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Monte Carlo simulation and experimental validation of the Finapp Model 3 cosmic-ray neutron sensor

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Abstract

This work summarizes reference measurements, Monte Carlo (MC) particle transport modeling, and validation of the Finapp Model 3 cosmic-ray neutron sensor (CRNS). The MC calculations and reference measurements were performed independently in the broad-range radionuclide reference neutron fields of Czech Metrology Institute and Slovak Institute of Metrology. The validated model outputs were subsequently verified using monoenergetic neutron reference fields with energies ranging from 24 keV to 1.2 MeV at the Physikalisch-Technische Bundesanstalt, Germany, confirming the predicted response agreement within 13% of the experimental results. To demonstrate the applicability of the validated and verified models, they were used to predict the probe behavior in a virtual reference neutron field simulating realistic conditions with relative volumetric soil moisture levels ranging from 1% to 50%. The obtained results matched the Universal Transport Solution model across the whole soil moisture range. Single parameter power equation which, together with on-site calibration, can be used to convert the relative count rate of the Finapp 3 probe to volumetric soil moisture is proposed.

1. Introduction

Soil moisture is an essential climate variable (ECV) [1] whose effective monitoring is hampered by significant harmonization issues across different scales, particularly due to the systemic lack of metrological rigor applied to emerging intermediate-scale technologies like cosmic ray neutron sensing (CRNS) [2, 3].

The critical metrological gap is the lack of traceable validation for commercial CRNS probes, which has resulted in unknown detector response functions and compromised the physical grounding of neutron transport models used for crucial environmental corrections.

The SoMMet (Soil Moisture Metrology) project [4], funded by EURAMET (European Partnership on Metrology), provides the necessary metrological intervention by Monte Carlo (MC) modeling and testing of commercial CRNS probes in SI-traceable reference neutron fields maintained by National Metrology Institutes (NMIs). Such validated models are essential for quantifying and predicting the behavior of these devices in complex outdoor conditions.

2. Finapp Model 3 CRNS probe

This work summarizes the reference measurements, MC particle transport modeling, and validation of the Finapp Model 3 CRNS probe [5]. The MC calculations and reference measurements were performed independently in the broad-range radionuclide reference neutron fields of the Czech Metrology

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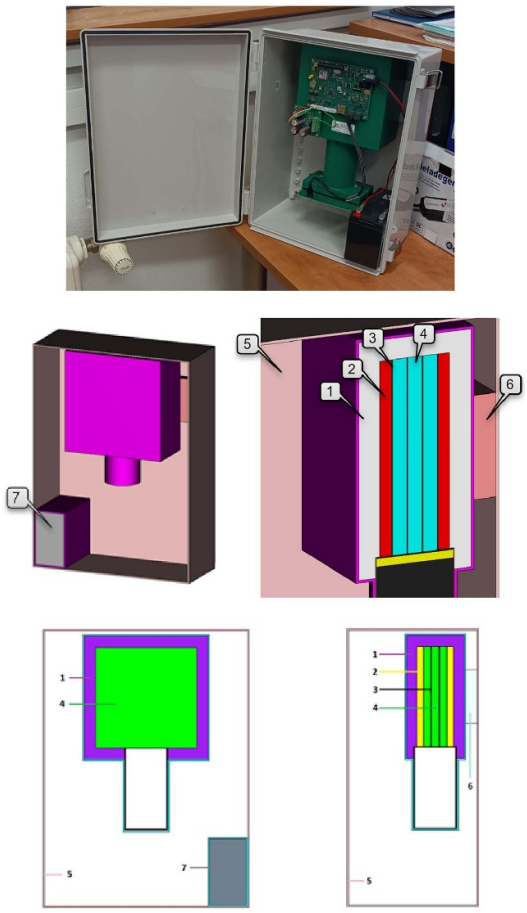


Figure 1. Photo of the Finapp 3 detector (top) and visualization of its MC model prepared by CMI (middle) and SMU (bottom). See text for the description.

