

Fiducial Reference Measurements for Soil Moisture (FRM4SM)

Contract No. 4000135204/21/I-BG.

Executive Summary Report

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Centre d'Études Spatiales de la BIOsphère (CESBIO)

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Acronyms

AWST Angewandte Wissenschaft, Software und Technologie GmbH.

BAFG Bundesanstalt für Gewässerkunde.

CEOS Committee on Earth Observation Satellites.

CESBIO Centre d'Études Spatiales de la BIOsphère.

DOIs Digital Object Identifiers.

EO Earth observation.

ESA European Space Agency.

FPP-SM FRM Protocols and Procedures for Soil Moisture.

FRM Fiducial Reference Measurement.

FRM4SM Fiducial Reference Measurements for Soil Moisture.

GEO Group on Earth Observations.

GMU George Mason University.

ISMN International Soil Moisture Network.

NPL National Physics Laboratory.

QA4EO Quality Assurance for Earth Observation.

QA4SM Quality Assurance for Soil Moisture.

QI Quality Indicator.

R&D Research and Development.

ROI Return On Investment.

SAG Scientific Advisory Group.

SMOS Soil Moisture and Ocean Salinity.

TU Wien Technische Universität Wien.

USDA US Department of Agriculture.

WMO World Meteorological Organization.

1 Introduction

This is the executive summary report of the Fiducial Reference Measurements for Soil Moisture (FRM4SM) project, which was carried out by Angewandte Wissenschaft, Software und Technologie GmbH (AWST), Technische Universität Wien (TU Wien), and Centre d'Études Spatiales de la BIOsphère (CESBIO), it ran from May 2021–April 2023 (Phase 1) and was extended as part of a Contract Change Notice from May 2023–December 2024 (Phase 2) under European Space Agency (ESA) contract No. 4000135204/21//I-BG. This report provides a synthesis of all work done in the FRM4SM project. An in-depth description of the project results is provided in the final report and the respective work package technical notes, which can be found on the project website (https://www.geo.tuwien.ac.at/project-frm4sm/resources/documents/).

This document is built up in the following sections:

- Section 2 provides the scientific background that has led to the FRM4SM project.
- Section 3 describes the initial FRM4SM project phase:
  - Section 3.1 details the goals, tasks, structure, and timeline of FRM4SM.
  - Section 3.2 describes activities related to in situ measurements and the assessment and characterization of their quality.
  - Section 3.3 describes activities related to the assessment and analysis of traceable uncertainty budgets for FRMs.
  - Section 3.4 describes maintenance and evolution activities of the Quality Assurance for Soil Moisture (QA4SM) online validation platform.
  - Section 3.5 details validation case studies based on the Soil Moisture and Ocean Salinity (SMOS) mission.
  - Section 3.6 reports on dissemination activities of the project.
  - Section 3.7 concludes the project and provides a roadmap for future scientific developments.
- Section 4 describes the extended FRM4SM project phase:
  - Section 4.1 describes the evolution of FRM Methodologies.
  - Section 4.2 describes maintenance and evolution activities of the Quality Assurance for Soil Moisture (QA4SM) online validation platform.
  - Section 4.3 details validation case studies based on the Soil Moisture and Ocean Salinity (SMOS) mission.
  - Section 4.4 reports on dissemination and outreach activities of the project.

2 Scientific background

Despite the recognized importance of satellite soil moisture data products (*WMO*, 2022), little regard has been given so far to a clear definition of what constitutes a "good" product and how accuracy ought to be assessed. Until this day, the almost universally-cited (*Entekhabi et al.*, 2010) and officially-endorsed (*WMO*, 2022) satellite retrieval accuracy requirement of 0.04 m^2m^{-2} for satellite soil moisture data products is not justifiable on scientific grounds and usually ill-defined as to how it ought to be assessed (*Gruber et al.*, 2020).

To address the lacking consensus on validation practices, the satellite soil moisture community has recently developed good-practice guidelines for the validation of satellite soil moisture products, including recommendations for ground sampling, sensor calibration, in situ–satellite intercomparison, metrics to be used, data preprocessing, and various other issues (*Gruber et al.*, 2020; *Montzka et al.*, 2020). However, statements on ground sampling and calibration only partly complement the recommendations laid out by the World Meteorological Organization (WMO) Guide to Instruments and Methods of Observation (*WMO*, 2021), which endorse the adherence to metrological practices (*BIPM et al.*, 2008) but provide little actual

guidance regarding calibration, operation, and maintenance other than statements to follow manufacturer's recommendations.

At the same time, awareness about metrology has been growing in the EO community more generally (*Merchant et al.*, 2017). To foster the application of metrological principles to satellite data validation, the Quality Assurance for Earth Observation (QA4EO) framework has been established, which is endorsed by the Group on Earth Observations (GEO). QA4EO aims at providing a consistent approach across disciplines to establish fully-traceable Quality Indicators (QIs) for fundamental data records, thematic data products, and FRMs so users can assess suitability for their applications, i.e., the "fitness for purpose". A central element of these guidelines is the traceability of uncertainty and so-called fiducial reference measurements (FRMs).

ESA defines FRMs as "a suite of independent, fully characterized, and traceable ground measurements that follow the guidelines outlined by the GEO/ CEOS 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. FRM4SM is one such project aiming at:

- assessing existing, and defining new QIs that provide the best possible understanding of in situ soil moisture data quality;
- defining protocols and procedures to establish traceability for soil moisture product uncertainty, and to select FRM "super sites";
- developing and evolving the QA4SM online validation service for both satellite soil moisture products and in situ data; and
- demonstrating the project findings through dedicated SMOS validation case studies.

These individual activities were continued from and based on earlier activities by the partners of the project team: TU Wien has managed and evolved the ISMN network for more than ten years and has been working on evolution and standardisation of quality control principles for the ISMN in several earlier projects. AWST, together with TU Wien, has originally developed the QA4SM validation service with funding from the Austrian Research Promotion Agency's Space Applications Programme to reduce the validation effort for satellite soil moisture products while ensuring a clearly defined validation standard and full traceability between inputs and results. CESBIO has been heavily involved in the production and validation of SMOS soil moisture products from the start of the SMOS mission. FRM4SM aims to bring the experience from these areas together, and focus on soil moisture data validation and FRMs from all relevant perspectives to eventually set up a full FRM-based validation system for soil moisture data on a solid and well-defined basis. While this may be a far reaching objective, the FRM4SM project has indeed made substantial steps in this direction, which will be described in the following sections.

3 Initial project phase

The initial FRM4SM project was carried out from May 2021 through June 2023. The three main areas of activity were:

1. R&D on ISMN quality indicators & FRM specification (TU Wien);
2. QA4SM evolution (methodological R&D and implementation) and maintenance (AWST, TU Wien);
3. R&D to further develop the validation methodology for SMOS Soil Moisture products (CESBIO).

3.1 FRM4SM Project overview

The FRM4SM project was organised in five major tasks for a total period of two years, where each task was defined by objectives, which were mapped to requirements. Figure 1 shows an overview with the mapping of project tasks to their pertinent objectives and requirements.

