Fiducial Reference Measurements for Soil Moisture (FRM4SM)

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DT2-1

FRM Protocols and Procedures for Soil Moisture (FPP-SM)

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Reference documents

Deliverable	Full name	availability
DT1-1	WP1 Technical Note — ISMN QC/flagging and R&D	https://www.geo.tuwien.ac.at/project-frm4sm/resources/documents/
DT3-1	QA4SM Software User Manual	https://www.geo.tuwien.ac.at/project-frm4sm/resources/documents/
DT4-3	QA4SM Evolution Verification Report	https://www.geo.tuwien.ac.at/project-frm4sm/resources/documents/

Acronyms

Acronym	Full name
AACES	Australian Airborne Cal/val Experiment for SMOS
AD	Applicable Document
AMMA-CATCH	African Monsoon Multidisciplinary Analysis – Coupling the Tropical Atmosphere and the Hydrological Cycle

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Acronym	**Full name**
ARM	Atmospheric Radiation Measurement Climate Research Facility
AWDN	Automated Weather Data Network (name of in-situ network in the USA)
BIEBRZA_S-1	Instytut Geodezji i Kartografii
BfG	German Federal Institute of Hydrology
BNZ-LTER	Bonanza Creek Long-Term Ecological Research
BMU	The German Ministry of Environment
BMVI	The Federal Ministry of Transport and Digital Infrastructure
CALABRIA	Name of in-situ network in Italy
CAMPANIA	Name of in-situ network in Italy
CARBOAFRICA	Name of in-situ network in Sudan
CCI	Climate Change Initiative
CEOP	Coordinated Energy and Water cycle Observations Project
CEOS LPV	Committee on Earth Observation Satellites (CEOS) Land Product Validation subgroup (LPV)
CHINA	Name of in-situ network in China
COSMOS	COsmic-ray Soil Moisture Observing System (network in USA)
CTP_SMTMN	Central Tibetan Plateau Soil Moisture and Temperature Monitoring Network (name of in-situ network in China)
DAHRA	Name of in-situ network in Senegal
DOI	Digital Object Identifier
FLUXNET_AMERIFLUX	Name of in-situ network in USA
FMI	Finnish Meteorological Institute (name of in-situ network in Finland)
FR_Aqui	Name of in-situ network in France
GB	Gigabyte
GROW	Grow observatory citizen science project - name of in-situ network located within Europe (based in the Great Britain)
GTK	Geological Survey of Finland (name of in-situ network in Finland)
HOAL	Name of in-situ network in Austria
HiWATER_EHWSN	Heihe Watershed Allied Telemetry Research Wireless Sensor Network (in China)
HOBE	Hydrological Oberservatory in Denmark
HSC_SEOLMACHEON	Hydrological Survey Center (HSC) in –situ network in South Korea
HWSD	Harmonized World Soil Database
HYDROL-NET_PERUGIA	Name of in-situ network in Italy
HYU_CHEONGMICHEON	Name of in-situ network in South Korea
ICN	Illinois Climate Network (name of in-situ network in USA)
ICWRGC	The International Center for Water Resources and Global Change

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Acronym	Full name
IIT_KANPUR	Indian Institute of Technology Kanpur (name of in-situ network in India)
IMA_CAN1	Name of in-situ network in Italy
IOWA	Name of in-situ network in USA
IPE	Instituto Pirenaico de Ecologia, name of in-situ network in Spain
iRON	Roaring Fork Observation Network
ISMN	International Soil Moisture Network
KHOREZM	Name of in-situ network in Uzbekistan
KIHS_CMC	Name of in-situ network in South Korea
KIHS_SMC	Name of in-situ network in South Korea
LAB-net	Laboratory for Analysis of the Biosphere Network (name of in-situ network in Chile)
MAQU	Name of in-situ network in China
METEROBS	Met European Research Observatory (name of in-situ network in Italy)
MOL-RAO	Lindenberg Meteorological Observatory, Richard-Aßmann Observatory
MONGOLIA	Name of in-situ network in Mongolia
MySMNet	Name of in-situ network in Malaysia
NAQU	Name of in-situ network in China
NGARI	Name of in-situ network in China
NRT	Near Real Time
NVE	Name of in-situ network in Norway
NWCC	National Water and Climate Center
ORACLE	Name of in-situ network in France
OZNET	Name of in-situ network in Australia
PBO_H2O	Plate Boundary Observatory (Name of in-situ network in USA)
PHP	PHP: Hypertext Preprocessor
PTSMN	Name of in-situ network in New Zealand
QC	Quality Control
RD	Reference Document
REMEDHUS	Name of in-situ network in Spain
RISMA	Real-time In-situ Soil Monitoring for Agriculture Network in Canada
RSMN	Romanian Soil Moisture Network
Ru_CFR	Russia Central Forest Reserve (name of in-situ network in Russia)
RUSWET-AGRO	Name of in-situ network in Former Soviet Union
RUSWET-GRASS	Name of in-situ network in Former Soviet Union
RUSWET-VALDAI	Name of in-situ network in Former Soviet Union
SASMAS	Name of in-situ network in Australia

Table – continued on next page

Acronym	Full name
SCAN	Soil Climate Analysis Network
SI	International System of Units
SKKU	Name of in-situ network in South Korea
SM	Soil Moisture
SMOS	Soil Moisture and Ocean Salinity
SMOSMANIA	Name of in-situ network in France
SNOTEL	SNOwpack TELemetry
SOILSCAPE	Soil Moisture Sensing Controller and Optimal Estimator Network in the USA
SQL	Structured Query Language
SWC	Soil Water Content
SWEX_POLAND	Soil Water Experiment Poland (name of in-situ network in Poland)
SW-WHU	Name of in-situ network in Poland
TAHMO	Trans-African HydroMeteorological Observatory (name of in-situ network in Africa)
TCA	Triple Collocation Analysis
Telespazio (VEGA)	European spaceflight services company
TERENO	Terrestrial Environmental Observatories (name of in-situ network in Germany)
TUW	Technische Universität Wien
UDC_SMOS	Upper Danube Catchment SMOS (name of in-situ network in Germany)
UMBRIA	Name of in-situ network in Italy
UMSUOL	Umidita del Suolo (name of in-situ network in Italy)
USCRN	US Climate Reference Network
USDA_ARS	Research Watersheds Supporting Soil Moisture Remote Sensing Network in USA
VAS	Valencia Anchor Station
VDS	Name of in-situ network in Myanmar hosted byVanderSat
VWC	Volumetric Water Content
WEGENERNET	Name of in-situ network in Austria
WMO	World Meteorological Organization
WP	Work Package
WSMN	Wales Soil Moisture Network in the UK

1 Introduction

1.1 Purpose and Scope

This document forms deliverable DT2-1 of the Fiducial Reference Measurements for Soil Moisture (FRM4SM) project. Its purpose is to detail Fiducial Reference Measurement (FRM) protocols and procedures for soil moisture (FPP-SM). The goals of the FPP-SM are to:

- describe methods, instruments, calibration procedures, and reference standards for measuring soil moisture in situ (Section 2);
- define criteria to assess whether a set of soil moisture (SM) ground measurements can be considered "fiducial" (Section 4);
- provide guidelines to ensure the traceability of FRM uncertainties and to calculate an FRM uncertainty budget (Section 5); and
- provide guidelines for how to use FRMs to evaluate space-borne radiometer-based soil moisture products (Section 6).

1.2 FRM definition

The European Space Agency (ESA) defines fiducial reference measurements (FRMs) as "a suite of independent, fully characterized, and traceable ground measurements that follow the guidelines outlined by the GEO/CEOS Quality Assurance framework for Earth Observation (QA4EO)". Furthermore, FRMs should "provide the maximum Return On Investment (ROI) for a satellite mission by delivering, to users, the required confidence in data products, in the form of independent validation results and satellite measurement uncertainty estimation, over the entire end-to-end duration of a satellite mission" (Banks et al. 2020).

To that end, FRMs ought to:

- have documented SI traceability using metrology standards and/or community-recognized best practices;
- have documented and maintained uncertainty budgets that are openly available;
- be independent from the satellite geophysical retrieval process;
- be accompanied by measurement protocols, procedures, and community-wide management practices (measurement, processing, archive, documents, etc.) that are defined, published, and adhered to by FRM instrument operators;
- be accessible to other researchers allowing the independent verification of processing systems; and
- be used to to quantify the in-orbit uncertainty characteristics of satellite geophysical measurements via independent validation activities.

In the recent years, ESA has been funding numerous activities related to the establishment and utilization of FRMs for various land, ocean, and atmosphere variables. A list of other ESA-funded FRM-related projects is provided in Table 3.

Table 3: List of other ESA-funded FRM projects; last updated: December 2023.

Acronym	Full name	Reference
FRM4VEG	Fiducial Reference Measurements for Vegetation	https://frm4veg.org/
FRM4SOC	Fiducial Reference Measurements for Satellite Ocean Colour	https://frm4soc.org/
FRM4ALT	Fiducial Reference Measurements for altimetry	https://www.frm4alt.eu/
FRM-BOUSSOLE	Buoy for the acquisition of long-term optical time series	http://www.obs-vlfr.fr/Boussole/html/project/strategy.php
FRM4DOAS	Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations	https://frm4doas.aeronomie.be/
FRM4GHG	Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations	https://frm4ghg.aeronomie.be/
FRM4STS	Fiducial Reference Measurements for validation of Surface Temperatures	http://www.frm4sts.org/
Pandonia FRM	Fiducial Reference Measurements for Ground-Based Direct-Sun Air-Quality Observations	https://www.pandonia-global-network.org/

1.3 FRM4SM ground reference data

The FRM4SM project does not deal with the installation or operation of in situ SM sensors. Instead, it relies upon measurements drawn from the International Soil Moisture Network (ISMN), which is an international data hosting facility for in situ surface and subsurface SM measurements. Currently, the ISMN contains globally-distributed measurements of SM and other variables (precipitation, temperature, snow, etc.) from more than 3000 stations that are operated by 76 different independent networks (last updated: December 2022). As acknowledged by the CEOS Land Product Validation Group, it is the most important reference database for satellite soil moisture validation (Dorigo et al. 2021).