Institute (CMI) and Slovak Institute of Metrology (SMU). A photography and both models are depicted in figure 1.

2.1. Description of the Finapp 3 MC model

The Finapp 3 device is built as a stack of four EJ-426 [6] scintillator layers interlayered by three EJ-280 [7] wavelength shifters connected to the photomultiplier tube at the bottom. The whole sandwich is covered by polyethylene and enclosed in a water proof plastic case.

The calculations were performed using the general-purpose particle transport codes MCNP6.3 [8] (CMI) and MCNP6.2 [9, 10] (SMU) with data library ENDF/B-VIII.0 [11] at temperature of 296 K (S(α,β) treatment of low energy neutrons). The composition of the main model parts follows (numbering corresponds to figure 1):

1. High-density Polyethylene; CH_2; density 0.97 g cm^{-3}
2. PVC; C_2H_3Cl; density 0.007 g cm^{-3} (CMI)
   EPS; C_8H_8; density 0.007 g cm^{-3} (SMU)
3. EJ-426 thermal neutron detector [6]; LiF:ZnS in ratio 1:3; density 1.544 g cm^{-3}
4. EJ-280 wavelength shifter [7]; Polyvinyltoluene; density 1.023 g cm^{-3}
5. PVC; C_2H_3Cl; density 1.406 g cm^{-3} (CMI)
   PP; C_3H_6; density 0.9 g cm^{-3} (SMU)
6. Al alloy EN-AW-5083; density 2.66 g cm^{-3} (CMI)
   Al alloy EN-AW-2024; density 2.78 g cm^{-3} (SMU)
7. Battery approx. by lead alloy; density 3.05 g cm^{-3} (CMI)
   Battery approx. by lead; density 11.35 g cm^{-3} (SMU).

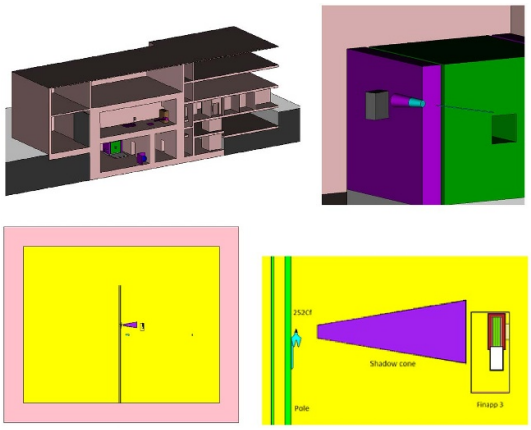


Figure 2. MC model of the CMI irradiation room (top left) and the detail with the Finapp 3 probe (top right) and SMU irradiation room (bottom left) and central detail (bottom right).

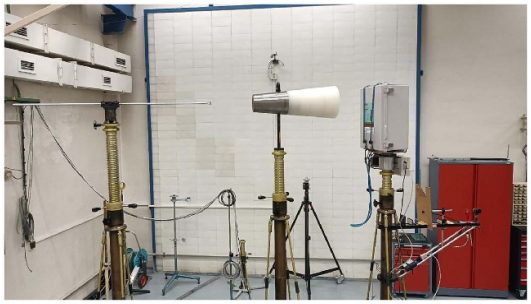


Figure 3. Example of irradiation setup of the Finapp 3 probe front irradiation by a ^{252}Cf neutron source with the shadow cone at a distance of 100 cm at CMI.

The calculated quantities were in both cases a number of ^{6}Li(n,α)T interactions, neutron absorption in scintillator, proton recoil counts in the scintillator, alphas and tritons in the scintillator (per sheet + total).

CRNS instrumentation is sensitive mostly to epithermal neutron energies [12] and the standardly used shadow cone method for correction of the instrument readings to the neutron scattering component is associated with very large uncertainties. Therefore, it was considered necessary to model not only the instrument but the whole irradiation room (see model on figure 2) as well.