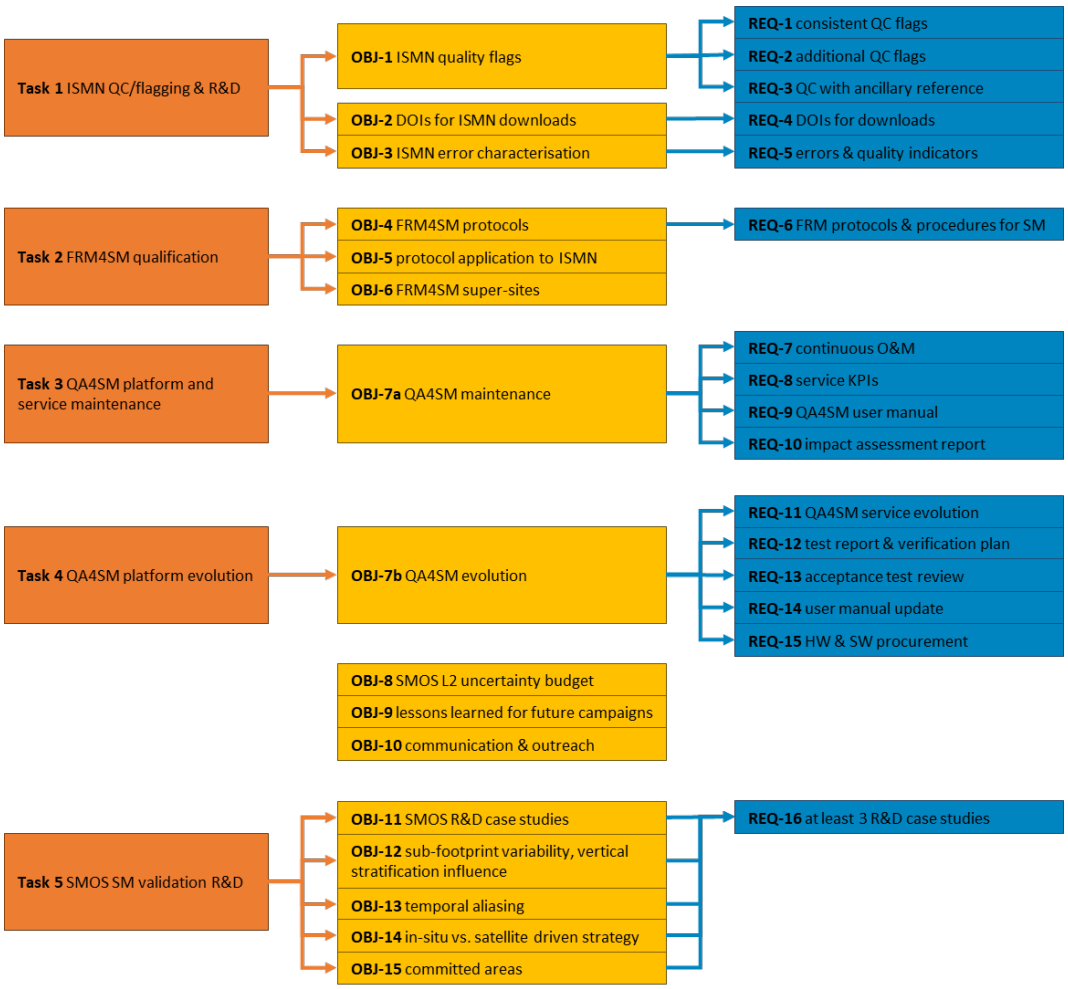


Figure 1: FRM4SM project tasks, objectives and requirements

Task 1 focused on Research and Development (R&D) activities to qualify FRM in-situ data from the ISMN stations network. The objectives were to develop relevant quality flags, to define and improve the error characterisation and to introduce Digital Object Identifiers (DOIs) for ISMN data downloads.

Task 2 was geared towards the specification of FRM protocols and procedures for soil moisture data. The initial focus was on the ISMN in-situ data and on the identification of FRM super-sites within ISMN. In a next

stage, the procedures were extended by best practices for validation of satellite-based soil moisture products for both intercomparison of several products and validation against FRM in-situ data. These activities resulted in the FRM Protocols and Procedures for Soil Moisture (FPP-SM) document.

Task 3 and 4 both focused on the Quality Assurance for Soil Moisture (QA4SM) online service, with Task 3 covering continuous maintenance and operations activities of the QA4SM software and hardware platform and Task 4 geared towards the technical and scientific evolution of the service. This evolution started from a baseline, which had already been developed in earlier projects and produced a series of scientific and technical service enhancements, which were made available at https://qa4sm.eu in two major releases.

Task 5 focused on R&D activities to specifically improve the validation methods for soil moisture products retrieved from the SMOS satellite. The pertinent objectives specified a specific set of R&D goals, which were organised into three distinct studies, each resulting in a technical note reporting the outcome.

Each task was led by one of the project partners, with **TU Wien** leading Tasks 1 and 2, **AWST** leading Tasks 3 and 4 and **CESBIO** leading Task 5. AWST also managed the project, while TU Wien had the scientific lead. In order to foster the active exchange with the scientific community, a **Scientific Advisory Group (SAG)** consisting of ten representative members of the international soil moisture data validation, modelling and metrology communities was formed. The SAG also served as a group of key stakeholders to engage the scientific user community of the QA4SM service.

Figure 2 shows, in the form of a symbolic work flow, how all tasks come together, with **ISMN** (left) and **SMOS** (right) R&D activities leading to **FRM and validation protocols** (centre), which are implemented and directly made accessible in the **QA4SM service**, which provides the links between satellite and in-situ data and validation methods. The activities and outcomes of each task are described further in the following sections.

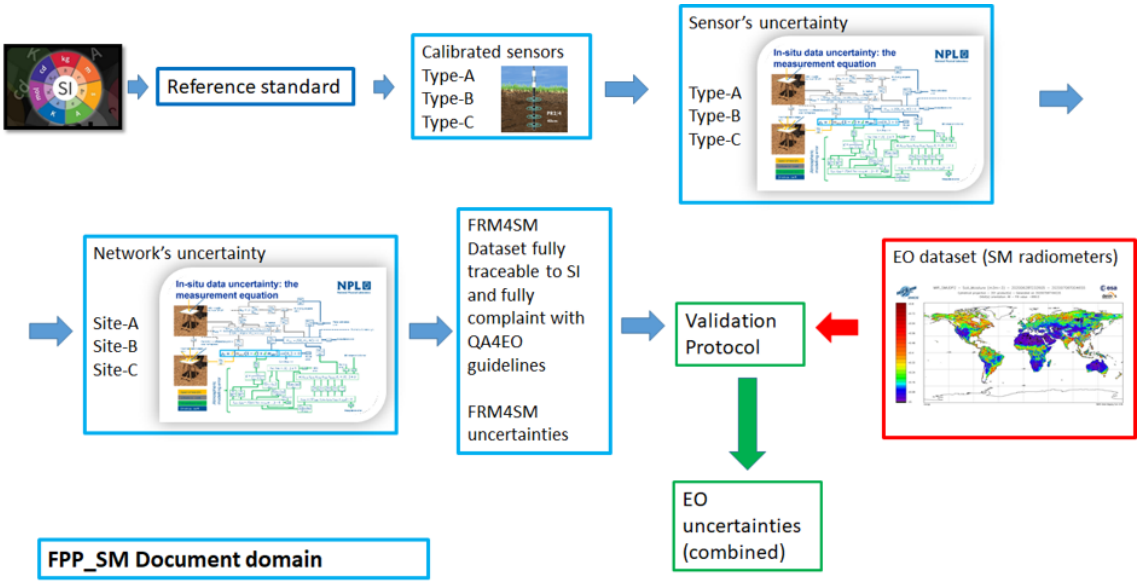


Figure 2: FRM4SM project work flow

3.2 ISMN Quality control and flagging R&D

The main goals of this task were the investigation and further development of the existing International Soil Moisture Network quality control system, the implementation of automatically-generated DOIs, and the assessment of ISMN measurement uncertainties and their description via new and/or improved QIs. The ISMN (https://ismn.earth; *Dorigo et al.* (2021)) is the main source for long-term, reliable in situ soil moisture datasets for the validation and improvement of global satellite products, and land surface, climate, and hydrological models. Therefore, the ISMN also builds the base for understanding in situ soil moisture uncertainty and error traceability studies within the FRM4SM project. TU Wien was the host of the ISMN operations from its initial start in 2009 until end of December 2022. This means that during the project phase 1 of the FRM4SM, a transfer of the ISMN to the new host was also ongoing, shifting certain tasks to an earlier focus while it was still possible to access the backend of the ISMN operations from TU Wien side.