Important to note, however, is that the various independent local and regional in situ networks that provide data to the ISMN often do not follow standardized measurement techniques or protocols and are collecting data in different units, at different depths, and at various sampling rates. Besides, quality control is rarely applied and accessing the data is often difficult. The ISMN has been created to address most of these issues: Within the ISMN, in situ SM measurements (surface and sub-surface) are collected, harmonized in terms of units and sampling rates, advanced quality control is applied (Dorigo et al. 2013), and the data is stored in a database and made available online free of costs.

To address the limited information about the reliability and uncertainty of ISMN data, several new quality indicators (QIs) have been developed within the FRM4SM project, described in project deliverable DT1-1 (Himmelbauer et al. 2023). The present FPP-SM document is intended to provide guidelines for how to draw reliable FRM subsets from the ISMN for the purpose of validating space-borne radiometer-based SM products (Section 4). Note, however, that the quality indicators described in DT1-1 and the FPP-SM described here can be applied more generally to any in situ soil moisture data base.

2 Measuring Soil Moisture

2.1 Soil moisture definition

Soil Moisture (SM) is described as "all water that is present in the soil layer between the surface and the groundwater table". This soil layer is the so called vadoze zone, which describes the unsaturated zone of soil excluding the saturated state that is called the phreatic zone. The unsaturated soil state describes a mixture state of soil, air, and water (technically solids, gases, and liquids), while the saturated soil state describes a mixture of soil and water only (technically solids and liquids) where all cracks, holes, and pores are filled. Groundwater is part of the saturated zone where atmospheric pressure is equal (at groundwater surface) or smaller than water pressure, whereas in the unsaturated zone, atmospheric pressure is always greater than water pressure; and the water pressure is varying depending on the amount of soil moisture. Put more succinctly:

- Soil moisture:
  - Vadoze zone
  - Unsaturated soil state
  - Mixture of soil, air, and water
  - Atmospheric pressure > water pressure
    - Water pressure varying depending on soil moisture amount
- Ground water:
  - Phreatic zone
  - Saturated soil state
  - Mixture of soil and water
  - Atmospheric pressure ⩽ water pressure
    - Ground water surface: atmospheric pressure = water pressure

Soil moisture can be better understood when understanding the water movement in the soil-air-water mixture, which is highly dependent on: (a) the soil structure; (b) a grouping of so-called aggregates (sand, silt ,clay, organic matter, and fertilizers); (c) the distribution of cracks and pore space sizes (the free space); and (d) three different physical forces to describe water flows and retention within the soil (Howe & Smith (2021), Montzka et al. (2021), WMO (2018), additional source USGS, status May 2023), which are explained in the following.

1 Gravitational water

Gravitational water describes the free water flow in soil pore spaces. It can be described as water that is absorbed and trickling away to lower soil layers due to gravitation or as an abundance of water in such quantities that the soil is saturated enough and free water flow is possible.

Saturation $\sim$ 0 kPa (macropores and micropores filled with water)

2 Capillary water

The Capillary water is soil moisture that is retained against gravity in soil pore spaces due to capillary force. Capillary force is greater than gravity and is further described as a force where cohesive forces between liquid molecules are not as strong as adhesion to the soil pores. Capillary water is the water storage in soil that is available for plants and is highly dependent on the soil texture (sand, silt, clay, organic matter). For sandy soils less than 10 volume percent of water might be available for plants while in high organic soils more than 40 volume percent could be available. General water movement is caused here partly from liquid water, partly from water vapour (at phase of distillation; vapour pressure; depending on soil temperature), and sometimes by plant root transport.

3 Hygroscopic water

Hygroscopic water is the moisture that is held in soil particles due to adhesion forces (zero vapour pressure). These forces are so strong that plants cannot even extract the water from the soil particles. It is therefore describing a state of water / soil moisture that is unavailable for plants.

The rate at which water can be extracted - or the energy that is needed to extract water from the soil is described as the so-called Soil Water Potential (SWP). SWP is different per soil texture (sand, silt, clay, organic matter) and can be further classified into soil states from "wet" to "dry", with the following generalized thresholds (Howe & Smith 2021):

Wet: Saturation: $\sim$ 0 kPa

$\uparrow\downarrow$ Gravitational water

Field capacity = soil moisture equivalent = 100% plant available water: for most soils at -33 kPa

$\uparrow\downarrow$ Capillary water

Plant stress

$\uparrow\downarrow$ Capillary water

Permanent wilting point (PWP) = 0 % plant available water = hygroscopic coefficient: -1500 kPa

$\uparrow\downarrow$ Hygroscopic water: below -1500 kPa

Dry: Oven dry

A saturated soil describes a soil-water state with no air left in the soil (most of the plants will suffer since they need also air to grow, with a few exceptions). Drainable soil is defined between saturation and field capacity. Field capacity describes the full water retention capacity of the soil from 100 to 0 % after gravitational drainage (2 -3 days after events of liquid precipitation / snow melting/ irrigation) where bigger soil pores are filled with both water and air, but smaller pores are full of water (Rai et al. 2017). Field capacity is highly varying for different soil textures and can be given in matric potential [ψ_m] (WMO 2018):

-1 $\mathrm{J\,kg^{-1}}$ for organic soils

-10 $\mathrm{J\,kg^{-1}}$ for loamy sands

-33 $\mathrm{J\,kg^{-1}}$ for most soils

-100 $\mathrm{J\,kg^{-1}}$ for heavy clay soils

The permanent wilting point (PWP) describes the threshold of the lower limit of plant available water at 0 % field capacity which most occurs at -1.5 MPa SWP [ψ_h] (WMO 2018).

When there is even no hygroscopic water present in the soil any longer and the soil state is composed out of purely soil and air then this is called oven dry.

2.2 Soil moisture target metric

Soil Moisture (SM) can be measured in many different ways. To harmonize the measurements in terms of units, the Satellite Soil Moisture (SSM) community has established Volumetric Water Content (VWC) [θ_v] as a standard unit for SSM retrieval products as well as for the in situ reference datasets to make them comparable. In general, expressing water content in volumetric units VWC can be more useful since precipitation, evapotranspiration and solute transport variables are commonly expressed in terms of flux (WMO 2018). In respect to all above-mentioned arguments, this document will also consider all different measurement techniques and the transformation steps needed, i.e., calibration functions, to reach VWC.

Note that 100 % VWC (= 1 $\mathrm{m^3\,m^{-3}}$) is 100% water without soil or air in a given volume, i.e., pure water, while 0 % VWC is what has been described in the chapter 2.1 as oven-dry soil with no water present in a given volume, i.e., only mineral or organic constituents with gas-filled pores.

Although, VWC is dimensionless, it is usually given in $\mathrm{m^3\,m^{-3}}$ indicating $\mathrm{m^3}$ water per $\mathrm{m^3}$ soil. VWC can be derived as follows:

$$\theta_v = \frac{\mathbf{V}_{water}}{\mathbf{V}_{sample}} = \frac{\left(\frac{\mathbf{M}_{\mathrm{water}}}{\mathbf{d}_{\mathrm{water}}}\right)}{\mathbf{V}_{solid} + \mathbf{V}_{liquid} + \mathbf{V}_{gas}} \qquad \mathrm{m^3\,m^{-3}} \tag{1}$$

where V_{water} is the volume of water contained in a soil volume V_{sample} (including dry soil, air, and water); m_{water} is the mass of the water; and d_{water} the water density.

2.3 Measuring soil moisture

Volumetric Water Content (VWC) can be measured only indirectly. Therefore, several different measurement techniques have been developed detecting either directly or indirectly (Montzka et al. (2021), Robock et al. (2000), WMO (2018), Meter sensor producer (May 2023)) one of the following:

1 **Soil Water Content (SWC) [θ_g]**

- amount of water in soil (relative to the amount of soil)
- extensive variable (changing with size and situation)

2 **Soil Water Potential (SWP) [ψ_h]**

- The energy state of water (= determination of dynamic movement of the water in the soil)
- An intensive variable (= intensity or quantity of matter or energy)
- SWP is basically the energy that needs to be expended to get water out of soil sample.
- Applied for irrigation since it is well applicable to understand the comfort level of plants

Both, SWC [θ_g] and SWP [ψ_h] describe the water status in soil related to density and texture (WMO 2018)(Copyright © 2022 Decagon Devices, Inc.. All rights reserved.).

SWC [θ_g] is measured by means of the gravimetric mass **m** of wet and oven-dried soil:

$$\theta_g = \frac{\mathbf{m}_{water}}{\mathbf{m}_{soil}} = \frac{\mathbf{m}_{\text{wet soil}} - \mathbf{m}_{\text{oven dry soil}}}{\mathbf{m}_{\text{oven dry soil}}} \qquad \text{kg kg}^{-1} \quad (2)$$

As mentioned above SWP [ψ_h] is another form of measuring soil moisture, or more correctly the energy state of water and can be derived from the total water potential equation:

$$\psi_t = \psi_g + \psi_m + \psi_O + \psi_P \qquad \text{J kg}^{-1} \quad (3)$$

where [ψ_g] is the gravitational potential (elevation above sea level / reference level); [ψ_m] is the matric or capillary potential (interaction of soil particles with water); [ψ_O] is the osmotic potential (energy effects due to solutes dissolved in the soil water); and [ψ_P] is the pressure potential (hydro static pressure below a water surface).