2.2. Irradiations in the reference neutron fields

CRNS probes are designed to measure in environments where neutron fluence rate is in the order of 10^{-2} cm^{-2} s^{-1} with a resulting count rate of ∼1000 cph. However, neutron metrology laboratories standardly operate within the fluence rate range of 10^{2}–10^{4} cm^{-2} s^{-1} which is too high for testing. The optimal fluence rate for CRNS probe testing was found to be ∼0.5 cm^{-2} s^{-1} corresponding to ∼10 cps which require neutron sources with an emission rate of about 3 orders of magnitude lower than usually.

In order to benchmark the prepared MC models, it was necessary to obtain the reference data under different irradiation conditions. This was achieved by combining the following parameters:

- Am–Be and ^{252}Cf source type,
- direct irradiation and irradiation with a shadow cone,
- different detector orientation with respect to the source (front, side, top, bottom),
- source to detector distance from 75 cm up to 250 cm.

The CMI model was tested with 84 different combinations of irradiation conditions, and SMU used 44 different combinations. One example is shown in figure 3.

3. Validation of the Finapp 3 MC model

For each ith combination of irradiation conditions, the MC-calculation-to-measurement-ratio was calculated with the following formula:

$$S_i = \frac{M_i}{R_i/B},$$

where:

M_i is the MC calculated number of neutron absorptions in scintillator sheets per source neutron,
R_i is the Finapp 3 detector neutron channel rate [cps],
B is the neutron emission rate of the source used for irradiation [s^{-1}].

The average of the S_i was determined as:

$\bar{S}_{CMI} = 1.47 \pm 10\%$, $k = 1$ for the CMI model,
$\bar{S}_{SMU} = 1.29 \pm 13\%$, $k = 1$ for the SMU model.

The results show that the MC models predict by 47% (CMI) or 29% (SMU) more events than what was actually measured. This has been expected because MCNP calculations do not reflect all the influences in the detection chain (light collection efficiency, pulse shape discrimination (PSD) based neutron selection algorithm, etc.). The uncertainty of the average has the following main components:

- combined uncertainty of the emission rate B: ∼1%
- statistical uncertainty of MC calculation: ∼0.5%
- systematic uncertainty of the MC model: 2%–5%
- variation of the S_i average: 10%–12%.

These values were used to scale the results of MC calculations in order to get absolute responses under different irradiation conditions.

3.1. Verification of the validated MC model

The scaled predictions of MC models of Finapp 3 probes were subsequently verified using experimental results from the irradiation campaign in neutron reference fields of monoenergetic neutrons with energies ranging from 24 keV to 1.2 MeV at the PIAF [13] facility of Physikalisch-Technische Bundesanstalt (PTB), Germany—see figure 4.

Comparison of measured Finapp 3 detector responses per reference unit of neutron fluence rate to the output of MC calculations, scaled by a factor corresponding to CMI and SMU models, shows that both models agree with the experimental results within estimated uncertainties.

3.2. Energy response function of Finapp 3 probe

One of the applications of the validated MC models is to calculate quantities which are difficult or impossible to measure experimentally. A typical example in neutron metrology is the full-range energy response function—see figure 5.

However, in the case of CRNS probes, such a detailed energy response function cannot be directly used for the estimation of the instrument response at the different soil moisture conditions and it is necessary to use a different approach.

4. Example of the use of the validated MC model for environmental applications

To demonstrate the practical applicability of the validated MC models, they were used to predict the expected probe responses in a virtual reference neutron field simulating realistic conditions with relative volumetric soil moisture levels ranging from 1% to 50%.

4.1. Description of the virtual reference field

The MCNP transport code used for the laboratory characterization of the Finapp 3 probe is not optimized for environmental applications. Therefore, the transport of the cosmic neutrons through the atmosphere and in the soil was calculated by the URANOS (Ultra Rapid Adaptable Neutron-Only Simulation) [14] code v 1.25. Using the output of the URANOS calculations in MCNP, the concept of the virtual reference CRNS field is introduced with the following parameters.

