The required numbers of sampling days found in the previous section could possibly be reduced if certain wetness states that yield relatively poor calibration solutions are avoided, and preferred wetness states for good sampling days are chosen. To identify such preferred wetness states, we used depth-weighted average soil moisture content (Bogena et al., 2013) as indicator of wetness conditions. We used the Cumulative Density Function (CDF) approach as employed for parameter sensitivity analysis (Demaria et al., 2007), but instead applied it to soil moisture content states. We split the MAE_{val} populations into groups of 25 % increments, ranked from best (0–25 %) to worst (75–100 %). We calculated a CDF describing the distribution of weighted average soil moisture contents for each of the MAE_{val} groups for the 1DAY temporal strategy (Fig. 9). We computed CDFs describing the absolute difference between the soil moisture contents of the paired days for the 2DAY strategy (Fig. 10), while for the 4–16DAY strategies we used the SDs over the soil moisture contents of the combined days. Notice that all metrics are somewhat related to a dispersion measure from the mean value (or the mean value itself for 1DAY), and are hence related to each other. The figures can be understand by realising that at soil moisture contents where the CDF of a certain group is steep, relatively more solutions are obtained.

The CDFs of the 1DAY strategy showed differences between the worst 25 % solutions (75–100 %) and the other groups for all site-parameterisation combinations except N_{0mod} at WB. At SR relatively dry conditions seemed to yield a better chance of relatively good calibration solutions for HMF and COSMIC; for instance, 50 % (CDF = 0.5 (–)) of the solutions of the best 25 %-group of both param-

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eterisations had $\theta < 0.035\,\mathrm{cm^3\,cm^{-3}}$, while 50 % of the solutions of the worst 25 %-group had $\theta > 0.05\,\mathrm{cm^3\,cm^{-3}}$. Relatively dry to average wetness conditions ($0.03 < \theta < 0.04\,\mathrm{cm^3\,cm^{-3}}$) yielded relatively good calibration solutions for $N_{0\mathrm{mod}}$ at SR. The worst solutions (75–100 % groups) originated mostly from relatively dry conditions ($\theta < 0.35\,\mathrm{cm^3\,cm^{-3}}$) for all three parameterisations at RB, while the better solutions (0–75 % groups) were mostly obtained under average wetness conditions ($0.37 < \theta < 0.41\,\mathrm{cm^3\,cm^{-3}}$). At WB this was only the case for HMF and COSMIC. We therefore recommend to avoid relatively dry conditions at RB and WB and to sample under more average conditions instead. It is unlikely that the worse calibration solutions obtained under drier conditions at RB and WB were caused by changes in above ground hydrogen pools (e.g. litter layer), because Bogena et al. (2013) found such hydrogen pools become less dominant under drier conditions. Instead, this could be related to sensitivity of HMF to changes in measurement depth as discussed in Sect. 3.1.

The calibration for $N_{0\mathrm{mod}}$ and COSMIC at all three sites was improved when paired days with distinct soil moisture contents were used, because the CDFs of the groups of worst (50–75 and 75–100 %) calibration solutions showed relatively sharp increases for similar soil moisture contents (SR: $\Delta\theta < 0.01\,\mathrm{cm^3\,cm^{-3}}$; RB and WB: $\Delta\theta < 0.05\,\mathrm{cm^3\,cm^{-3}}$), whereas better solutions were obtained under relatively drier conditions (Fig. 10). This might be expected because different soil moisture profiles are taken into account, as well as variations in other hydrogen pools. HMF showed opposite results in all cases. The better solutions for HMF were relatively often obtained from combinations of days with similar wetness conditions (SR: $\Delta\theta < 0.015\,\mathrm{cm^3\,cm^{-3}}$, RB and WB: SR: $\Delta\theta < 0.05\,\mathrm{cm^3\,cm^{-3}}$). Figures 11 (4DAY) and 12 (16DAY) show that increasing the number of days decreased the effects of different wetness conditions of the constituting days. Similar to the 2DAY strategy, for the 4DAY strategy different wetness conditions were more likely to yield a relatively good calibration solution for $N_{0\mathrm{mod}}$ and COSMIC while for HMF the opposite behaviour was found again.

We could not identify a clear reason for the opposite effects of wetness variability on HMF compared to the other two parameterisations. No temporal variation in hydrogen

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pools other than soil moisture was taken into account, and for the 1DAY strategy HMF showed no overall preferred wetness states.