A more comprehensive description of the equation 3 will follow in the next CCN project phase.

As for now, the overall hydraulic potential [ψ_h] is not related to either water or soil and can be expressed in saturated soil as (higher potential, wetter):

$$\psi_h = \psi_g + \psi_P \qquad \mathrm{J\,kg^{-1}} \qquad (4)$$

as well as in unsaturated soil (lower potential, dryer) when soil water is below field capacity as (Howe & Smith 2021):

$$\psi_h = \psi_g + \psi_m \qquad \mathrm{J\,kg^{-1}} \qquad (5)$$

Total water potential or hydraulic water potential is usually given in $\mathrm{J\,kg^{-1}}$ which, transferred to base SI units, is $\mathrm{m^2\,s^{-2}}$.

SWP (ψ_h) can be calculated either in gravimetric [ψ_g], matric [ψ_m] or osmotic [ψ_O] equivalents of negative units of pressure or with positive units of tension given in bars and converted either into kPa or MPa (Howe & Smith 2021).

Most of the SWP [ψ_h] sm sensors measure matric potential [ψ_m] which is then further converted to VWC [θ_g].

To summarize this chapter, SWC [θ_g] $\mathrm{kg\,m^{-3}}$ and SWP [ψ_h] kPa built the two groups of measurement types and will be further explored as well as explained within the individual subchapters for the measurement techniques (see chapter 2.4). Therefore, a more comprehensive understanding of the measured physical parameters, and the respective equations used, will be included per these subchapters in a step-by-step process starting in the next project phase.

Furthermore, the linkage from the measured parameter back to VWC [θ_g] $\mathrm{kg\,m^{-3}}$ (= the target metric) will be included in chapter 2.6. This will be also done as a step-by-step process per physical parameter measured which is either the subgroup of measurement technique if possible (e.g., gravimetric, apparent permittivity, lysimetric, matric potential, etc.), or per individual measurement technique if needed (e.g., gravimetric, cosmic ray, etc.).

2.4 Measurement techniques

Numerous SM measuring techniques exist and are continuously developed basing their techniques either on measurements of Soil Water Content (SWC) or Soil Water Potential (SWP) directly or indirectly. The list below summarizes currently existing techniques in the most important categories and subcategories found in the literature as well as explains the measuring techniques in a general form (Montzka et al. 2021, Petropoulos et al. 2013, SU et al. 2014, Walker et al. 2004, WMO 2018, Yu et al. 2021):

- **Soil Water Content SWC [θ_g]:**

- Direct measurement of SWC [θ_g]
  - * Thermal
    - → Gravimetric water content = thermo-gravimetric method
- Indirect measurement of SWC [θ_g]
  - * Dielectric = relative permittivity [ϵ_r]

    Direct:

    → Time Domain Reflectometry (TDR)

    Indirect:

    → Time Domain Transmission (TDT)

    → Frequency Domain Reflectometry (FDR)

    → Standing Wave Ratio (SWR)

    → GNSS reflectometry

    → Electrical Resistance Hydrometric

    → Impedance

    → Transmission Line Oscillator (TLO)
  - * Radiological/ Nuclear
    - → Neutron scattering method
    - → Gamma-ray attenuation
    - → Magnetic resonance
    - → Cosmic ray neutron

- **Soil water potential (SWP) [ψ_h]:**
  - Indirect measurement of SWP [ψ_h]:
    - * Thermal:
      - → Heat dissipation: -9.8 to -100000 kPa (-0.1 to -1000 bars)
      - → Heat pulse
      - → Psychrometers: -98 to -3000 kPa (-1 to -30 bars)
    - * Tensiometer: 0 to -80 kPa (0 to -0.8 bars) $\sim$ -800 cmd
    - * Resistivity (gypsum): 0 to -890 or -1500 kPa (0 to -10 or -15 bars)

2.4.1 SWC direct: gravimetric water content [θ_g]

The gravimetric water content method, also known in literature as the thermo-gravimetric method, is the only know measurement technique to date, deriving SWC [θ_g] directly. It is an invasive method requiring to retrieve a soil sample of a known volume (e.g., 0.15 m diameter, 0.3 m height and a bulk density [ρ_b] of 1.3 $\mathrm{g\,cm^{-1}}$ (Pikul Jr 2003, Xaver et al. 2020)), carefully from the field, and measure the soil mass against the dry soil mass (see equation 2). In order to get the soil dried mass, the sample is oven dried (electrical oven) with 105 $\pm$ 5 °C until the mass stabilizes at a constant value (usually between 16 and 24 hours (WMO 2018)). The derived SWC measurement can be further transferred to VWC, the target metric, with equation 19 (see also equation 21 to 22).

Although moisture can still be bound to the soil sample due to hygrometric forces introducing uncertainties (= random errors) to the measurement, this method is an international-accepted standard by the International Organization for Standardization ISO (global federation of national standard bodies developing and document international standards within the ICS catalogue, status May 2023):

* **ISO 11461:2001(en) (©ISO 2001)**
  - Soil quality — Determination of soil water content as a volume fraction using coring sleeves — Gravimetric method
  - Prepared by Technical Committee ISO/TC 190, Soil quality, Subcommittee SC 5, Physical methods.
* **ISO 11464:2006(en) (©ISO 2006)**
  - Soil quality — Pretreatment of samples for physico-chemical analysis
  - Prepared by Technical Committee ISO/TC 190, Soil quality, Subcommittee SC 3, Chemical methods and soil characteristics.
* **ISO 11465:1993/Cor.1:1994(en) (©ISO 1994)**
  - Soil quality — Determination of dry matter and water content on a mass basis — Gravimetric method
  - Prepared by Technical Committee ISO/TC 190, Soil quality, Subcommittee SC 3, Chemical methods and soil characteristics.

These three documents describe how to properly conduct the measurement and how to prepare the soil samples accordingly, to get observations that are theoretically free of systematic errors. It is recommended to repeat the whole procedure many times to get unbiased readings, making sure to have higher quality of the measurement. Since gravimetric measurements are independent of soil texture and salinity, they are assumed to be the most accurate measurement techniques to date.

However, it is very time-consuming and disruptive to the soil, as well as quite labour intense to get long time series for soil moisture measurements which is usually required for the validation process of satellite soil moisture products. Therefore, this method is usually used for calibrating non-intrusive soil moisture sensors (e.g., dielectric sensors, radiological sensors, tensiometers, etc.) before the installation in the field, to account for the soil texture at the location (see 2.7; Montzka et al. (2021)).

However, some biases can remain especially when the readings are compared with measurements from other facilities (e.g., handling of soil sample, etc.). Considering also the retention capacity of the soil (hygrometric water) under drying conditions, the ISO standard is not yet a full standard but the closest that the community can currently achieve to a standard. This means that some uncertainties remain. Therefore, the gravimetric technique is always further developed and improved upon. making comparing measurement results also not straight forward since it is usually not stated what method has been used (e.g., ISO standard, self-developed method, etc.).

2.4.2 SWC [θ_g] indirect: Dielectric = relative permittivity [ε_r]

Soil moisture can also be measured with the so-called dielectric method, which means usually the direct or indirect measurement of relative permittivity [ϵ_r] (= apparent dielectric permittivity [K_a] or [κ_a] or [κ]; also called dielectric constant in older literature; sometimes the accuracy of the real dielectric permittivity is given in a sensor user manual which is referring to the real part of the relative permittivity - see 2.4.2.1).

Many different techniques have been developed to measure relative permittivity [ϵ_r]:

- Indirect measurement of SWC [θ_g]
    - * Dielectric = relative permittivity [ϵ_r]

        Direct:

        → Time Domain Reflectometry (TDR)

        Indirect:

        → Time Domain Transmission (TDT)

        → Frequency Domain Reflectometry (FDR)

        → Standing Wave Ratio (SWR)

        → GNSS reflectometry

        → Electrical Resistance Hydrometric

        → Impedance

        → Transmission Line Oscillator (TLO)
    - * Radiological/ Nuclear

→ Neutron scattering method

→ Gamma-ray attenuation

→ Magnetic resonance

→ Cosmic ray neutron

All individual techniques, the physical parameter of the sensor output as well as the measurement is planned to be documented in a comprehensive way in the next CCN project phase. This will help to understand the uncertainties to be considered and the gaps still missing, getting a traceable understanding of the direct sensor output before the transferral into the target metric VWC [θ_V].

2.4.2.1 The physical principle behind the measurement

This chapter still is work in progress and will be completed within the next CCN project phase. Therefore, units and explanations for some variables can still be missing.

Within the Maxwell's Equations (1960s) the dielectric permittivity (also known as permittivity) was mathematically quantified for the first time, explaining the propagation of an electrical wave within a material where a complex wave vector $\vec{k}$ is introduced, describing the wave distribution within the real part of the equation as well as the damping through the material by the imaginary part of the equation.

Therefore, the Maxwell Equations were simplified/ modified for the electrical field of a material $\vec{E}$ to:

$$\vec{E} = \vec{E_0} * e^{i(\vec{k}\vec{x}-\omega t)} \qquad \mathrm{F\,m^{-1}} \tag{6}$$

where $\vec{E}$ is the electrical field in a material and $\vec{E_0}$ is the electrical field in vacuum. The orientation is built around the $\vec{k}$ wave vector, pointing into the direction of the wave propagation for $\frac{2\pi}{\lambda}$ length (where λ is the wave length), $\vec{x}$ is the location, and **t** is the time. The variable **i** is the imaginary unit ($= \sqrt{-1}$) and ω is the angular frequency (see equation 8).

The complex wave vector $\vec{k}$ can be expressed as:

$$k = \vec{k}' + i\vec{k}'' \tag{7}$$

where $\vec{k}'$ represents the real part (orange) and therefore, the wave distribution in a media, while $i\vec{k}''$ represents the imaginary part (blue), describing the damping in the media (this case soil).