For example, the finalisation of the transfer of the operational Quality Control module (QC) from IDL to python was completed and is now openly available as a python package on GitHub called "flagit" `https://github.com/TUW-GEO/flagit`. The flagit module allows direct collaboration with the new ISMN team in respect to future development of ISMN flags on a time stamp level (per measurement, which in the case of ISMN is mainly hourly). Furthermore, the ISMN data-viewer was modified in the backend and frontend to allow filtering for the best possible dataset for a user's purpose with the option to directly download the filtered data when logged in. This newly created additional advanced filtering option `https://ismn.earth/en/dataviewer/#` is also constructed as a framework to allow easy and sustainable inclusion of new variables in the future e.g., as an outcome of the FRM4SM project, while not disturbing other ISMN initiatives for other communities.

Certain tasks could not be implemented into the ISMN operations as planned since this falls now under the scope of the new ISMN team, the German Federal office for Hydrology (BFG), and the connected International Center for Water resources and global change (ICWRGC). For example, several analyses were conducted to understand data quality on a time series level and to develop new Quality Indicators (QIs). One such QI that was developed and deemed useful to characterise in situ station quality is the spatial representativeness indicator, which is defined as four classes of spatial representativeness for ISMN stations (see Figure 3) estimated using triple collocation analysis (*Gruber et al.*, 2013, 2016, 2020). This QI could not be included in the ISMN as preferred, but has been included instead in the Quality Assurance for Soil Moisture online validation service (QA4SM; `https://qa4sm.eu`; Section 3.4).

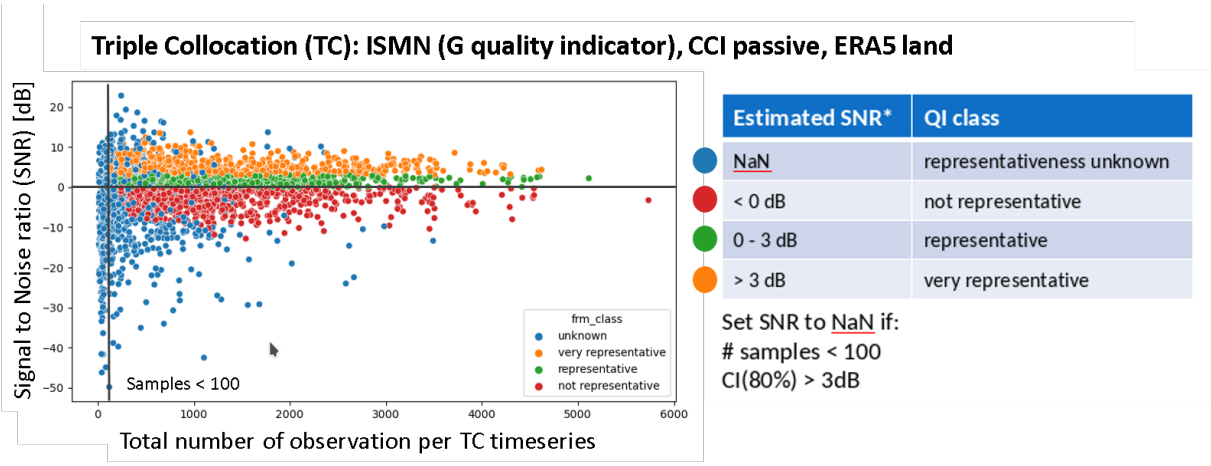


Figure 3: Scatter plot of individual ISMN time series when QI representativeness classification is applied for a Confidence Interval (CI) of 80 % for sensor time series in the upper 10 cm soil.

The investigation of neighbouring in situ sensor behaviour by cross-comparing sensors on the basis of autocorrelation and spatial decorrelation (*Dirmeyer et al.*, 2016) for sensors (i) at them same soil layer, (ii) at the same station but within different depths, and (iii) in proximity to the station, did lead to inadequate results to create trustworthy correlation coefficients for the prediction of faulty sensors or sensor degradation. Furthermore, the investigation of the creation of a highly flagged time series indicator could not be completed due to time constraints, but also since this task is highly dependent on the adequate handling of data gaps within time series, which needs to be investigated further and is in general a big question that the satellite community has not yet addressed (e.g., thresholds for data gaps in reference datasets). The creation of an irrigation QI per time series / per station has also been conducted. Such information is not provided by the data originator of the ISMN at the moment and efforts were put into collecting this information which was only possible to some extent and has been forwarded to the new ISMN team. It was found that a general classification of irrigation information (irrigated, not irrigated, or unknown) is more appropriate due to the delicate and political nature of sharing this information openly (e.g., sharing the amount of water per irrigation cycle could lead to legal consequences, etc.).

In order to make ISMN data usage more comparable and reproducible, three different in house versioning systems to version "arbitrary subsets of dynamical data" (*Rauber et al.*, 2021) were implemented and tested (*Staudinger*, 2023). All three systems—referred to as "integrated", "hybrid", and "separated" approach—are in full alignment with the recommendations of the Working Group on Data Citation (WGDC, *Rauber et al.* (2015)) of the Research Data Alliance (RDA) and the Go-FAIR principles, but differ in terms of data storage needs, query performance, the complexity of implementing the system, and the complexity of implementing future changes to the data base structure. After thorough testing, it was concluded that the "separated" approach seems to be the best choice for the productive ISMN system. This approach provides the most flexibility and ease for future changes to the ISMN data base structure without loosing on performance, but requires the largest additional storage space. This overhead is unlikely to be of any concern, however, because data volumes of in situ data are minuscule compared to those of satellite data. This versioning system was then complemented with an in-house issuing Digital Objective Identification (DOI) system for ISMN downloads, which was developed in accordance to the Datacite metadata schema v4.4 https://doi.org/10.14454/3w3z-sa82. The new ISMN team has been included in all discussions and outcome of this task, and they are planning to implement the new modifications in the near future. For more detail, see deliverable DT1-1 on ISMN QC and flagging RD (available at https://www.geo.tuwien.ac.at/project-frm4sm/resources/documents/, last accessed June 2023).

The ISMN data quality module was tested for flags D03 (sm for frozen soil conditions), and D05 (sm rise without precipitation event). These flags were derived with the ECMWF's ERA5 land data product (spatial resolution of 0.1° ; https://climate.copernicus.eu/climate-reanalysis) and compared to the results of the currently used NASA's GLDAS-Noah dataset with spatial resolution of 0.25° (*Rodell et al.*, 2004). The results were unexpected since the spatially coarser data product GLDAS-Noah seems to perform better than the higher

resolution product of ERA5-land, because the former appears to be more restrictive and therefore more in line with the currently stricter set ISMN quality control procedures (over-flagging rather than under-flagging).