Based on our results, we can conclude that the required number of days could be limited by choosing appropriate wetness conditions, or wetness variability. However, this does not affect the numbers of days identified in Sect. 3.2 because differences were mostly limited to between the worst 25 and the 75 % best solutions, while in Sect. 3.2 we looked only at the 75 % best solutions to identify numbers of sampling days needed. The preferred choice depends on the site chosen and the parameterisation used and hence no general recommendation can be given.

4 Conclusions

We investigated the performance of three widely used CRNS parameterisation methods (modified N_0, HMF, and COSMIC) at three sites characterised by distinct climate and land use. When calibrated with data from all days available from one year, the COSMIC and $N_{0\mathrm{mod}}$ methods performed better than HMF at the two more temperate and humid sites, while at the semi-arid site COSMIC performed better than both other methods. The soil profile approach of COSMIC gave an advantage at the site with higher soil moisture variability.

We found that it is advisable to collect soil moisture samples on more than a single day regardless of which parameterisation is used. However, sampling on more than six to ten days would, despite the strong increase in work effort, improve parameterisation quality only little. COSMIC needed the least number of days to meet the set performance threshold at each site, which confirms the advantage of the soil profile approach. For instance, at the semi-arid site between two and four days were needed for COSMIC, while $N_{0\mathrm{mod}}$ and HMF needed between ten and sixteen days and between six and ten days respectively. COSMIC needed between four and six days at the humid forest site whereas the other two methods needed between six and ten days.

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Sampling on days or combinations of days with appropriate soil wetness conditions can reduce the required number of sampling days, and especially avoiding certain wetness conditions can decrease the chance of obtaining poor calibration results. The preferred choice depends on the site and the parameterisation used. At the semi-arid site, the N_{0mod} method was better calibrated better under average wetness conditions, whereas HMF and COSMIC were calibrated better under drier conditions. Average soil wetness condition gave higher chances for better calibration results for all three parameterisations at the humid grassland site, and for HMF and COSMIC at the humid forest site. We could not identify a preferred soil wetness condition for N_{0mod} at the humid forest site.

The calibration results for the HMF method were better when calibrated with combinations of days with similar soil wetness conditions, opposed to N_{0mod} and COSMIC, which profited from using days with distinct wetness conditions. These differences decreased with an increasing number of days, and were not found for the sixteen days sampling strategy.

By providing a first general guideline of how often and under which wetness conditions soil moisture should be sampled, the outcomes of this study will help researchers to validate old calibration results and to reliably calibrate new CRNS-sites and such as in the UK, as part of the AMUSED project (http://www.bris.ac.uk/news/2014/august/soil-moisture-and-cosmic-rays.html). Our discussion on differences between the three CRNS parameterisation methods can be used to identify which parameterisation can be used best to relate neutron intensities to footprint average soil moisture contents. Further work at additional sites is required to validate our conclusions.

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Table 1. Temporal sampling strategies and their theoretical numbers of combinations.

Strategy	Number of days from data series	Theoretical number of combinations for SR
1DAY	any 1 day	362
2DAY	any combination of 2 days	6.5×10^4
4DAY	any combination of 4 days	7.0×10^8
6DAY	any combination of 6 days	3.0×10^{12}
10DAY	any combination of 10 days	9.4×10^{18}
16DAY	any combination of 16 days	3.0×10^{27}

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Table 2. Some characteristics of the three study sites. Data for SR is from Shuttleworth et al. (2013); Franz et al. (2013b); Scott et al. (1990); Cavanaugh et al. (2011); WRCC (2006), data for RB and WB is from Baatz et al. (2014).

Site	Latitude (dec. degr.)	Longitude (dec. degr.)	Altitude (m a.s.l.)	P_{avg} (mm y^{-1})	T_{avg} (°C)	ρ_s (g cm^{-3})	lw + w_{SOM} (cm^3 cm^{-3})	AGB$_{wet}$ (kg m^{-2})
SR	31.9085° N	110.839° W	989	415	17.8	1.46	0.041	1.12
RB	50.6219° N	6.304° E	515	1300	7.9	1.09	0.067	0.70
WB	50.5035° N	6.333° E	615	1400	7.5	0.83	0.068	68.2

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Table 3. Parameter calibration ranges.

Method	parameter	lower bound	upper bound
N_{0mod}	b_0 (cph cm^3 g^{-1})	35	800
	b_1 (cph)	300	1700
	b_2 (cm^3 g^{-1})	0.02	0.15
HMF	N_s (cph)	200	2000
COSMIC	N (cph)	50	1500
	α (–)	0.2	0.4

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Table 4. Parameter values for the best solutions of the reference strategy (Ref.) and the original (Orig.) solutions. Parameters a_0, a_1 and a_2 are constants in N_0 and are hence not shown.