The angular frequency ω can be described as follows:

$$\omega = 2\pi f = \frac{2\pi}{T} \tag{8}$$

where **f** is the frequency and **T** is the period.

If Maxwell's Equation 6 is now combined with the defined complex wave vector $\vec{k}$ as shown in equation 7, it can be split up into the real (orange) and imaginary (blue) part as follows:

$$\vec{E} = \vec{E_0} * e^{i(\vec{k}'\vec{x}-\omega t)} * e^{-\vec{k}''\vec{x}} \quad \mathrm{F\,m^{-1}} \tag{9}$$

Since the wave distribution in a media is considered with a certain velocity, the measured relative permittivity **[**ε_r**]** can be included as a variable in the wave vector $\vec{k}$ equation like this:

$$\vec{k} = \frac{\omega}{c_o} * \sqrt{\varepsilon_r' + i(\varepsilon_r'')} \tag{10}$$

This is possible since speed of light c can be expressed as follows:

$$c = \frac{\omega}{\vec{k}} \rightarrow \vec{k} = \frac{1}{c_m} * \omega = \frac{\omega}{c_0} * \sqrt{\varepsilon_r} \tag{11}$$

where c_m is the speed of light in a media, and c_0 is the speed of light in vacuum which can be further expressed as:

$$c_0 = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \quad \mathrm{s\,m^{-1}} \tag{12}$$

where ε_0 is permittivity in vacuum, and μ_0 is permeability in vacuum (~ 1 and therefore negligible). This leads to the light speed in a medium c_m :

$$c_m = \frac{1}{\sqrt{\varepsilon\mu}} = c_0 * \frac{1}{\sqrt{\varepsilon_r \mu_r}} \quad \mathrm{s\,m^{-1}} \tag{13}$$

where μ_r is relative permeability (again ~ 1 therefore negligible). The velocity can be combined with the complex wave vector as follows:

$$c_m = \frac{1}{\sqrt{\varepsilon\mu}} = c_0 * \frac{1}{\sqrt{\varepsilon_r \mu_r}} \quad \mathrm{s\,m^{-1}} \tag{14}$$

and $[\varepsilon_r]$ can be further expressed as:

$$\varepsilon_r'' = \varepsilon_{\mathrm{rel}} + \frac{\sigma_{\mathrm{dc}}}{\omega\varepsilon_0} \tag{15}$$

The variable $\sigma_{\textbf{dc}}$ is the electrical conductivity (the direct current) while ε_0 is the permittivity in vacuum. As for what ε_{rel} stands will be further investigated in the next CCN project phase.

The reason why the relative permittivity [ε_r] can be included as such in the Maxwell's Equations is because dielectric permittivity [ε] measures the electrical polarization of a dielectric which is determining the capacitance of a capacitor. The dielectric permittivity therefore, is the ability of a material to hold an electrical charge. While absolute permittivity [ε] is described as :

$$\varepsilon = \frac{\vec{E}}{\vec{D}} \qquad \text{dimensionless} \qquad (16)$$

where $\vec{E}$ is the electrical field and $\vec{D}$ is the electric flux density, the dielectric permittivity [ε] can be further expressed as:

$$\varepsilon = \varepsilon_r * \varepsilon_0 \qquad \text{dimensionless} \qquad (17)$$

which can then be further expressed as the relative permittivity [ε_r] as follows

$$\varepsilon_r = \frac{\varepsilon}{\varepsilon_0} \qquad \text{dimensionless} \qquad (18)$$

The measured relative permittivity [ϵ_r] in air is 1 and in distilled water $\sim$ 80 (at room temperature $\sim$ 25 °C).

2.4.2.2 Direct [ϵ_r]: Time Domain Reflectometry TDR

To be finished in next CCN phase.

2.4.2.3 Indirect [ϵ_r]: Time Domain Transmission TDT

To be finished in next CCN phase.

2.4.2.4 Indirect [ϵ_r]: Frequency Domain Reflectometry FDR

To be finished in next CCN phase.

2.4.2.5 Indirect [ϵ_r]: Standing Wave Ratio SWR

To be finished in next CCN phase.

2.4.2.6 Indirect [ϵ_r]: GNSS Relectometry

To be finished in next CCN phase.

2.4.2.7 Indirect [ϵ_r]: Electrical Resistance Hydrometer

To be finished in next CCN phase.

2.4.2.8 Indirect [ϵ_r]: Impedance

To be finished in next CCN phase.

2.4.2.9 Indirect [ϵ_r]: Transmission Line Oscillator (TLO)

To be finished in next CCN phase.

2.4.3 SWC [θ_g]: Radiological/Nuclear

To be finished in next CCN phase.

2.4.3.1 Neutron scattering method

To be finished in next CCN phase.

2.4.3.2 Gamma-ray attenuation

To be finished in next CCN phase.

2.4.3.3 Magnetic resonance

To be finished in next CCN phase.

2.4.3.4 Cosmic ray neutron

To be finished in next CCN phase.

2.4.4 SWP [ψ_h]: Thermal

To be finished in next CCN phase.

2.4.4.1 Heat dissipation

To be finished in next CCN phase.

2.4.4.2 Heat pulse

To be finished in next CCN phase.

2.4.4.3 Psychrometers

To be finished in next CCN phase.

2.4.5 SWP [ψ_h]: Tensiometer

To be finished in next CCN phase.

2.4.6 SWP [ψ_h]: Resistivity

To be finished in next CCN phase.

2.5 Validating/Calibrating the sensor output = inter-sensor variability

This chapter will be highlighting the findings on how the direct sensor output (per measurement technique group/ individual technique) is evaluated by the sensor producer and if and how this could be potentially also be done by the sensor users to test the sensor before converting the direct output to VWC [θ_v] (e.g., standard liquid method - dielectric method, etc.). First effort is put into the dielectric method and will be more investigated and documented within the next CCN project phase.

2.6 Transformation to target metric = calibration functions

Sensors reading need to be calibrated in order to convert sensor output to the desired target SM output. This is usually done in the laboratory by the manufacturer, who either applies the calibration function directly so that the end user only obtains the final SM output, or one or more calibration functions/parameters are provided which can provide some flexibility to choose the correct calibration for specific soil types. Since manufacturers usually provide only little information about how exactly calibration functions have been derived and their limits of validity, it is generally recommended to calibrate sensors for a particular purpose, either in the laboratory, or if possible directly for specific field conditions.

2.6.1 SWC [θ_g] to VWC [θ_V]

SWC [θ_g] can then be converted into VWC [θ_v] as follows:

$$\theta_v = \theta_g \left(\frac{\rho_{dry}}{\rho_w}\right) \qquad \mathrm{m^3\,m^{-3}} \quad (19)$$

where [ρ_{dry}] is the dry soil bulk density in kg m^{-3} and [ρ_w] is the soil water density in kg m^{-3} (unit weight of water).

Soil water density [ρ_w] can be derived as follows:

$$\rho_w = \frac{\mathbf{m}_{\text{water}}}{\mathbf{V}_{\text{water}}} = \frac{\mathbf{m}_{\text{total}} - \mathbf{m}_{\text{oven dry}}}{\mathbf{V}_{\text{water}}} \qquad \mathrm{kg\,m^{-3}} \quad (20)$$

Bulk density [ρ_b] is the total mass of the soil sample per total volume of the sample (comprising of solid, liquid, and gaseous constituents) and is therefore an estimate for the combination of:

- Water storage capacity
- Soil texture: sand, silt, clay (organic matter)

- Infiltration rate
- Compactness
- Aeration

$$\rho_b = \frac{\mathbf{M}_{sample}}{\mathbf{V}_{sample}} = \frac{\mathbf{M}_{solid} + \mathbf{M}_{liquid}}{\mathbf{V}_{solid} + \mathbf{V}_{liquid} + \mathbf{V}_{gas}} \qquad \mathrm{kg\,m^{-3}} \quad (21)$$

Dry soil bulk density [ρ_{dry}] is then the oven dry mass of the sample per total volume of the sample:

$$\rho_{dry} = \frac{\mathbf{M}_{\text{oven dry}}}{\mathbf{V}_{\text{total sample}}} \qquad \mathrm{kg\,m^{-3}} \quad (22)$$

2.6.2 Relative permittivity [ϵ_r] to VWC [θ_V]: Dielectric mixing models

Dielectric mixing models describe the physical relationship between the relative permittivity [ϵ_r]. An overview of different dielectric mixing models is provided by Van Dam (2014). The most commonly used model for SM sensor calibration and transferral of the relative permittivity [ϵ_r] into VWC θ_V is the TOPP equation (Topp et al. 1980) and the Complex Reflective Index model CRIM (Roth et al. 1990). These calibration functions can be readily applied by the sensor user.

The TOPP 1980 equation represents the empirical relationship between relative permittivity [ϵ_r] and VWC [θ_V] (frequency independent for sensors in the range of approximately 1 MHz to 1 GHz). It is most commonly used for mineral soils with a full saturation threshold of 0.5 $m^3\,m^{-3}$ and does not account for the effects of soluble salt content, soil temperature, varying texture, and bulk density. This, however, can be problematic since the rather inexpensive low-frequency probes tend to be indeed sensitive to these effects (Vaz et al. 2013).

The Complex Reflective Index model (CRIM, Roth et al. (1990)) is estimating the bulk permittivity of heterogeneous materials. The CRIM is rather popular due to its simplicity, yet its accuracy has never been rigorously tested.