Moreover, a pattern search was conducted to understand possible influences of soil, land cover, and climate for ISMN station locations. However, these analyses hinge on the quality of the used ancillary data for these land surface parameters. To investigate the influence of ancillary data for soil texture, the currently used Harmonized World Soil Database version 1.1 (HWSD; FAO/IIASA/ISRIC/ISSCAS/JRC, 2012, FAO, Rome, Italy and IIASA, Laxenburg, Austria) was compared to the ISRIC world soil information dataset SoilGrid version 2 (www.isric.org;*Hengl et al.* (2017); *Ribeiro et al.* (2018)) at ISMN station locations. This comparison was conducted in order to understand how well soil information is represented for the ISMN stations. Further investigations are needed to understand the validity of individual datasets used for soil influences on sensor readings and the overall creation of FRM4SM datasets. As for the influences of land cover, it was found that the ISMN data is much more represented in cropland and grassland for the used ESA Climate Change Initiative (CCI) land dataset (`https://www.esa-landcover-cci.org/`), which needs to be considered and therefore properly weighted in the validation process of satellite data products. Recommendations are given to the new ISMN team to include networks located also in other land cover classes such as e.g., forests, shrubs, etc, to improve validation results. Furthermore, the Köppen-Geiger Climate class dataset from *Peel et al.* (2007) is used within the ISMN and has been updated to the newest version within this project phase. Overall, no clear patterns could be found yet regarding the influence of climate, land cover, and soil texture on soil moisture uncertainty assessments, which could potentially hint at certain influences on data quality but will be further investigated in the next project phase.

3.3 FRM qualification, protocols, and procedures

The main goals of this task were to develop the so-called FRM Protocols and Procedures for Soil Moisture (FPP-SM) to establish traceability for satellite soil moisture uncertainty assessments, and to define criteria to assess whether a given set of in situ data can be considered fiducial. The following FRM selection protocol has been proposed and implemented in QA4SM to select the most reliable subset from the ISMN based on existing and newly-developed QIs for the purpose of satellite soil moisture validation.

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 Section 3.2).
3. Mask out all in situ measurements that are not marked as "good" by the automated flagging system[1] (*Dorigo et al.*, 2013).
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[2].

Metrological traceability is defined in the International Vocabulary of Metrology (VIM; *JCGM*, 2012) 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 define a protocol for obtaining a traceable uncertainty budget for SM FRMs, we followed 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). These guidelines recommend to first

[1] 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] 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

define the measurand and measurement model, which can then be analysed by means of a so-called traceability diagram. This diagram shall then be used to identify all possible sources of uncertainty, also referred to as effects, which can then be assessed quantitatively and summarised in an effects table.

Since SM FRMs are intended to validate satellite SM retrievals, the measurand is 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 can be written as:

$$\begin{aligned} SM^{g}_{t_g} &= c(\mathbf{X^g_{t_g}}, \mathbf{C}) + 0 \\ SM^{g'}_{t_g} &= u(\mathbf{SM^g_{t_g}}, \mathbf{U}) + 0 \\ SM^{g'}_{t_s} &= t(\mathbf{SM^{g'}_{t_g}}, \mathbf{T}) + 0 \\ SM^{s}_{t_s} &= s(\mathbf{SM^{g'}_{t_s}}, \mathbf{S}) + 0 \end{aligned} \tag{1}$$

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 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 $\mathbf{U}$. $t(\cdot)$ 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 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.

The traceability diagram for the measurement model that we developed for SM FRMs is shown in Figure 4. The uncertainty effects that were identified, together with estimates of their magnitude and the confidence in these estimates, are summarised in Table 1.

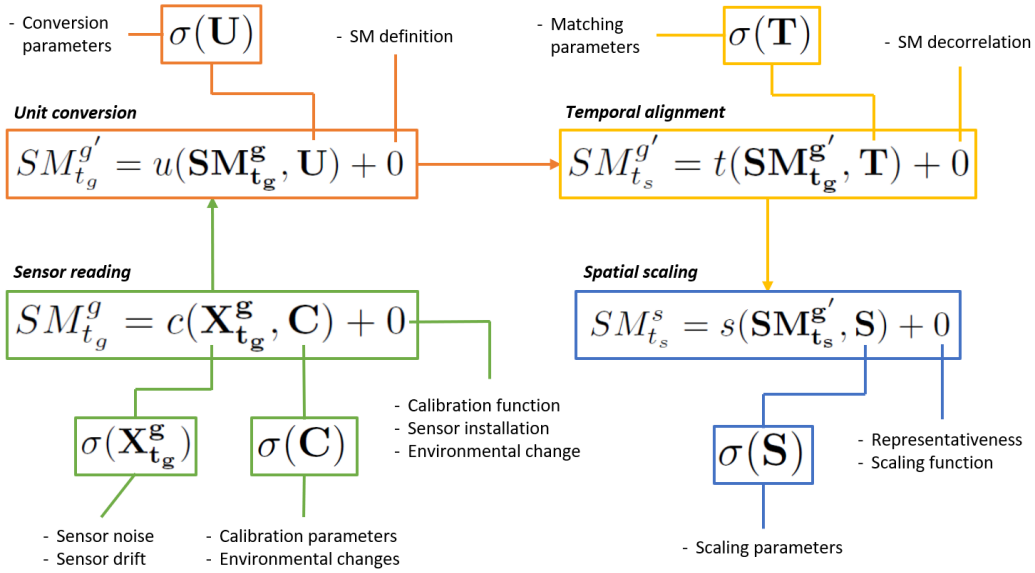


Figure 4: Traceability diagram for SM FRMs.

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

Table 1: 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 $\mathrm{m}^3\,\mathrm{m}^{-3}$; * assuming that some experience with sensor installation is given; ** not including total sensor loss.

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). For a detailed discussion on the various effects, see the FRM Protocols and Procedures for Soil Moisture (FPP-SM, available at https://earth.esa.int/eogateway/activities/frm4sm-fiducial-reference-measurements-for-soil-moisture/project-deliverables). Confidence levels are defined as follows:

0: Effects are known to exist but no quantitative estimates are available.

1: Only qualitative estimates are available, e.g., from visual data inspection or expert communication.

2: Some preliminary laboratory or field analyses have been performed to obtain quantitative estimates for the effect, but the experiment setup may be overly simplified, results were not yet published and/or replicated, or other factors may limit confidence in these estimates.

3: Rigorous experiments have been carried out to estimate the effect size, and the results have been published and replicated by independent groups.

3.4 QA4SM maintanance and evolution

The Quality Assurance for Soil Moisture (QA4SM) online validation service (https://qa4sm.eu, Figure 5) was originally developed with support of the Austrian Research Promotion Agency (FFG) and then further evolved in the FRM4SM project. The service responds to the requirements of the Quality Assurance for Earth Observation (QA4EO)[3] framework for global earth observation of soil moisture.

The QA4SM evolution activities have been aligned with all other FRM4SM activities and results and were structured into two development cycles, each resulting in a major release of the QA4SM service and consisting of the following elements:

1. **Design and implementation**: Evolution items are planned and implemented based on the agile Scrum[4] framework. Continuous software development, testing and integration is performed in a separate test environment while the operational service is continuously operated and kept stable.

2. **Testing and verification**: A Test Plan is developed and executed. Test results are summarised in a Verification Report and observed deficiencies are fixed and retested. A formal Acceptance Review is performed before deployment of the new release to the public QA4SM service.