Site	N_{0mod}			N_0	HMF		COSMIC					
	b_0	b_1	b_2	N_0	N_s		N		α		L_3	
	Ref.			Orig.	Ref.	Orig.	Ref.	Orig	Ref.	Orig	Ref.	Orig
SR	122	1004	0.028	2945	870	862	469	390	0.200	0.251	113.5	114.8
RB	61	504	0.062	1208	478	479	247	213	0.201	0.293	76.6	76.6
WB	44	384	0.021	936	706	699	195	166	0.201	0.320	50.8	50.8

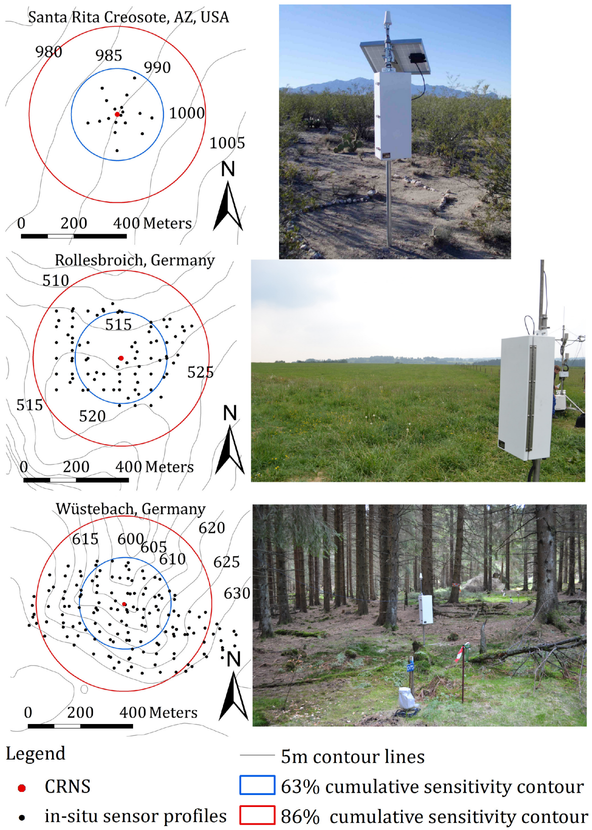

Figure 1. Maps and photos of the three research sites; Santa Rita Creosote (SR), Rollesbroich (RB) and Wüstebach (WB). The cumulative uncertainty contours indicate the relative areal contributions to the CRNS-signal. The 86 % contour represents the theoretical CRNS footprint (Zreda et al., 2008).

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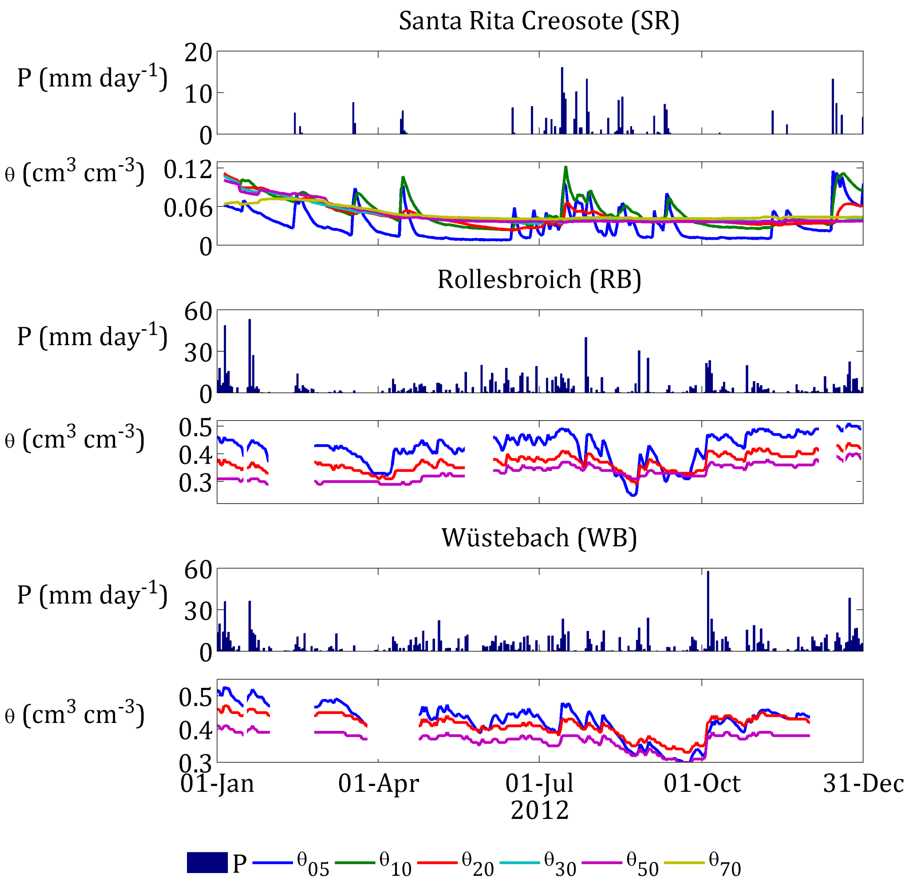