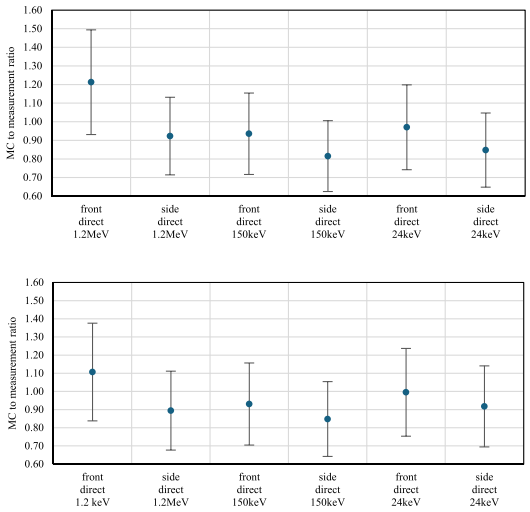


Figure 4. MC to measurement ratio from irradiation at the PIAF monoenergetic beam facility at PTB. CMI model (top) and SMU model (bottom). The error bars correspond to the $k = 2$, i.e. ∼95% coverage for normal distribution.

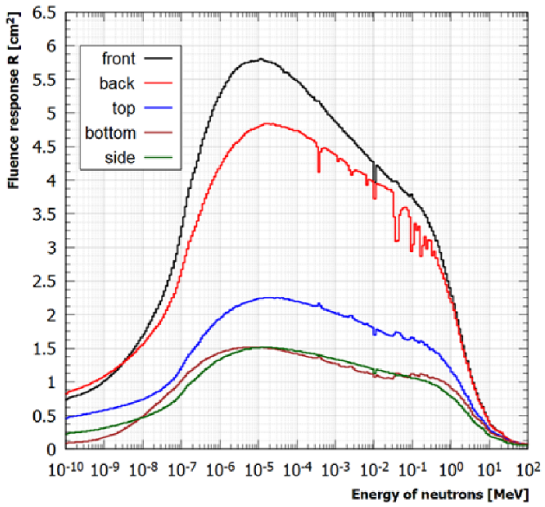


Figure 5. Response functions of Finapp 3 device for different irradiation directions calculated from SMU model.

4.1.1. Soil parameters

- Planar geometry with domain diameter: 800 m.
- Soil depth: 1.7 m.
- Soil consists of 50%$_{\text{Vol}}$ solids and a scalable amount of H_2O.
- The solid domain is comprised of 75%$_{\text{Vol}}$ SiO_2 and 25%$_{\text{Vol}}$ Al_2O_3 at a compound density of 2.86 g cm^{-3} [15].
- The total density depends on the volumetric water content.
- The 100% volumetric water content represents a theoretical case without solid domain in the soil, so that the whole 'soil' volume is composed of water.

4.1.2. Atmosphere parameters

- Thickness: 1600 m.
- 78%$_{\text{Vol}}$ nitrogen, 21%$_{\text{Vol}}$ oxygen, and 1%$_{\text{Vol}}$ argon at a pressure of 1020 mbar [15].
- Air humidity of 10 g m^{-3}.

4.1.3. Neutron source parameters

- Dimension (diameter) of the domain: 800 m.
- Source height: 650 m.

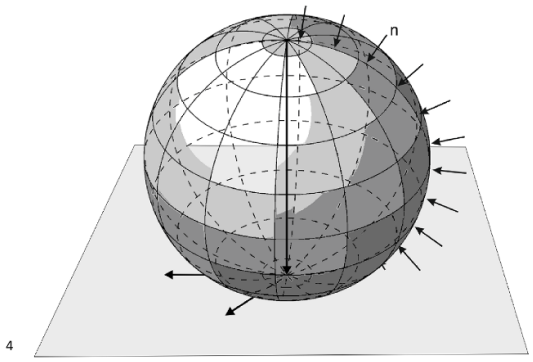


Figure 6. Virtual sphere, 2 m in diameter, used for the calculation of the reference CRNS neutron field used for the detailed MCNP calculation of CRNS probe responses.