High-frequency measuring techniques (above 1 GHz) may benefit from using microwave-specific soil dielectric models that are also used in satellite SM retrieval algorithms, such as the Mironov model (Mironov et al. 2004). Measurements obtained with high frequency sensors are deemed as more sensitive to the soil texture in literature. Since the Mironov model does allow the usage of soil information from an additional source, the general usage of this model for also low frequency measuring techniques could improve the data quality when applied, specifically also when the same soil information dataset is used as for the satellite observation dataset transferral into volumetric water content (VWC) [θ_V]. However, this is not commonly applied and needs to be investigated.

While most literature is explaining the used frequencies of the sensors in relationship to the usage of the dielectric mixing models, or rather its little effect, it is still confusing to understand the influences (e.g., soluble salt content, soil temperature, varying texture, and bulk density) that need to be considered when using different dielectric mixing models for the conversion in respect to the used sensors with a specific frequency.

Within the next project phase, effort will be put into the inclusion of additional mixing models that can be found in literature as well as by talking to experts. Furthermore, it is planned to give a more comprehensive overview of the individual models.

From the literature and from talking to in situ soil moisture experts and sensor producers, it is evident that it is of great interest to the community to get clear recommendations for what the most accurate dielectric mixing models for transferring sensor outputs $[\epsilon_r]$ of a specific frequency into $[\theta_V]$ are, and why. Conducting experiments in order to answer these questions are, therefore, highly recommended for a future project, which could also help to better understand the uncertainties associated with such models.

2.7 Laboratory-based calibration: considering the soil at the station

Since the soil composition does have a big impact on soil moisture measurements, and due to the nature of soil not being homogeneous even within proximity to one and another, considering the soil structure per station can improve the sensor reading quality. In order to do so, it is required to take a soil sample directly next to the station because the sensor should ideally be only installed in non-disturbed soils. However, for taking a soil sample, one would need to disturb the soil, digging a whole and bring this sample back into the laboratory. Therefore, a soil sample is taken right next to where the sensor should be installed, hereinafter referred to as a proxy soil sample, which can already differ from the real sensor location, but it is at least a better proximity to correct the sensor reading rather than standard calibration/validation functions which usually only considering mineral soils of a more homogeneous nature.

This strategy has been proven to improve the sensor reading when considered. Even for this method, most of the current techniques calibrate soil moisture behaviour against mineral soils (sand, silt, and clay), extracting the organic component from the soil sample, but it is getting increasingly more common to account for the soil organic carbon content (SOC) due to its capacity for storing large water quantities that can cause sensors to saturate quickly.

Accounting for SOC is especially important for the satellite SM community because it is contained mainly in the first few centimetres of the soil, for which satellites are most sensitive. The following lab-calibration strategies are most commonly used:

Calibration for mineral soils

* gravimetric water content measuring technique (see chapter 2.4.1)

Calibration for high organic soils

* To be included in next CCN phase

More literature review is currently needed to understand different techniques used

2.7.1 Calibration considering mineral soils only

The collected proxy soil sample, taken next to where the sensor will be installed, is brought back to the laboratory.

to saturation, and oven-drying it while using gravimetric weight measurements to obtain a high-quality reference. In both cases, an empirical relationship throughout the entire SM range is established between the sensor that is to be calibrated and the reference measurements, which can then be applied as a correction factor that is applied to any subsequent measurements taken during regular use.

Note, however, that the quality of gravimetric samples can vary significantly depending on the precision of the soil sample drying, the determination of its volume, and on the soil sample that is used ("fresh" versus sieved, disturbed versus undisturbed, organic content included or excluded, etc.). Established thresholds for the drying process regarding the temperature, time frame, and soil sample usage account for most of the above-mentioned issues, but inaccuracies may still remain since bound water in the soil sample may remain. Nevertheless, the gravimetric water content measuring technique is accepted as the gold standard for measuring SWC in a given soil volume. This method is therefore commonly used as a reference to calibrate SM probes for most of the measuring techniques.

2.7.2 Calibration including high organic soils

To be finished in next CCN phase.

2.8 Sensor installation

Depending on the sensor measurement group/ technique the installation can differ.

The gravimetric technique is an intrusive technique where soil samples are taken from the field. Therefore, this method is not consistent of a permanent installed sensor. For this method, ISO standards do exist that should be followed to get the best possible measurement as further explained and linked to the appropriate documents in chapter 2.4.1.

For the installation of dielectric sensors, lysimeters, tensiometers, resistance sensors and psychrometers, the contact with the soil is of utmost importance as well as the positioning in the soil (e.g., position of sensor itself in soil, interference of other sensors in proximity, taking into consideration the topography of the area and the natural water flows, etc.), which can differ again per technique. Furthermore, the cable management and the right positioning of the data logger and antenna is also of great importance.

For the radiological group of sensors, the installation is a bit different again and can again vary per individual technique.

Therefore, this chapter is planned to be steadily extended by measurement group/ technique within the next CCN project phase and probably beyond. But it is already clear that experience and training is key for the installation of sensors, to get the best possible data quality. Very interesting and important to identify will be how to handle the installation in different soils as well as understanding thresholds for sensor installation per technique per individual soils. For example, dielectric sensors need full contact with the soil which is not possible for sandy soils (high organic soils) at a specific threshold (currently not known to the authors). However, for cosmic ray neutron sensors this could still work as long as the installation rod is installed in a stable manner.

Quantifying uncertainties for the sensor installation requires dedicated field experiments, which are currently out of scope of the FRM4SM project.

2.9 Sensor ageing / sensor drifts over time

At the moment there is no clear understanding of how long a sensor lifetime is in literature and when taking to sensor users. In just recent conducted first talks with sensor producers, there also seems not a clear threshold for a sensor replacement, but the five-year warranty is mentioned as it is the general threshold of guaranteed lifetime of any electric hardware. More investigations are needed to get here a more well-rounded statement.

Furthermore, when talking to the ISMN sensor provider, it was mentioned that most of them do not have the budget to exchange the hardware every few years (just to make sure the measurements are trustworthy). This led to the observation, that in general the current sensor techniques on the market are quite good and stable running for $\sim$ 10 years and beyond at least for the current dielectric methods. It was further noted that when purchasing new sensors, it is important to test them all individually because it even newly-bought sensors rather often don't function properly. However, once the tests show a stable behaviour, one can confidently use them for the next $\sim$ 10 years.

In general, many of the sensor providers install two to three sensors at the same depth at the same station to test for drifts, or average the observations and provide only this average as the measurement (Bogena et al. 2018, Montzka et al. 2021). However, since sensor interference needs to be considered as well as the influence of soil even for sensors in proximity is extremely high, further literature review as well as talks with experts are needed to get here a clear understanding within the next CCN project phase.

3 Reference standards and SI traceability

The WMO Guide to Instruments and Methods of Observation (WMO 2018) states that soil moisture instruments must undergo laboratory or on-site calibration, under stable, defined and known conditions, against a standard traceable to the SI[1], where such a traceable standard exists. Calibration must be performed over the instrument's field operational range, at time intervals consistent with the stability of the instrument. Calibration intervals should initially be as recommended by the manufacturer and then be adjusted based on analysis of calibration performance. Furthermore, instruments should have their performance verified when they are removed from the field, and must be maintained to retain the desired measurement uncertainty. Maintenance intervals should initially be based on manufacturers' recommendations and then be adjusted based on analysis of the system performance.

To our best knowledge, no institution has yet been accredited by a metrological laboratory to provide SI-traceable reference standards for soil moisture sensors. Some sensor manufacturers claim their provided uncertainty estimates to be SI traceable, yet information about how uncertainty information was obtained or how traceability has been established is usually unavailable.

Alternatively, reference standards for sensor calibration can be obtained by gravimetric sampling, which is, as mentioned earlier, currently the gold standard in the soil moisture community (Montzka et al. 2021). Collecting such a gravimetric reference standard in an SI-traceable manner requires taking traceable weight measurements in kg while oven-drying a test soil sample. These weight measurements then need to be converted further into volumetric units ($m^3\,m^{-3}$), which requires taking also traceable measurements of the soil volume (m^3) and temperature (K).

Note, however, that this faces further challenges because (a) it is difficult to cut out and measure a perfectly cube-shaped sample of natural soil, and (b) the weight-volume relationship is subject to change due to soil compression and dilatation. Finally, even though SI traceability could be established properly in the laboratory, it remains unclear how representative the used soil sample is, in terms of soil composition, for the conditions in the field where the evaluated sensor ought to be used.

More research is needed to quantitatively assess the uncertainties related to deviations from the soil type assumed in the sensor calibration, or with the conversion of gravimetric to volumetric units. Nevertheless, these effects can be expected to be

[1]SI traceability is defined in the International Vocabulary of Metrology (Vocabulaire International de métrologie; VIM; JCGM 2012) as "the property of the result of a measurement or the value of a standard whereby it can be related to stated references, usually national or international standards, through an unbroken chain of comparisons all having stated uncertainties".

largely systematic and small compared to spatial and temporal representativeness (see Section 5), and thus probably won't have a significant impact on a SM FRM uncertainty budget.

4 Soil Moisture FRM Criteria

This section provides a guidance protocol on how to derive an FRM subset from the ISMN by defining the intended purpose and utilizing quality indicators associated with the stations. Even though referring to the ISMN here, this protocol could be generalized to any available in situ data.

4.1 Purpose

Recall that FRMs should "provide the maximum Return On Investment (ROI) for a satellite mission by delivering, to users, the required confidence in data products, in the form of independent validation results and satellite measurement uncertainty estimation, over the entire end-to-end duration of a satellite mission". Therefore, the selection of FRMs depends upon the spatial and temporal extent of the satellite product that ought to be validated. Spatial extent, in this context, refers to the area for which the mission is committed to provide reliable soil moisture retrievals.