Figure 2. Precipitation, and in-situ sensor soil moisture content time series from the three research sites, for the used year 2012.

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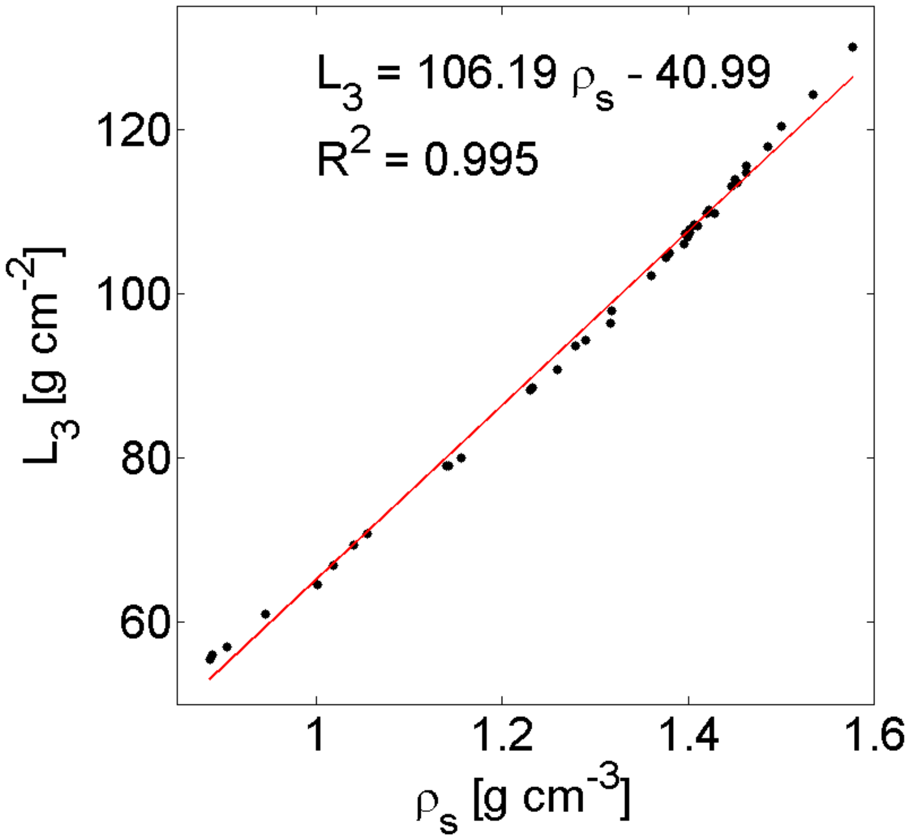

Figure 3. Relationship (red line) between soil bulk density ρ_s ($g\,cm^{-3}$) and COSMIC parameter L_3 ($g\,cm^{-2}$), adapted from Shuttleworth et al. (2013). Two volcanic Hawaïan sites from Shuttleworth et al. (2013) were ignored in this case because of their aberrant physical characteristics. The black dots represent the pairs of measured soil bulk densities and MCNPx calibrated L_3 values of the used sites.

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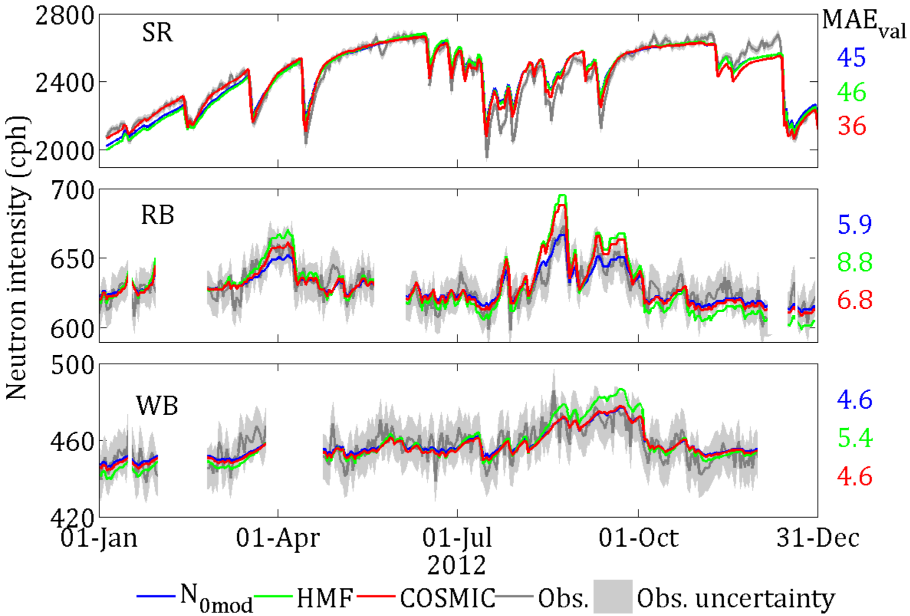