[3] https://qa4eo.org/
[4] https://www.scrum.org/resources/scrum-guide

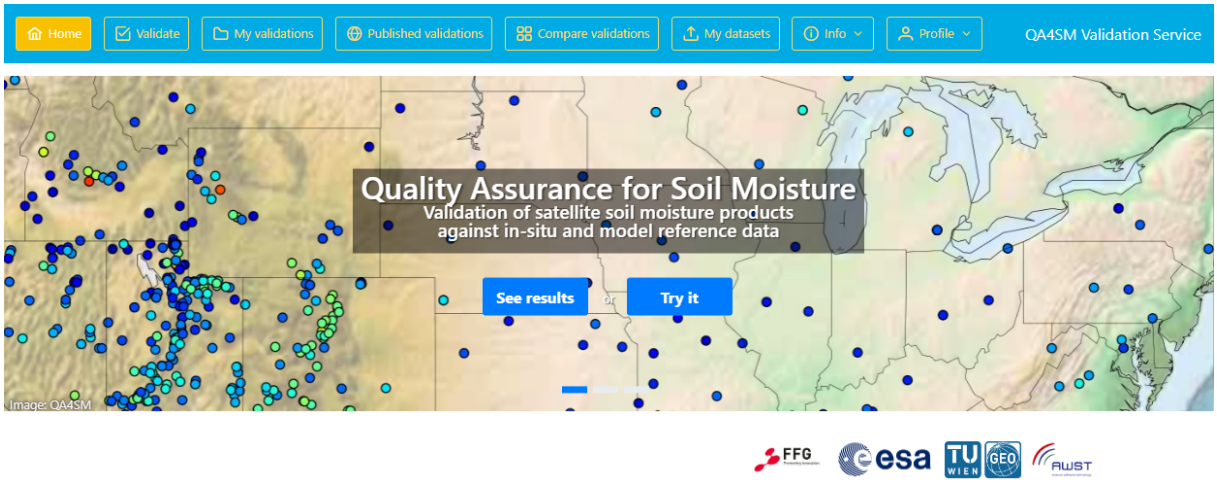


Figure 5: QA4SM online validation service

3. **Deployment and maintenance**: The service release is deployed and made publicly available. The public service is continuously maintained and users are supported via a QA4SM helpdesk. After deployment, the next development cycle begins.

QA4SM Release 1[5] and 2[6] were deployed in June 2022 and March 2023. Figure 6 shows the main phases of QA4SM service maintenance and evolution and the tasks which were carried out in each phase.

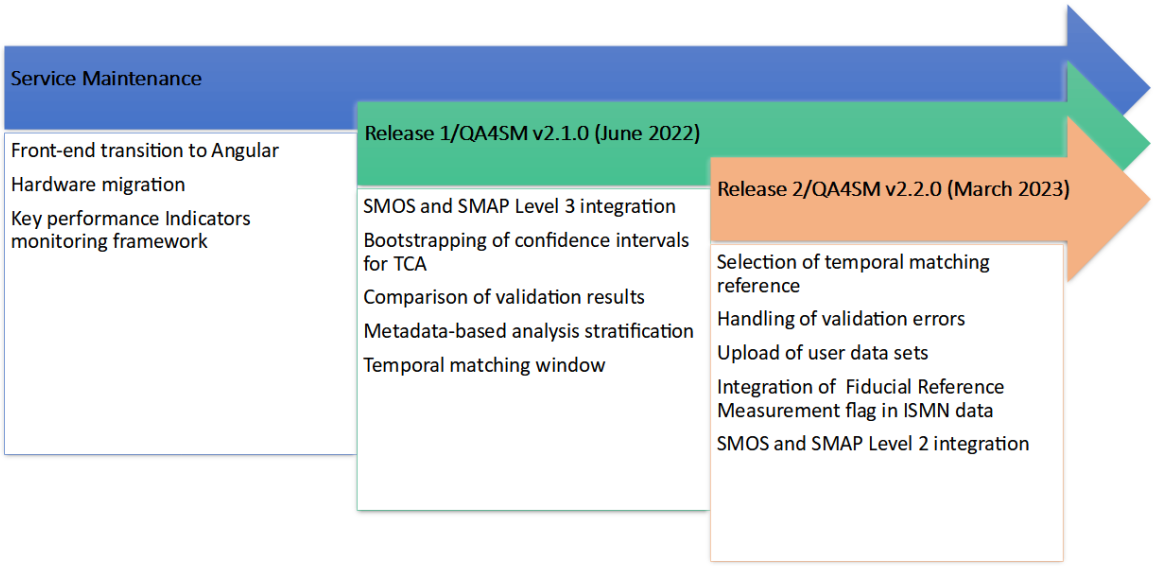


Figure 6: Major development activities, added features and public releases of the QA4SM service.

The following features and enhancements were implemented in QA4SM releases 1 and 2:

- **Software architecture upgrade and service migration:** The QA4SM user interface was newly

[5] qa4sm version 2.1.0
[6] qa4sm version 2.2.0

implemented using the Angluar framework to make the service better extensible for future features and to improve both the service usability and the operational maintainability.

- **Upload of user data for validation:** A feature to upload and validate user data was implemented. Users can upload data in NetCDF format or time series data in CSV format, where detailed format descriptions are provided in the QA4SM service. This was the the most requested enhancement by users and led to increased user activity after its implementation in release 2.
- **Comparison of multiple validation results:** A module was introduced that allows users to compare the results of different validations which were performed in QA4SM. The metrics of the selected validations are quantitatively compared and outputs are provided in a table as well as in graphical maps.
- **Handling of validation errors:** There is a range of possible reasons why the data validation may not be possible for certain locations. Nine specific error conditions have been specified and QA4SM was enhanced to detect these error conditions. The validation results include a distribution of validation errors by type and a map showing the geographic distribution of error cases.
- **FRM Quality Indicator Classification:** An FRM quality indicator was developed for ISMN data to characterise ISMN stations as "very representative", "representative" or "not representative". In QA4SM, users can set a filter option to include only "representative" and "very representative" ISMN stations in their validation.
- **Aggregation by ISMN metadata:** A range of ISMN metadata classification diagrams has been added to QA4SM to provide users with additional box plots showing how their validation data locations are stratified by land cover class, Köppen-Geiger climate class, soil type and sensor depth, and FRM class (representativeness).
- **Bootstrapping of confidence intervals:** In certain cases, e.g., for triple-collocation metrics, the confidence intervals cannot be analytically calculated. However, they can be estimated from a synthetic reconstruction of the score distribution using statistical resampling. This bootstrapping method has been implemented where analytic confidence intervals are not available. The resulting confidence intervals are provided in the NetCDF output for validations and in the box plots for each validation metric.
- **Update of the temporal matching routine:** Additional controls have been implemented for users to fine tune the temporal matching method for their validations: Users can separately select spatial and temporal reference data sets and they can adjust the temporal matching window in a range from 1 to 24 hours.
- **Integration of new data sets:** A number of additional soil moisture data sets have been integrated into QA4SM and was made available with QA4SM releases 1 and 2. Most prominently, these include SMOS and SMAP Level 2 and Level 3 products, as well as an updated version of the ISMN data set. In total, there are currently 16 featured data sets available in QA4SM, which can be intercompared or validated against each other. Additionally, user data can be validated against one or more selected featured data sets.

A complete description of QA4SM features and validation options is available in the QA4SM Software User Manual v2.0, FRM4SM deliverable DT4-1.

By the time of writing, 176 users from 32 countries have registered in the QA4SM service. More than 750 validations have been performed with QA4SM, 33 validation results were published with a DOI and QA4SM is referenced in 10 scientific publications. The user activity and feedback has increased with the availability of the option to validate user data in QA4SM release 2.

3.5 SMOS soil moisture validation R&D

The SMOS satellite mission *Kerr et al.* (2001), launched in 2009, was the first satellite dedicated to monitor the absolute value of surface soil moisture at the global scale. Based on an L-band radiometer (1.4 GHz), it provides surface soil moisture estimates from Brightness Temperatures (Vertical and Horizontal polarizations)

from a footprint of ∼43 km, and with a global coverage in three days. The expected accuracy, i.e. the mission requirement, is 0.04 $m^3.m^{-3}$, which is assumed to be achievable for the soil top layer (∼5 cm) only for the specific surface conditions of i) a vegetation water content $\leq$ 5 $kg.m^{-2}$ and ii) a homogeneous land cover distribution within the footprint. To evaluate this accuracy and assess SMOS uncertainties, often called "validation", the method usually consists in comparing the SMOS soil moisture to a reference. The present analysis benefits from the International Soil Moisture Network (ISMN) that provides in situ measurements in various climate conditions (see the red points on the map Figure 7), which are considered as the reference. The objectives are to better understand and assess the SMOS Level 2 v700 performances and uncertainties, and their variability in relation to several geophysical and sampling conditions.