4.2 Quality indicators (QIs)

QIs can and should be used to filter out unreliable sensor readings or entire stations that are inapt for satellite product validation. The ISMN has developed an automated flagging system that detects and flags suspicious sensor measurements, which is available on GitHub (https://github.com/TUW-GEO/flagit) and described in Dorigo et al. (2021, 2013). It is recommended to use this flagging system for the selection of FRMs. In addition, new QIs have been developed within the FRM4SM project, which are described in the deliverable DT1-1 (Himmelbauer et al. 2023). So far, among all tested options, only the "representativeness" QI, which determines the degree to which an in situ station is representative for the satellite scale, is recommended to be used to select FRMs. Note, however, that these investigations are ongoing and recommendations will be continuously updated throughout the project.

4.3 FRM selection protocol

The following protocol is proposed to extract an FRM subset from a given ground reference database, in the case of this project the ISMN.

1. Select all stations that fall within the region of interest and fully cover the time period of interest.
2. Mask out all in situ stations that are not deemed "very representative" by the representativeness QI (see RD DT1-1; Himmelbauer et al. 2023, Sec. 2.2.6).
3. Mask out all in situ measurements that are not marked as "good" by the automated flagging system[2] (see RD DT1-1; Himmelbauer et al. 2023, Sec.

[2] The masking of data due to the use of a "frozen soil flag" is suspected to be excessive in high latitudes and/or regions with high organic soil content. Therefore, for the sake of data availability, this flag may be relaxed in these regions.

2.1.1)..

4. Use any additional information available to mask out measurements or stations that appear unreliable (e.g., manual visual time series inspection, recommendations from data providers, etc.).
5. If multiple in situ stations fall within a satellite grid cell, their measurements should be averaged.
6. Collocate in situ measurements with satellite observations following community-agreed guidelines for temporal matching (Gruber et al. 2020)
7. Mask out all stations for which no reasonable sample size remains after collocation (A common sample size threshold is 100 (Gruber et al. 2020), yet this may be relaxed in difficult regions with limited reference data availability, such as Northern latitudes).

Ad 6. (I): Averaging multiple stations faces several challenges, for example how to deal with missing data, how to account for bad sensor readings, or how to weigh sensors according to spatial representativeness. More research is needed to provide clear guidelines to address these issues, which may be conducted in a future phase of the project.

Ad 6. (II): The SMAP community has established several so-called core validation sites. These sites are densely-sampled areas where a large number of in situ sensors have been placed within SMAP 36 km EASE v2 grid cells to provide footprint average soil moisture estimates at 3 km, 9 km, and 36 km resolution using sophisticated spatially-weighted averaging techniques (Colliander et al. 2017a,b) (the EASE v2 match-up data base is accessible at https://nsidc.org/data/nsidc-0712/versions/1; last accessed: December 2022). These core validation sites are considered to be the most reliable ground reference measurements at the satellite scale. However, they are limited to only a few locations worldwide, which do not suffice to assess global uncertainty characteristics comprehensively and with statistical significance.

4.4 Practical considerations and limitations

4.4.1 Traceability

Recall that FRMs ought to have a fully-traceable uncertainty budget. However, attaining full traceability for FRM uncertainties faces two issues. First, many in situ data providers (including virtually all data providers of the ISMN) do not provide any information about sensor installation or calibration. Experiments are needed to quantify the possible range of uncertainty associated with unknown sensor installation and calibration. Second, in situ SM sensors provide point measurements, which should be used to validate SM retrievals from space-borne microwave instruments that represent SM averages within ill-defined footprints of hundreds of square kilometres. The difference between SM at these two vastly different scales, referred to as representativeness error, often exceeds the actual measurement uncertainty of in situ SM sensors (Miralles et al. 2010) and varies greatly in space (Gruber et al. 2013).

A full account on traceability for SM FRMs is provided in Section 5. For this section, suffice it to say that the representativeness QI, calculated through triple collocation analysis (TCA), is currently accepted by the SM community as the only reliable way to estimate the combined sensor plus representativeness uncertainties of in situ stations in the absence of dense networks and intensive field work (Gruber et al. 2020, 2016). These TCA-based station uncertainty estimates have been validated extensively with data from the above-described core validation sites (Chen et al. 2016, Miralles et al. 2010).

4.4.2 Temporal data coverage

The recommendations about data coverage provided in Section 4.3 are concerned with total sample size only. No quantitative minimum sample size requirement is provided because absolute sample size recommendations are generally not meaningful. This is because sample size selection usually requires trade-offs that depend on the intended application. For example, in situ data coverage is already limited in many areas (see the next section), and imposing strong sample size requirements may lead to a complete reference data loss in regions such as high-latitudes due to prolonged frozen periods. Instead, sample size requirements should be chosen carefully depending on data availability while putting special attention on the estimation of confidence intervals (Gruber et al. 2020).

Moreover, total sample size requirements do not account for possible irregularities in data coverage and its relation to the intended application. For example, one generally requires reference data that is reasonably well distributed over the entire seasonal SM cycle. However, this might not be feasible especially during the winter where several month of data might be missing due to soil freezing. On the other hand, in agricultural areas reliable reference data is generally more important during the growing period than during the fallow winter time.

No metrics have yet been developed to quantify the aptness of the temporal data coverage of SM reference data to properly represent the temporal dynamics within a given period of interest. Accordingly, no guidelines can be provided here yet. This is subject of ongoing investigations and the FRM4SM project aims to provide such recommendations in the near future.

4.4.3 Spatial data coverage

As mentioned, the ISMN is the most important reference database for large-scale satellite soil moisture validation. Nevertheless, there is a strong spatial bias of station coverage (see https://ismn.earth/en/dataviewer/). The majority of in situ stations contained in the ISMN are located in grasslands or croplands (see Figure 1) while barren and woody areas remain underrepresented. Since satellite retrieval quality varies greatly depending on the land cover, care must be taken when interpreting summary statistics of supposedly "global" validation results obtained

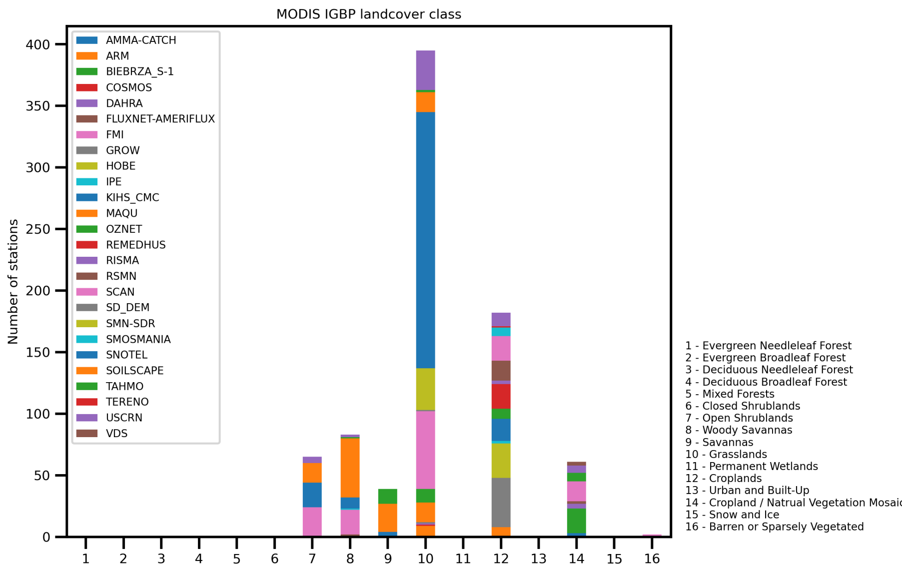

Figure 1: Number of ISMN stations per MODIS land cover class.

from the ISMN (or any other large-scale ground reference database). It is therefore recommended to summarize validation results per land cover class. The FRM4SM project also endorses any activities related to SM reference data collection in under-represented regions. Such data should be integrated in the ISMN.

4.5 Implementation

The Quality Assurance for Soil Moisture (QA4SM) online validation platform (https://qa4sm.eu/ui/home), which is an integral part of the FRM4SM project, adheres to the guidelines provided above. While reference station selection criteria can be changed manually, the FRM selection criteria proposed in this FPP-SM document are applied by default. More details about the QA4SM platform and its evolution within the FRM4SM project can be found in deliverables DT3-1 (AWST 2023b) and DT4-3 (AWST 2023a).

5 Traceability and Uncertainty Budget Analysis

This section applies the guidelines from the QA4EO framework (https://qa4eo.org/documents.php; last accessed: December 2022), which build upon the metrology "Guide to the Expression of Uncertainty in Measurement" (BIPM et al. 2008), to define a protocol for obtaining a traceable uncertainty budget for SM FRMs. These guidelines recommend the following 5 steps, which will be detailed in the following subsections.