Figure 4. Neutron intensity time series for the calibration solutions from the reference strategy plotted with observed neutron intensities and observed neutron intensity uncertainty bounds. The uncertainty boundaries represent 95 %-confidence intervals around the mean daily fluxes (Zreda et al., 2008) MAE_{val} values of each parameterisation are shown in the same color as the neutron intensity time series.

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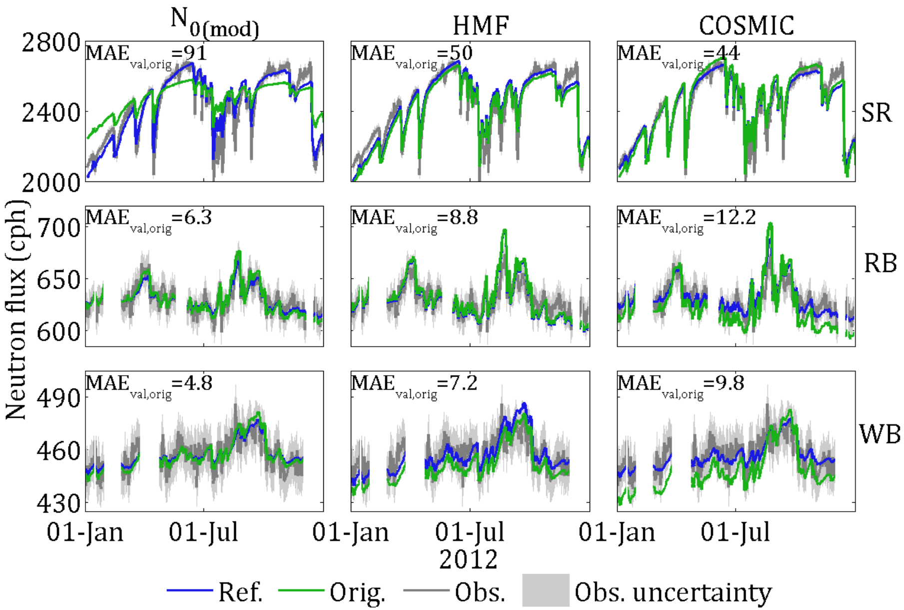

Figure 5. Neutron intensity time series for the calibration solutions from the reference strategy (Ref.) and from original (Orig.) calibration solutions plotted together with observed neutron intensities and associated uncertainty bounds. $MAE_{val,}$orig (cph) values for original solutions are included.

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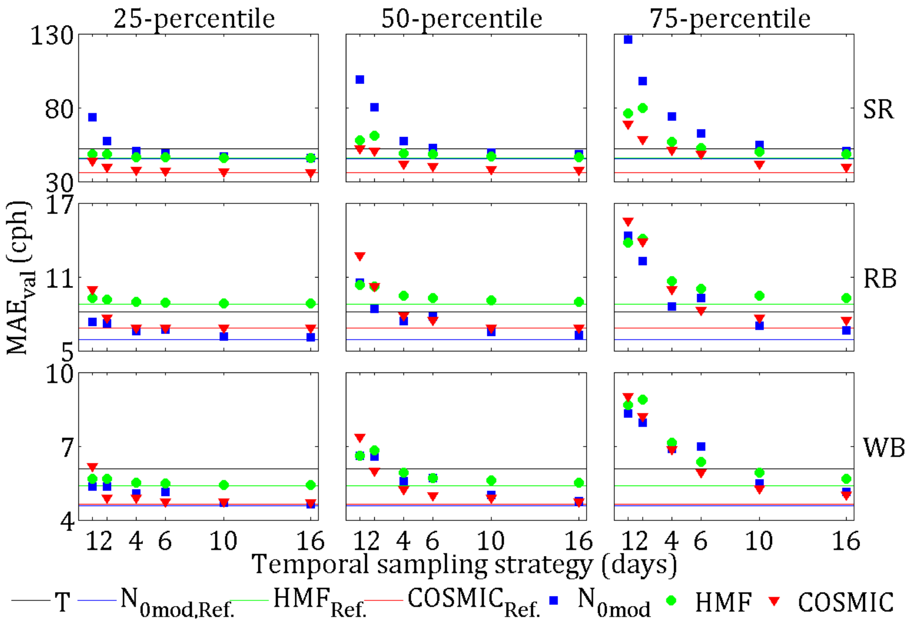