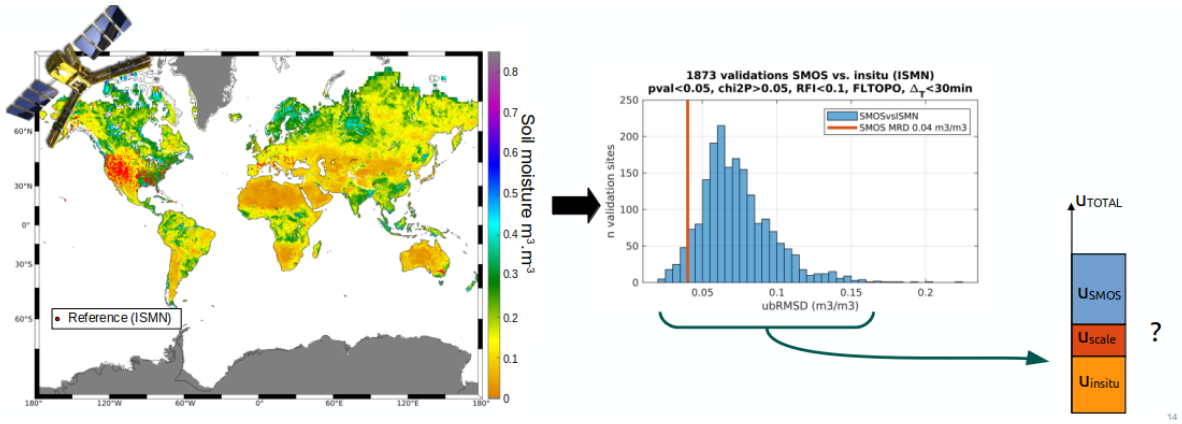


Figure 7: Overview of SMOS uncertainty budget

The analysis is conducted in the context of three case studies:

1. **Case study 1: SMOS committed areas** The first part focused on evaluating SMOS SM performances. A strategy is set up to compute the scores of validation (R, ubRMSD, bias, RMSD). It shows that SMOS is more related to surface soil moisture, which is well documented, but it also shows the impact of surface conditions, which significantly affects the scores. SMOS performs best for low vegetation, low topography, minor presence of water bodies, and sandier soils with a high bulk density within its footprint. Relationships are found between surface conditions and SMOS ubRMSD, which are used to estimate the SMOS uncertainties at a global scale (Figure 8). This allows to characterise SMOS uncertainties also in the controlled surface conditions specified in the mission requirements, whose accuracy is expected to be 0.04 $m^3.m^{-3}$. It is found that SMOS has uncertainties higher than such prescribed accuracy in these favourable areas. Further assessment is thus needed to redefine the geophysical regimes and boundaries within which a committed area can be specified (i.e., a geographical portion where mission requirements are accomplished). In addition to the dependence on the methodology, different sources of uncertainties can impact the validation scores (see Figure 7) such as the reference uncertainty and the scale mismatch. The methodology to derive the uncertainties at the global scale (Figure 8) is a first step towards a more robust one, that needs to be developed. It is the first time such uncertainties are estimated at pixel level, and it is planned to better define and combine the different relationships to assess the SMOS accuracy. A more accurate analysis of the influences of surface conditions will allow us to define the committed areas, and to identify a subset of in situ sites that will be recommended to evaluate coarse-scale satellite soil moisture.

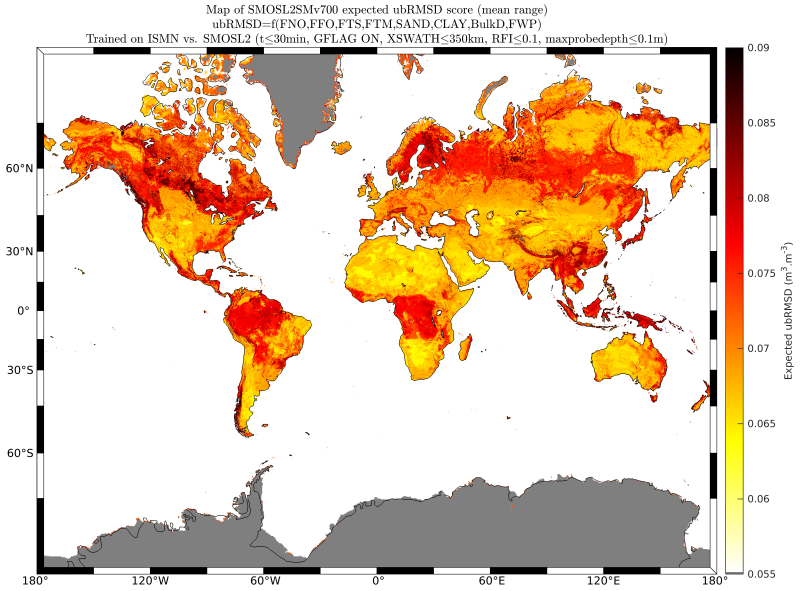


Figure 8: Map of estimated SMOS uncertainty as a function of the surface condition (yellow/low to red/high)

2. **Case study 2: SMOS performance in rich-organic soils** The second part of the analysis focuses on soils having a high organic content. The soil moisture (average and standard deviation) acquired by the in situ sensors does not show any relationship with the Soil Organic Carbon (SOC) content values. One explanation could be the quality of the calibrations and the empty gap within the time series (which can notably appear under snow presence). Indeed, these instruments are very sensitive to the soil type and a special calibration should be considered in rich organic soils.

   SMOS SM shows however a worsening of its performances in the context of organic soils (from SoilGrid database v2020), compared to mineral soils. Further investigations are then needed to better quantify the sensitivity of the dielectric constant models used in SMOS retrieval (Mironov or Bircher) for the particular case of high SOC.

3. **Case study 3: Representativeness and scale mismatch** Finally, the last part focuses on the scale mismatch between the in situ and the coarse scale satellite data. The issue of representativeness is fundamental to evaluate coarse-resolution data with very high-resolution references. The scale mismatches are twofold, as they concern the timescale ($\sim$days for SMOS vs. $\sim$min. for the probes) and the spatial scale ($\sim$43 km of diameter in average for SMOS vs. $\sim$cm for the probes). Several topics are initiated to estimate the different components of this uncertainty budget (seasonal effect, collocation strategy) with first analyses that need to be further developed. The first spatio-temporal scale mismatch analyses between SMOS and the probes provide i) elements on the SMOS performance sensitivity to different features and ii) potential criteria to classify the probes in a Fiducial Reference Measurement (FRM) perspective.

   Concerning the spatial scale mismatch, the use of a subset of probes that have the same surface conditions as the whole SMOS footprint, improves the validation scores, by reducing the uncertainty on the scale mismatch. It is planned to identify the probes and create a subset of in situ that are more representative. For instance, the subset of probes flagged as "good representativeness" from the Quality Indicator, improves the scores. The distance between probes and the SMOS footprint centre is not a good indicator as it does not show any impact on the scores. However, the strategies of spatial collocation (in situ driven versus SMOS nodes driven) is more interesting as they present a significant variability of the scores. Concerning the temporal scale mismatch, the validation scores are sensitive to the time window characteristics (i.e. beginning/end of the time window), especially in climates that are characterised by high seasonality.