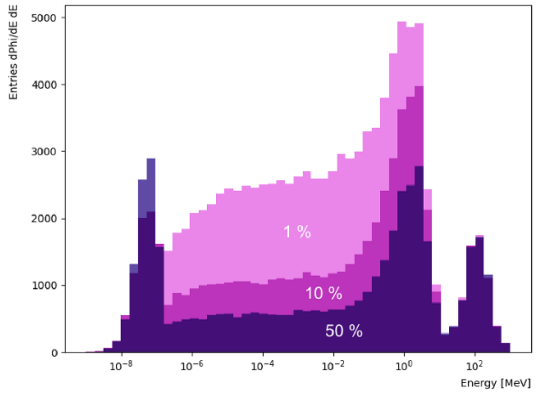


Figure 7. Neutron energy spectrum in the center of the virtual sphere for 1%, 10% and 50% volumetric water content.

- Source neutron energy and directional distribution [16, 17].
- Cutoff rigidity: 5 GV.

4.2. Neutron distribution on the virtual sphere

At the center of the domain and 1 m above the soil level, a virtual sphere 2 m in diameter was placed (see figure 6).

The following properties of each simulated neutron passing through the surface of this sphere were recorded forming the so-called 'Virtual reference CRNS neutron field': energy, intersection point with the sphere, directional vector, origin (for calculation of the footprint) and last interaction point before entering the sphere.

The footprint radius and the support volume depth, i.e. from where the CRNS probe sees the signal, changes with soil moisture. The typical range is from around 140 m to 240 m for the radius and 15 cm to 75 cm in depth [18].

In total, nine virtual CRNS reference neutron fields were calculated for different relative soil moistures expressed in terms of volumetric water content of 1%, 3%, 6%, 10%, 20%, 30%, 40%, 50% and 100%[5] and constant air humidity of 10 g m^{-3}.

The three examples of the energy spectrum of the neutrons entering the sphere are depicted in figure 7 for the same number of primary particles.

The influence of soil moisture is demonstrated by changes in the height of thermal and evaporation neutron peaks as well as a clear decrease in neutrons in the epithermal region with increasing soil moisture—the actual operation range of CRNS devices. The high energy neutron peak is not sensitive to soil moisture variations because it is composed of primary neutrons only.

[5] Theoretical case with no solid domain in the soil so that the whole 'soil' volume is composed of water.

Table 1. Finapp 3 detector response and relative response (rel. to 10% soil moisture) in different soil moisture virtual reference CRNS neutron field.

Volumetric soilmoisture [%]	R_{CMI} [counts per primary neutron $\times 10^{-9}$]	R_{CMI} (rel. to 10% soil moisture)	R_{SMU} [counts per neutron $\times 10^{-9}$]	R_{SMU} (rel. to 10% soil moisture)
1	30	1.99	35	2.03
3	22	1.44	25	1.46
6	18	1.19	21	1.19
10	**15**	**1.00**	**17**	**1.00**
20	13	0.86	15	0.86
30	10	0.69	12	0.69
40	9.9	0.66	11	0.64
50	9.3	0.62	11	0.62
100[a]	6.3	0.42	7.2	0.41

[a] Theoretical case with no solid domain in the soil so that the whole 'soil' volume is composed of water.