Figure 6. 25, 50 and 75 percentiles of MAE$_{val}$ best solution populations. The coloured horizontal lines represent the MAE$_{val}$ values of the calibration solutions from the reference strategy. The black horizontal lines represent thresholds (T) defined as the means of the reference strategy and original solutions for each site.

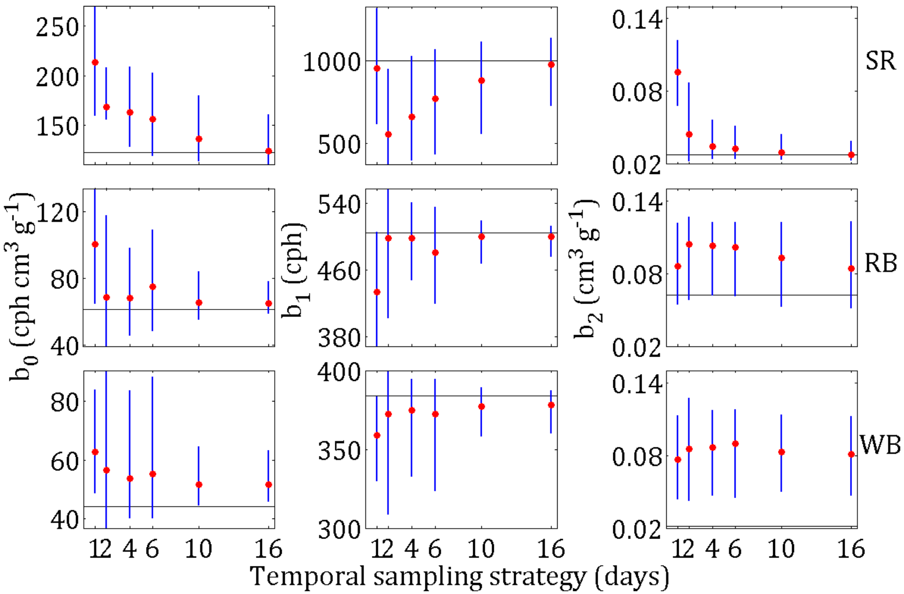

Figure 7. Boxplots showing, for each site, for each temporal sampling strategy, the interquartile ranges (vertical blue bars), and the medians (red dots) of the best solution populations of N_{0mod} parameters b_0, b_1, and b_2. The parameter values of the reference strategy solutions are represented by black horizontal lines.

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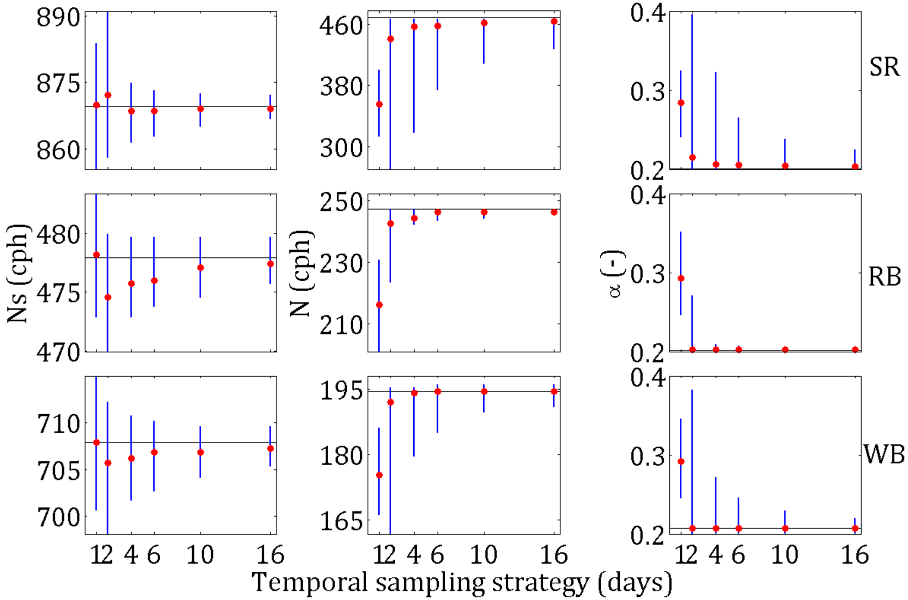

Figure 8. Boxplots showing, for each site, for each temporal sampling strategy, the interquartile ranges (vertical blue bars), and the medians (red dots) of the best solution populations of HMF parameter N_s (left column), and COSMIC parameters N, and α (middle and right columns). The parameter values of the reference strategy solutions are represented by black horizontal lines.