1. Define the measurand and measurement model
2. Establish the traceability with a diagram
3. Evaluate each source of uncertainty and fill out an effects table
4. Calculate the data product and uncertainties
5. Record information about the uncertainty analysis for long-term data preservation purposes (implicit above) and summarise for today's users

5.1 Measurand and measurement model

SM FRMs are intended to validate satellite SM retrievals. The measurand is thus the average soil moisture within a satellite footprint at the time of satellite overpasses. The measurement model is thus best considered as comprising four steps: (i) calibration of the sensor reading; (ii) unit conversion (optional); (iii) temporal alignment with satellite overpass times; and (iv) (up)scaling to the satellite footprint scale. Formally, this could be written as:

$$\begin{aligned} SM^{g}_{t_g} &= c(\mathbf{X^g_{t_g}}, \mathbf{C}) + 0 \\ SM^{g'}_{t_g} &= u(\mathbf{SM^g_{t_g}}, \mathbf{U}) + 0 \\ SM^{g'}_{t_s} &= t(\mathbf{SM^{g'}_{t_g}}, \mathbf{T}) + 0 \\ SM^{s}_{t_s} &= s(\mathbf{SM^{g'}_{t_s}}, \mathbf{S}) + 0 \end{aligned} \tag{23}$$

where the superscripts refer to the measurement support at the ground (g) and satellite scale (s); g' refers to the unit-converted ground measurement; and the subscripts refer to the measurement times of the ground sensors (t_g) and the satellite overpasses (t_s). $c(\cdot)$ is the application of the measurement calibration function (see Section 2) using the sensor readings $X^g_{t_g}$ and calibration parameters $\mathbf{C}$. $u(\cdot)$ is the unit conversion from the calibrated SM readings $SM^g_{t_g}$ into the satellite retrieval space using the unit conversion parameters U. $t(\cdot)$ is the temporal alignment of the unit-converted sensor SM readings $SM^{g'}_{t_g}$, possibly using temporal interpolation or aggregation methods that require the parameters $\mathbf{T}$. $s(\cdot)$ is the (s)scaling function that converts the temporally-aligned SM readings $SM^{g'}_{t_s}$ to the satellite scale, possibly averaging measurements from different sensors that fall within the footprint, using the parameters $\mathbf{S}$. The "plus zero" term acknowledges the inadequacy of the functions to account for all phenomena that actually affect the measurement but are unknown in magnitude.

Recall that, as described in Section 2, a plethora of SM sensing technologies exist which rely on distinctive measurement techniques (from dielectric measurements to gravimetric measurements to the counting of slow neutrons) and calibration strategies (e.g., laboratory-based vs. field-based). Since most in situ network operators (including virtually all ISMN networks) do not provide any information on sensor installation or calibration, no specific functional shape for the calibration can be provided in Eq. 23. Similarly, different methods exist for the temporal alignment with satellite overpass times (e.g., averaging all measurements within a day, temporal interpolation, imposing different maximum-distance thresholds, etc.) and the upscaling to the satellite footprint scale (e.g., simply assuming a single sensor to be representative or averaging multiple sensors with different weighting strategies).

No strict guidelines exist for these issues, nor would such guidelines always make sense because the methods required are often circumstantial and require trade-offs that are, to some degree, subjective and application dependent. Therefore, the uncertainty budget analysis framework provided here is kept general to be applicable to any given SM reference dataset and application. Note, however, that the FRM4SM project is actively working towards providing standardized guidelines wherever meaningful.

5.2 Traceability

Metrological traceability is defined in the International Vocabulary of Metrology as the "property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty". To establish this "documented unbroken chain of calibrations", the QA4EO framework recommends using so-called traceability diagrams to identify all sources that contribute to the uncertainty of the measurements. A traceability diagram for the measurement model of SM FRMs is provided in Figure 2. Its components are discussed in the next section.

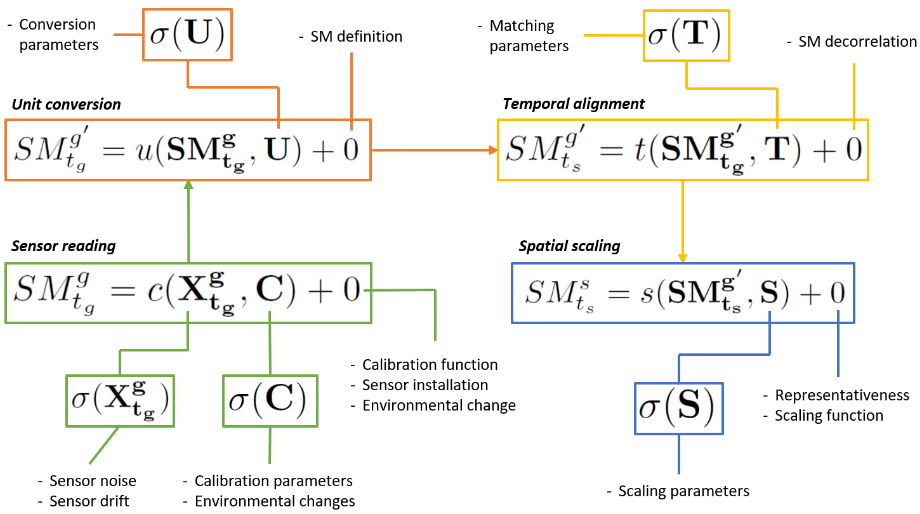

Figure 2: Traceability diagram for SM FRMs.

5.3 Sources of uncertainty

The QA4EO framework recommends summarizing all sources of uncertainty identified in the traceability diagram, also referred to as effects, together with their characteristics in a so-called effects table. Such an effects table associated with the traceability diagram in Figure 2 is shown in Table 4.

Table 4: Effects table. The following coding is used. Type: R=Random, S=Systematic; Correlated: Y=Yes, N=No, P=Potentially; Confidence: 0=Effects identified, no quantification; 1=Estimates only; 2: Some analysis performed to evaluate; 3: Rigorous analysis performed. Magnitudes are given in $m^3 m^{-3}$; * assuming that some experience with sensor installation is given; ** not including total sensor loss

Effect	Type	Correlated	Magnitude	Confidence
Sensor noise	R	N	0.01–0.1	2
Sensor drift	S	N	0	1
Calibration function	S	P	0.01–0.07	2
Calibration parameters	S	P	0.0–0.07	2
Sensor installation	S	P	0–0.5*	1
Environmental factors	R+S	P	0–0.7**	1
Conversion parameters	S	P	0.01 –0.03	1
SM definition	S	P		0
Matching parameters	S	P	0–0.01	1
SM decorrelation	R	P	0–0.04	2
Scaling parameters	S	P	0.05–0.1	1
Scaling function	S	P	0.05–0.1	1
Spatial representativeness	R	P	0.01–0.07	3

Random effects are errors that are independent of one sensor measurement to the next whereas systematic effects are errors that persist over some periods of time. Non-correlated effects are errors that affect only individual soil moisture sensors whereas correlated effects are errors that may affect several sensors at the same time (usually sensors in proximity). The following subsections discuss the various effects in more detail.

5.3.1 Effects related to sensor reading and calibration

5.3.1.1 Sensor noise and drift

Like all electronic instruments, SM sensors are subject to random instrument noise and sensor drift due to ageing. Estimates for the uncertainties of the sensor SM readings are often provided by the manufacturer (see effects table 4). However, since there seems to be no standard in how to provide technical specifications for the sensors, comparison of sensor manuals and the specifications given from different producers is challenging, also because usually little information is given about how they were obtained. Based on personal communication with sensor produces and operators, sensor drift due to aging electronics appears to be negligible for at least 5 - 10 years.

One challenge in interpreting sensor noise specifications is that the sensor producers usually refer to unknown conditions (probably laboratory) using some soil sample with only generic specifications of the properties. That is, it is unclear whether specifications refer to a medium-specific calibration, inorganic or mineral soils, soil specific calibration for fine textured soils, etc.. Therefore, it can be assumed that the conditions used by the sensor producer to estimate uncertainties resemble the conditions for which a sensor is going to be used lateron. Further investigations and collaborations with the sensor producers are needed and planned to be conducted in the next CCN project phase to obtain reliable and traceable estimates of the influence of these effects.

5.3.1.2 Calibration function and parameters

The relationship between sensor readings (i.e., a measurand such as capacitance or permittivity) and VWC is established through a calibration function, which can introduce additional, mostly systematic, uncertainties if the calibration function is not appropriate for the soil conditions (e.g., a calibration function for mineral soils is applied to sensor readings made in organic soils), or if calibration parameters (e.g., sand or clay content) are inaccurate. Also, even if sensors have been field-calibrated using e.g., gravimetric samples, as is commonly recommended (Montzka et al. 2021), SM sensors only measure proximal variables (e.g., capacitance) that are related, but not identical, to VWC. Experiments are needed to obtain reliable and fully traceable estimates of the uncertainties associated with these effects.

5.3.1.3 Sensor installation and environmental factors

Additional uncertainties are introduced once a sensor is placed in the field, which may be both random and systematic. Soil properties will not entirely match the reference sample, the sensor installation is subject to various sources of error (e.g., unintended compression of the soil, bad soil contact of the rods, water flowing down badly placed cables, etc.), and the sensor is under continuous environmental influence (soil erosion, freezing and thawing, animals, extreme weather events such as washout after floods or soil cracking during drought, gravity-induced soil movement, etc.).

Little is known about the magnitude of the uncertainties associated with these effects, but they are expected to be potentially large. For example, if not properly installed, sensors placed in the topmost soil layer might be washed out entirely by severe rainfall. A first estimate for the effect of sensor installation was made assuming the person has some experience on how to install a sensor properly. However, it is highly recommended to conduct experiments to understand common magnitudes of uncertainties related with poor sensor installation better.

Furthermore, estimates for the impact of environmental factors have been made with care (not included is total sensor loss, see table 4) with the assumption that they can have similar results as improper installation effects, since a sensor can lose contact due to extreme weather events especially for sensors in the upper soil layer (e.g., during a heat wave).

While it is generally recommended to verify the proper functioning of sensors placed in the field and to recalibrate them regularly (Thorne et al. 2018, WMO 2018), experiments are needed to obtain traceable estimates of uncertainty related to environmental influence.

5.3.2 Effects related to unit conversion

In situ sensors use diverse measurement techniques that measure properties related to soil moisture (e.g., resistance, capacitance, or cosmic ray neutrons), which are converted into soil moisture using calibration functions (see Section 2). However, soil moisture can be expressed in different ways (e.g., soil water content, SWC, or soil water potential, SWP). The satellite SM community has established VWC as a standard unit for soil moisture in which most products are provided. SM FRMs, therefore, might need to be converted into this unit before they can be used to validate satellite products.