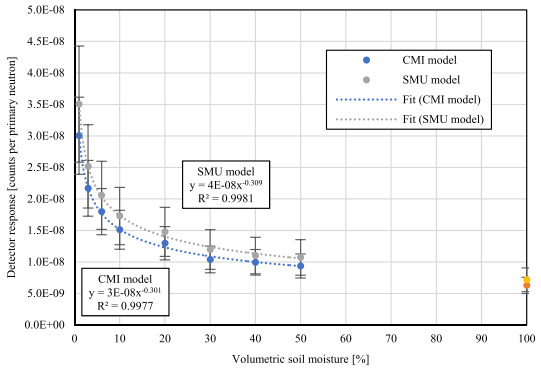


Figure 8. Finapp 3 detector responses calculated using CMI and SMU model and their fit. The error bars correspond to the $k = 2$, i.e. ∼95% coverage for normal distribution.

4.3. Finapp 3 response in virtual reference field

In the next step, the neutron fields calculated previously by URANOS (see section 4.1) were used as input (source definition) for MCNP calculation. The validated MCNP model of the Finapp 3 detector was placed in the center of the virtual sphere described in section 4.2 and irradiated by the virtual reference CRNS neutron field calculated for different volumetric soil moisture conditions.

The responses R normalized per one primary neutron of the URANOS calculation derived using both CMI and SMU validated MC models are summarized in table 1.

The calculated Finapp 3 detector responses normalized per primary neutron for both models are depicted in figure 8. Both models are equivalent within estimated uncertainties and can be reliably fitted (least squares) with a power function.

4.4. Comparison of the results to other available models

To determine the soil moisture in practice one needs to compare the detector response relatively to the response at known soil moisture conditions (obtained by a field calibration) both corrected for incoming neutron flux, air pressure and air humidity. Currently, several different models are used to determine soil moisture from the CRNS probes count rate. We have compared the MC model-based predictions to the following two models:

- N0 equation with the commonly used parameters 0.0808, 0.372, 0.115, recalculated to volumetric soil moisture, inverted and scaled relatively to 10% soil moisture [3]
- Universal Transport Solution (UTS) equation with a parameter set 'MCNP drf (full)' for air humidity of 10 g m^{-3} and scaled relatively to 10% soil moisture [19].

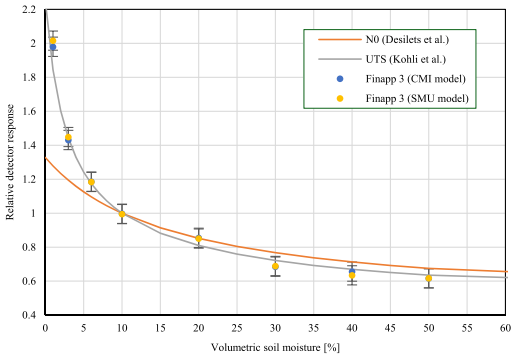


Figure 9. Comparison of the MC-based characterization of the Finapp 3 detector's relative response to different volumetric soil moistures to the two currently used models. The error bars correspond to the $k = 2$, i.e. ∼95% coverage for normal distribution.

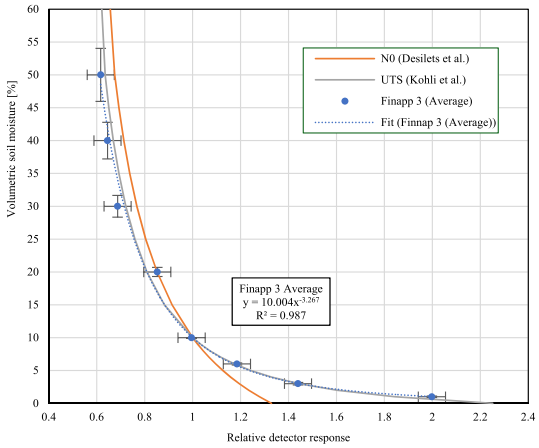


Figure 10. Soil moisture determined from the Finapp 3 relative detector responses (average of CMI and SMU model) calibrated at 10% volumetric soil moisture. The error bars correspond to the $k = 2$, i.e. ∼95% coverage for normal distribution.