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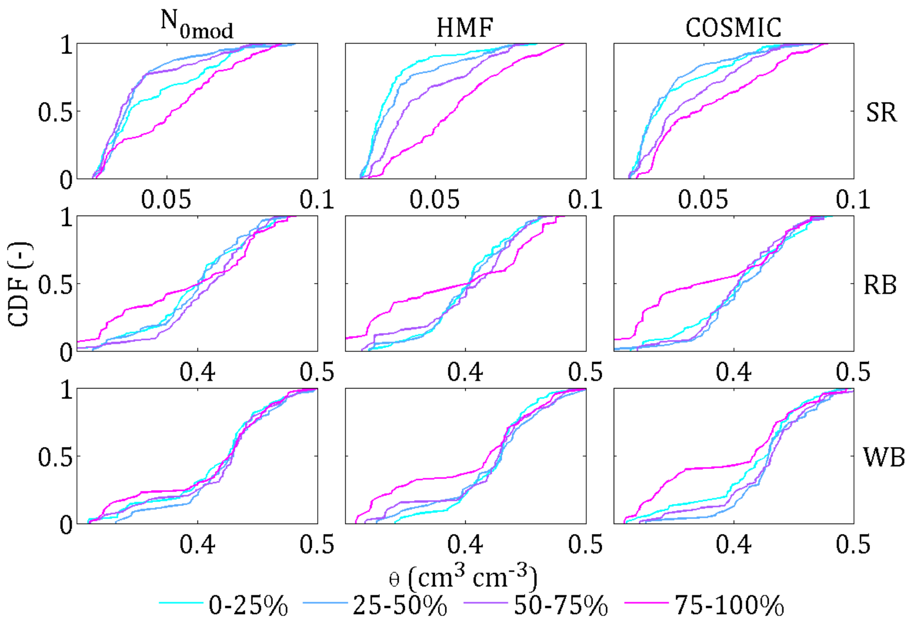

Figure 9. Cumulative Density Functions (CDF) of sub-groups from the 1DAY best solution MAE_{val} populations plotted against weighted average soil moisture content (θ) (Bogena et al., 2013).

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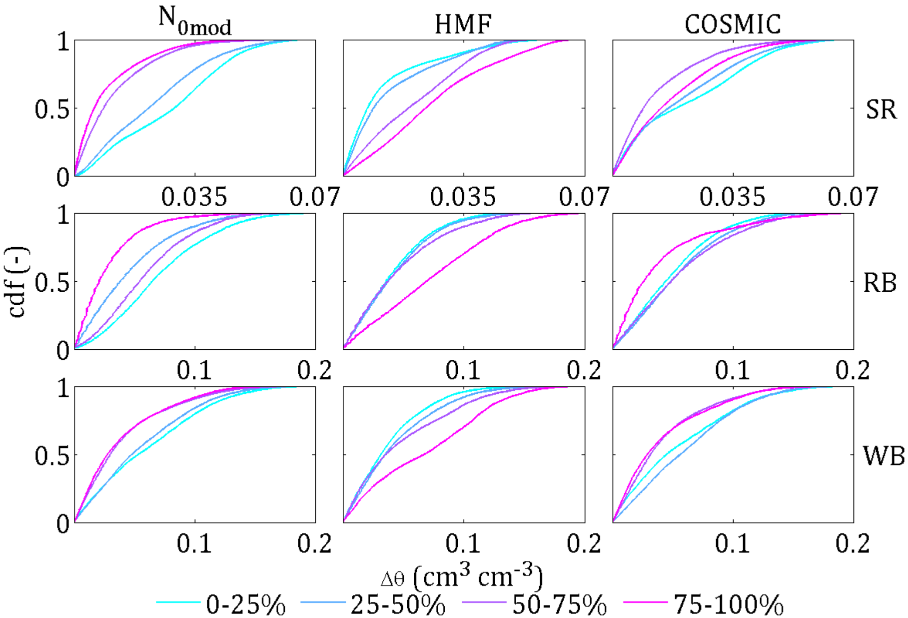

Figure 10. Cumulative Density Functions (CDF) of sub-groups from the 2DAY best solution MAE_{val} populations plotted against the difference (Δ) between the weighted average soil moisture contents (θ) of the paired days (Bogena et al., 2013).