5.3.2.1 SM definition and conversion parameters

There are two sources of uncertainty associated with this unit conversion: The possible inaptness of the conversion function to properly account for the differences between the respective definition, and inaccuracies in the conversion parameters. Both of these effects can be expected to be largely systematic, but no quantitative estimates of their possible magnitude exist yet.

5.3.3 Effects related to temporal alignment

Both in situ and satellite measurements are distinct snapshots with negligible measurement integration times. Ideally, one wants FRMs to be taken at the exact same time of the satellite overpass. Most in situ measurements provide data frequently (e.g., hourly), and the temporal offset to satellite overpasses is usually small. It is possible to interpolate between measurements to account for remaining time differences, yet this is not commonly done and it is not expected to be of any significant importance at a sub-hourly scale.

When comparing more than one satellite data product against ground reference measurements, however, it is generally recommended to use the exact same reference measurements to ensure fair comparison (Gruber et al. 2020). Since time differences between the observations of different satellite missions can reach from hours to days, choices need to be made about which reference measurement times to use for the comparison and how large a time difference is allowed before masking out data points. The intuitive solution of using ground reference measurements that fall exactly in the middle between satellite observation times is not necessarily the fairest option because temporal SM auto-correlation is asymmetrical due to the different SM behaviour before and after rainfall events. No clear recommendations exist yet for these choices, but the FRM4SM project aims at developing them in the future.

The temporal misalignment between reference measurements and satellite overpasses also introduces uncertainties that are both systematic (in situ measurements before a satellite overpass will usually be larger, measurements taken after will generally be smaller) and random (due to unpredictable rainfall events).

5.3.3.1 Matching parameters

The systematic component of these errors could partially be accounted for, e.g., by interpolation between measurement times. However, this is not been done and visual time series inspection of in situ measurements in different geographic regimes suggest that these effects are usually small. More research is needed, however, to obtain quantitative estimates.

5.3.3.2 Soil moisture decorrelation

The random error component originates from a decorrelation between soil moisture at different time stamps due to random precipitation events. The magnitude of these uncertainties will vary greatly with the characteristics of the land surface (soil texture, topography, etc.) and the atmosphere (rain fall probabilities, temperature patterns, etc.). The combined effect of these characteristics can be quantified using estimates of temporal SM auto-correlation (Gruber et al., in prep.). Since raw SM time series are correlated over periods of weeks to months, uncertainties introduced by a time offset of hours to days can be considered largely negligible. SM anomalies, however, usually decorrelate in a matter of days. Short time offsets can thus already introduce significant uncertainties that need to be considered in the uncertainty budget calculation. Preliminary analyses suggests that effects can reach up to 0.04 $m^3\,m^{-3}$.

5.3.4 Effects related to spatial scaling

The scale gap between in situ sensors and satellite footprints can be addressed by either assuming a station to be representative for the entire footprint or to aggregate multiple stations within the footprint. In most parts of the world, only single stations are available. In both cases, an additional adjustment of the mean, the variance, and possibly higher moments can be applied to account for systematic differences at the different scales (Gruber et al. 2020).

5.3.4.1 Scaling parameters and scaling function

Uncertainties might be introduced by the inaptness of the scaling function to properly describe the relationship between scales (e.g., not properly accounting for sub-pixel variations in land cover, topography, or soil texture) or by inaccurate scaling parameters (e.g., applying an unweighted average where more weights ought to be put on stations that are located closer to the footprint centre or in more representative areas. Experiments that assess the magnitude of uncertainty related to the spatial scaling function and parameters are still lacking. Nevertheless, studies that investigated the statistical properties of soil moisture suggest that failing to account for scale differences might result in a systematic difference in soil moisture of up to 0.05–0.1 $m^3\,m^{-3}$ (Famiglietti et al. 2008)

5.3.4.2 Representativeness error

In addition, no realistic number of measurement locations, let alone single stations, can sample the actual soil moisture variations that are observed by a satellite, not least because the measurement support of satellite instruments is ill-defined (penetration depth varies depending on moisture content, signal strengths decrease from the footprint centre outwards, etc.). Random differences between the SM signals observed by an in situ sensor and a satellite footprint are commonly referred to as representativeness error. As already mentioned, the SM community has established TCA as the standard method for quantifying the combined in situ measurement plus representativeness uncertainty (Chen et al. 2016, Gruber et al. 2020, 2013) as:

$$\sigma_{\varepsilon_i} = \sqrt{\sigma_i^2 - \frac{\sigma_{i,x}\sigma_{i,y}}{\sigma_{x,y}}} \tag{24}$$

where σ_{ε_i} is the combined in situ measurement plus representativeness uncertainty, σ_i^2 is the temporal variance of the in situ time series; and $\sigma_{i,x}$, $\sigma_{i,y}$, and $\sigma_{x,y}$ are the temporal covariances between the in situ time series and two auxiliary data sets x and y. These auxiliary data sets are usually either one active-microwave-based and one passive-microwave-based remote sensing soil moisture product, or one remote sensing soil moisture product and one modelled soil moisture data set. Importantly, the errors of all three data sets must be independent of one another. For more details on TCA, see (Gruber et al. 2016).

A study by Famiglietti et al. (2008) suggests in situ measurement errors are usually negligible compared to representativeness errors. A study by Gruber et al. (2013) thus suggests that representativeness uncertainty across ISMN stations often ranges from about 0.01 to about 0.07 $m^3\,m^{-3}$.

5.4 Calculating SM and its associated uncertainty

When calculating estimates for the measurand, all known uncertainties should be taken into account by propagating them through the measurement model using either the Monte Carlo method or the Law for the Propagation of Uncertainties BIPM et al. (2008).

However, for SM, most contributing effects have not been assessed with a sufficient level of maturity to do so. Instead, the SM community has established triple collocation analysis as an accepted method to provide Type B uncertainty estimates[3] for in situ SM reference measurements at the satellite scale (Chen et al. 2018, 2016, Gruber et al. 2016). These estimates are lumped estimates of the total uncertainty budget originating from all effects identified in Figure 2 and Table 4, and they are provided for ISMN stations in the QA4SM online validation platform. As discussed in Section 5.3, more research and experiments are needed to disentangle all these effects and obtain SI-traceable, quantitative estimates for all sources of uncertainty.

Note that the QA4EO SM has developed the CoMet python toolbox (https://github.com/comet-toolkit; last accessed: December 2022) to aid the calculation of uncertainty budgets according to metrological principles. This toolkit was developed to provide quality-assured code to store and propagate uncertainty and error-correlation information. Once all effect magnitudes and processing functions in the traceability chain (see Figure 2) are known, one could use the CoMet toolbox to propagate the uncertainties end-to-end to obtain the total error budget.

5.5 Data documentation and preservation

For consistency, continuity, and comparability purposes it is vital that products as well as their uncertainties are well documented and that these documentations remain accessible for long periods of time.

Within the FRM4SM project, a system has been developed that allows assigning DOIs to data downloads of the ISMN (see deliverable DT1-1; Himmelbauer et al. 2023). These DOIs allow the long-term access of the ISMN data as well as their associated QIs. Moreover, the QA4SM online validation platform allows the creation of DOIs for the results obtained with a chosen validation setup (see deliverable DT4-3; AWST 2023a). These results also include the above-described TCA-based estimates for in situ station uncertainty. In addition, any documentation of product uncertainty analyses should remain accessible and findable at least for as long as the assessed product is accessible and being used.

[3] Type A uncertainties refer to uncertainty estimated obtained by a statistical analysis of measured quantity values obtained under controlled measurement conditions, i.e., as the spread of repeated measurements of a known stable target. Type B uncertainties are uncertainty estimates obtained by any means other than a type A evaluation of measurement uncertainty (BIPM et al. 2008).

6 FRM4SM guidelines

The following provides a summary of all guidelines about how to select and use FRMs for validating radiometer-based satellite SM products.

- **Instruments and installation:** For operation of in situ soil moisture stations, We endorse the guidelines provided by the WMO Guide to Instruments and Methods of Observation (WMO 2018). In addition, specific recommendations about the establishment and maintenance (e.g., regular sensor re-calibration) of fiducial reference networks are provided by Thorne et al. (2018).
- **FRM selection:** FRMs ought to be selected following the protocols provided in Section 4. In addition, we endorse the use of SMAP Core Validation Sites (Colliander et al. 2017b) as the most reliable satellite footprint-average SM reference data.
- **Validation procedures:** We endorse the validation protocols provided by Gruber et al. (2020) and Montzka et al. (2021). We also endorse the QA4SM platform (https://qa4sm.eu/) to be used for satellite product validation, which adheres to the recommendations and guidelines in these and the present FPP-SM documents. For the evaluation of high-resolution soil moisture data sets, we endorse the methods proposed by Crow et al. (2022).

7 Roadmap

Significant progress has been made in the FRM4SM project to develop guidelines for selecting FRM stations and establishing traceability of their uncertainties. Advances have been made in particular concerning the characterization of uncertainties related to the spatial and temporal representativeness of FRMs, which are expected to constitute the largest fraction of their uncertainty budget.

The greatest obstacle for the estimation of a complete, traceable uncertainty budget, however, remains the lack of guidelines for installing, maintaining, assessing, and documenting FRM networks that comply with metrological principles. Some guidelines are provided by the WMO (see Section 3; WMO 2018), yet these mainly refer to manufacturer recommendations. Unfortunately, manufacturers themselves do not provide recommendations regarding the compliance with metrological practices. More detailled guidelines for the establishment and operation of "fiducial reference networks" are provided by Thorne et al. (2018).

However, as yet, most ground reference datasets do not comply with these recommendations and also do not provide any information about how sensors were installed and calibrated. Efforts will thus be undertaken to obtain reliable quantitative estimates of the magnitude of uncertainty associated with a lack of this information, as well as all other uncertainty sources that are yet poorly understood.

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