The obtained results are depicted in figure 9. It is clear that the MC model-based predictions for the Finapp 3 detector show better agreement with the UTS model in the full range of volumetric soil moisture. The N0 model might work satisfactorily but only in the partial soil moisture interval depending on the used parameters.

Figure 9 demonstrates that the relative agreement of both MC models (0.4% in average) is much better than the absolute comparison shown on figure 8 (13% in average). This indicates that the difference in the absolute predictions of both models is not caused by differences in MC definitions (choice of materials, dimensions, densities, etc.) rather than the model validation procedure i.e. a different selection of irradiation conditions combinations used for the model validation at CMI and SMU (see section 2.2).

To determine soil moisture from the CRNS probe count rate one needs to obtain the inverse function of the intensity-to-soil-moisture-ratio. This is rather difficult for the complex multiparametric UTS model [19]. However, the analysis presented in section 4.3 demonstrates that the Finapp 3 relative response to soil moisture can be reliably fitted with a power function which is simple to invert analytically.

4.5. Determination of soil moisture from Finapp 3 relative count-rate measurements

Since the relative predictions of both CMI and SMU MC models are almost identical, for the further calculations we will use the average of the relative responses from table 1.

The graph of inverse functions to the one presented in figure 9 is shown in figure 10. The relative volumetric soil moisture θ can be determined from the Finapp 3 relative detector response using following equation:

$$\theta = \theta_{\mathrm{cal}} \cdot \left(\frac{N}{N_{\mathrm{cal}}}\right)^{p} = \frac{\theta_{\mathrm{cal}}}{N_{\mathrm{cal}}^{p}} \cdot N^{p},$$

where:

θ is volumetric soil moisture,
θ_{cal} is volumetric soil moisture at calibration conditions,
N is Finapp 3 count rate,
N_{cal} is Finapp 3 count rate at calibration conditions,
p is a fit parameter specific for a particular CRNS device, operating above soil with composition similar to section 4.1.

The fit parameter p determined from the average of CMI and SMU MC model calculated relative responses is:

$$p = -3.267 \pm 2.6\%,\ k = 1.$$

The standard error of the fit parameter p was determined by least square method.

The total uncertainty of the volumetric soil moisture determination in outdoor conditions will depend on the uncertainty of the calibration, Finapp 3 counting statistics, uncertainty of various corrections to environmental conditions and uncertainty of the determined p parameter. The contribution of the p parameter to the total uncertainty will depend on the distance between the measured soil moisture and soil moisture at the calibration conditions. For the probe calibrated at 10% volumetric soil moisture the p parameter will contribute up to ~10% to the total uncertainty in the whole measurement range.

5. Summary and conclusion

The Finapp Model 3 CRNS probe was metrologically characterized by means of validation and verification of the MC model at the reference neutron fields. The pertinence of the used method was supported by independent validation of two different models by primary metrology laboratories of CMI and SMU which were subsequently verified at primary monoenergetic neutron fields at PTB.

Both models were used to predict the Finapp 3 response in a virtual reference neutron field simulating realistic operation conditions with relative volumetric soil moisture levels from 1% to 50%. The absolute predictions of both models are equivalent within estimated uncertainties.

It was found that the relative predictions of both models are almost identical and in agreement with the UTS equation [19] and can be reliably fitted by a power function.

A single parameter formula for determination of the volumetric soil moisture from Finapp 3 probe count rate corrected for incoming neutron fluence was proposed. The fit parameter p determined from the average relative response in the virtual reference neutron field calculated by CMI and SMU MC models is:

$$p = -3.267 \pm 2.6\%,\ k = 1.$$

This parameter was determined for specific soil composition and landscape geometry described in section 4.1 and can be applied in practice under similar conditions.

This work in the framework of the SoMMet initiative will help to transform CRNS from a specialized hydrological tool with unknown uncertainty into a standardized, metrologically assured environmental monitoring system capable of delivering the high-quality, harmonized data required for the sustained assessment of soil moisture as an ECV.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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