3.6 Communication, outreach, and promotion

SAG and QA4SM user engagement

A Scientific Advisory Group (SAG) was formed in the initial phase of the project to provide feedback from key stakeholders and the scientific community and to identify community needs and priorities. The SAG members were:

- Andreas Colliander, NASA
- Michael Cosh, USDA
- Wade Crow, USDA
- Stephan Dietrich, BAFG
- Paul Dirmeyer, GMU
- Carsten Montzka, FZ Jülich
- Emma Wooliams, NPL
- Joaquin Munoz Sabater, ECMWF
- Maria Piles, University of Valencia
- Lothar Schueller, EUMETSAT

The SAG was regularly informed about project activities, milestones and QA4SM service releases and was invited to the QA4SM users workshop in June 2022. A dedicated newsletter was distributed in December 2022. Feedback and input regarding community requirements was continuously collected, further discussed, prioritised and addressed throughout the project. Special emphasis was put on engaging scientific users to experiment with and assess the QA4SM online validation service. In this context, the SAG members took a role as key stakeholders and several SAG members assigned team members to work with QA4SM.

Both, the SAG and user engagement will continue in the next project phase and selected additional members have been invited to join the SAG.

In addition to scientific contacts on an individual basis, contact has also been made with several related projects. In particular, a regular information exchange and mutual discussions about potential areas of collaboration were started with the SoMMet project (https://www.sommet-project.eu/home and mutual points of contact were nominated to further elaborate these discussions in the next project phase.

In July 2022, two members of the FRM4SM project participated in the SMAP Validation Experiment (SMAPVEX22) in Amherst, USA. In November 2022, a presentation to introduce the FRM4SM project was given to the SMAP team.

In December 2022, ISMN operations has been transferred from TU Wien to BAFG, Germany. TU Wien continues to provide scientific advice and is in regular exchange with the new operations team at BFG and ICWRGC.

QA4SM user workshop

A dedicated QA4SM user workshop was organised after deployment of QA4SM release 1 in combination with the 6th Satellite Soil Moisture Validation and Application Workshop in June 2022 at Perugia, Italy. The QA4SM workshop was held with 21 participants on June 7, before the start of the general Soil Moisture Validation workshop. A comprehensive introduction to and demonstration of the QA4SM validation service was provided, followed by a questions and answers session. The main part of the workshop was a guided hands-on session where the participants performed their own validations with QA4SM. This was followed by an open feedback discussion to discuss the future evolution of the service and a survey to collect written feedback. The workshop concluded with a dedicated feedback discussion between the participating SAG members and the QA4SM team.

The feedback from the user workshop was included in the development plan for the next evolution phase and, in particular, the option to upload and validate user data was provided with QA4SM release 2, which was deployed in the public service in March 2023. After notifying the users, increased user activity was observed

in QA4SM, as users started to work with their own data in order to explore how QA4SM may support their respective projects. This also led to an increase in feedback and support requests and the QA4SM team will continue to engage users and to address feedback in the next project phase.

Websites and Social Media

- The QA4SM service is publicly and freely available at https://qa4sm.eu.
- ISMN is hosted at https://ismn.earth.
- An FRM4SM project website has been set up at https://project-frm4sm.geo.tuwien.ac.at and will be migrated to an ESA address soon after completion of this report.
- Information about FRM4SM project activities has also been published in ESA web stories, for example: https://earth.esa.int/eogateway/news/qa4sm-evolution-in-frm4sm-presented-at-sixth-soil-moisture-validation-workshop. Additional web stories are planned in the next project phase.
- Furthermore, project related news and links to relevant milestones, websites, events and workshops has been posted on social media, predominantly on Twitter, to increase the visibility of the information provided through other channels.

Publications

The following publication was accepted during the FRM4SM project:

- Dorigo, W., I. Himmelbauer et al. (2021), The International Soil Moisture Network: serving Earth system science for over a decade, https://doi.org/10.5194/hess-25-5749-2021.

A further publication on the definition of committed areas for SMOS soil moisture products is in preparation at the time of writing this report.

Conference and workshop contributions

Table 2 shows the conferences and workshops where the FRM4SM project was presented. In several cases, separate presentations and posters were presented with a focus on different project activities (ISMN, FRM, QA4SM, SMOS studies).

Conference/Workshop	Location	Date	Website
EGU General Assembly 2022	Vienna, Austria	23-27 May 2022	https://www.egu22.eu
ESA Living Planet Symposium	Bonn, Germany	23-27 May 2022	https://lps22.esa.int
6th Satellite Soil Moisture Validation and Application Workshop	Perugia, Italy	7-9 Jun 2022	https://venti-eventi.com
QA4SM user workshop	Perugia, Italy	7-9 Jun 2022	https://venti-eventi.com
Metrology for Climate Action	Vienna, online workshop	26-30 Sep 2022	https://www.bipm.org/en/bipm-workshops/bipm-wmo-workshop-2022
2nd GCOS Climate Observation Conference	online meeting	17-19 October 2022	www.eventsforce.net/eumetsat/
Global Terrestrial Network Hydrology (GTN-H) panel meeting	online	20 October 2022	https://www.gtn-h.info/about-us/
Introducing FRM4SM to SMAP	online	9 November 2022	https://smap.jpl.nasa.gov/

Conference/Workshop	Location	Date	Website
Kick off SoMMet EU project	online	21 November 2022	https://www.sommet-project.eu/home
ISMN provider workshop #2	online	24 - 25 November 2022	https://ismn.earth
National Physics Laboratory (NPL) meets the FRM4SM	online	12 December 2022	https://www.npl.co.uk/
9ème Colloque Interdisciplinaire en Instrumentation 2023	Grenoble, France	25-27 Jan 2023	https://c2i-2023.sciencesconf.org/
IDEAS-QA4EO Cal/Val Workshop	Potsdam, Germany	28 Feb - 3 Mar 2023	https://earth.esa.int/eogateway/events/ideas-qa4eo-cal-val-workshop-4
EGU General Assembly 2023	Vienna, Austria	23-28 Apr 2023	https://www.egu23.eu
ISMN DOI meeting with GEO, GTN-H and ISMN	Vienna, Austria	27 Apr 2023	https://www.earthobservations.org/index.php
ISMN in house versioning and DOI take over, new ISMN team	online	10 Mai 2023	no link available
SMOS Quality Working Group #36	Frascati, Italy	23-25 May 2023	no link available
LPVE23 - Workshop on Land Product Validation and Evolution	Frascati, Italy, Austria	12-14 Jun 2023	https://nikal.eventsair.com/lpve-2023

Table 2: Conferences and Workshops

3.7 Conclusions and outlook

ISMN and evolution of FRM methodologies

The existing ISMN quality control system was investigated thoroughly and new quality indicators have been proposed. However, several aspects of in situ data quality still need to be characterized better. This includes, for example, the investigation of highly-flagged time series, the development of new spatial and temporal scale-related QIs, such as sub-pixel heterogeneity of soil texture, land cover, or other relevant properties, or the assessment of temporal data gaps and their influence on uncertainty budget estimates.

What has also become clear during the project is that most existing soil moisture networks can not be considered 'fiducial' in the strictest metrological sense, predominantly for a lack of transparency regarding sensor installation and calibration. Little research has been conducted to assess the uncertainty associated with lacking (re)calibration, prolonged environmental influence, and—consequently—to assess satellite soil moisture uncertainty globally in an SI-traceable manner. This is reflected by the low confidence in effect magnitudes reported in Table 1.

By the same token, the ISMN data provider community has, over the past decade, continuously expressed the wish to be provided with more clear instructions on how to operate and maintain in situ sensors in a standardised way that is agreed upon by the community and international authorities (e.g., metrological laboratories, WMO, CEOS, and GCOS).