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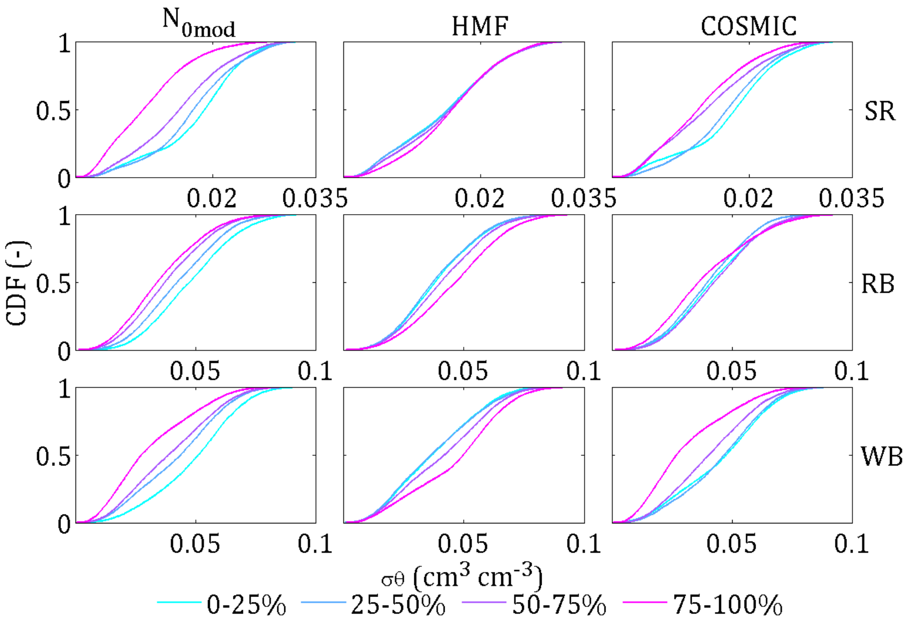

Figure 11. Cumulative Density Functions (CDF) of sub-groups from the 4DAY best solution MAE_{val} populations plotted against the SD (σ) of the weighted average soil moisture contents (θ) of the combined days (Bogena et al., 2013).

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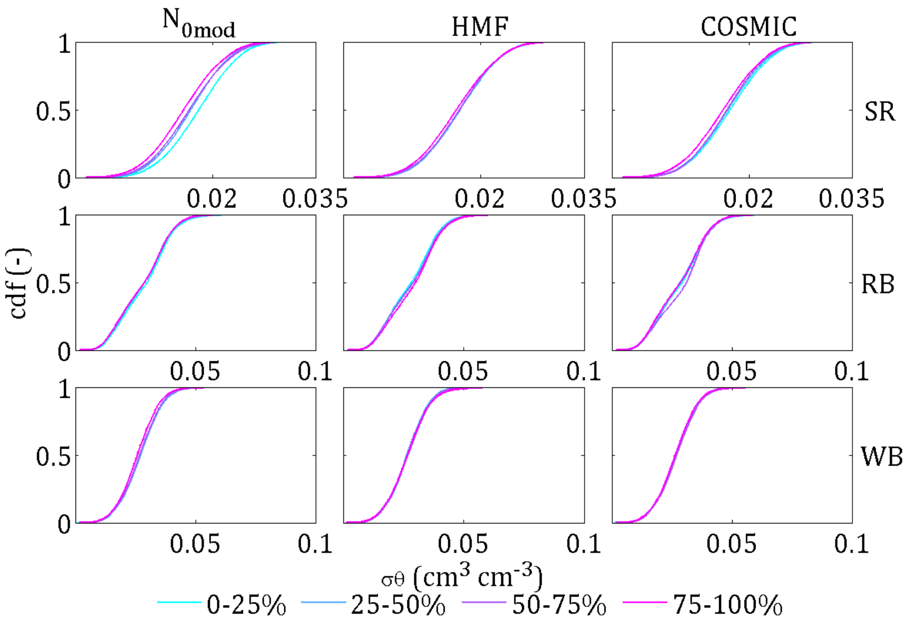

Figure 12. Cumulative Density Functions (CDF) of sub-groups from the 16DAY best solution MAE_{val} populations plotted against the SD (σ) of the weighted average soil moisture contents (θ) of the combined days (Bogena et al., 2013).