Taken as a whole, we identify the following research gaps that ought to be addressed in the near future (ordered by priority and feasibility):

- SI-traceable FRM uncertainty budget estimates for in situ networks that follow the FPP-SM guidelines need to be calculated, maintained, and provided publicly wherever possible.

- Guidelines are needed on how to install, operate, and maintain ground reference networks, so they can be considered 'fiducial'.
- Experiments are needed to better estimate and characterise the uncertainty associated with temporal and spatial scale mismatch.
- Experiments are needed to better estimate and characterise periodic uncertainty changes over time associated with annually-recurring events such as vegetation growth.
- Experiments are needed to quantify the uncertainty associated with inapt sensor calibration (e.g., using standard calibration functions over soils with high organic carbon).
- Long-term field experiments are needed to estimate the uncertainties associated with lacking sensor (re)calibration and prolonged environmental influence.
- New FRM networks need to be set up in underrepresented regions such as forests, deserts, or irrigated areas to allow for the estimation of *global* satellite soil moisture uncertainty budgets.

We aim to address (some of) these issues and continuously update community best practices according to the latest scientific developments and in close collaboration with scientific experts in the field over the course of the next project phase.

Finally, we emphasise the vital need for stable FRMs that are operated and maintained long term over diverse land surface conditions, and thus urge funding bodies to consider the benefit of supporting FRM networks for extended periods of time.

QA4SM evolution and maintenance

The QA4SM online validation service has performed reliably and with high availability throughout the full project period of two years. This was possible, as a fully operational baseline of the service was already available from earlier development. Building on this baseline, the iterative evolution effort in the FRM4SM project was structured into two main phases resulting in two major QA4SM service releases. With each release a number of technical, usability oriented, data oriented and scientific improvements were added to the service, including new featured data sets, a new FRM quality indicator, a feature to compare different validation results, the option to share and publish validation results, improved characterisation of uncertainties and more detailed error handling when the validation cannot be performed for certain locations in the data sets.

QA4SM release 2 was deployed in March 2023 and includes all evolution enhancements which were developed in the FRM4SM project. It is complemented with an online tutorial, descriptions of featured data sets, guidelines and format descriptions for uploading and validation of user data and a comprehensive QA4SM Service User Manual (FRM4SM deliverable DT-4.1).

A QA4SM user workshop was held in June 2022 in combination with the 6th Satellite Soil Moisture Validation and Application Workshop in Perugia. Valuable user feedback was collected during and after the workshop and assessed priority requirements were already addressed in QA4SM release 2, most prominently the option to validate user data. This has indeed led to an increase in user activity and additional feedback after release 2 deployment. Such feedback is highly valued and will be addressed in the further evolution of the QA4SM service. The following specific enhancements will be addressed in the next project phase:

- Regular data updates: The featured datasets in QA4SM will be updated in regular intervals to add new data and extend the covered time periods. New versions of data sets will be validated by comparison with the previous versions.
- Automated integration of operational products: Where technically supported by the data providers, we plan to automate the download and preprocessing processes to automatically integrate new data into QA4SM. Together with automatic validation reports, this will lift QA4SM to a Stage 4 validation service per the definition of the CEOS Land Product Validation subgroup (https://lpvs.gsfc.nasa.gov).
- Traceable sharing of data and results: QA4SM users will be enabled to share their uploaded data sets with other users, so that others can perform independent validations with the same data. As the data

owners can delete their uploaded data again, care will be taken to preserve the traceability between data and validation results.

- Inclusion of new quality indicators: We plan to implement additional FRM quality indicators which are not contained in the ISMN data, for example, in the areas of sub-pixel heterogeneity or vegetation and topographic changes around ISMN stations. Furthermore, we plan to add intra-annual and temporal stability validation metrics to QA4SM.
- Requirements for enhanced user data upload: In relation to QA4SM release 2, we noticed high user interest in the validation of user data. We will systematically assess the community requirements in this regard and will propose future service enhancements to best support the identified need.

SMOS validation studies

Research activities developed during this project on the SMOS SM validation have raised a number of caveats and directions to be explored. It was shown that coarse-scale SM uncertainty, such as SMOS, is sensitive to many factors including the satellite footprint content (in terms of vegetation, topography, bulk density, soil texture), but also to the uncertainty of the reference. In the present case, the reference is the ISMN in situ dataset, which is characterised by the probe configuration (as its depth, technology). Moreover, the methods of spatial and temporal collocation introduce another source of uncertainty due to the scale mismatch between the two sensors. All these factors impact the uncertainty budget, and they should be considered when assessing the performance of satellite-derived SM.

To take these activities a step further, and to better detail the uncertainty budget, we plan to focus on two main tasks: i) the refinement of the methodology to represent SMOS uncertainty at global scale and ii) the impact of the validation methodology on the results. The first one will be addressed by a better characterisation of the SMOS footprint in terms of spatial distribution of surface conditions, and fine-tuning of the methodology to represent the uncertainty. The second one will be addressed by a clear quantification of the impact of the different strategies of spatial and temporal collocation on the scores.

4 Extended project phase

The FRM4SM project was extended via Contract Change Notice No. 1 for the period July 2023 through December 2024. The main areas of activity were similar to those in the initial projects phase, but Work Packages were reorganised to some extent, in order to bring together thematically related activities and results across partners, datasets, and technologies used:

1. Evolution of FRM Methodologies;
2. QA4SM Evolution and Maintenance;
3. SMOS Case Studies;
4. FRM4SM Dissemination and Outreach.

4.1 Evolution of FRM Methodologies

Spatial Scale related Quality indicators

In this task, we tested whether a significant association exists between the spatial heterogeneity of various land surface features and the spatial representativeness of in situ soil moisture stations. The analyses were based on the premise that if variability in land surface features leads to variability in soil moisture, this variability in soil moisture might lead to a decoupling between soil moisture at single locations and average soil moisture within satellite footprint areas, i.e., limited spatial representativeness of individual locations.

We tested the correlation between the representativeness of ISMN stations and the heterogeneity of different surface features within the microwave radiometer footprint scale. To preserve information content about

spatial representativeness, we consider the signal-to-noise ratio (SNR) estimates for the ISMN stations directly instead of categorizing them into three 'representativeness' classes based on SNR thresholds (Technical Note on Evolution of Methodologies, to be made available at https://earth.esa.int/eogateway/activities/frm4sm-fiducial-reference-measurements-for-soil-moisture/project-deliverables).

Spatial variability measures were computed over 0.25x0.25 degrees around each SMOS grid point to represent the satellite footprint. Variability measures used in this analysis include mean, median, variance, standard deviation, interquartile range, and coefficient of variation. The results are depicted in Figure 9. The following heterogeneity proxies were tested:

- Soil texture (Blue): correlation between sand, silt, clay, and organic carbon fractions at individual ISMN FRM sites and their spatial representativeness was analyzed for two maps: the Harmonized World Soil Database (HWSD; (Scharlemann et al., 2009)) and the SoilGrids database (Hengl et al., 2017; Ribeiro et al., 2018).
- Vegetation (green): Both Vegetation optical depth (VOD) & the Normalized Difference Vegetation Index (NDVI) were used. VOD parameters represent temporal variability in the vegetation, whereas NDVI parameters represent spatial variability. Two NDVI products of the Copernicus Land Monitoring Service (CLMS) based on SPOT/PROBA-V were considered: Version 3 of the Long-Term Statistics (lts) and Short-Term Statistics (sts) datasets, which represent 1km spatial resolution NDVI climatologies in 10-day intervals for the years 1999–2019 and 2015–2019, respectively.
- Land cover (Red): To obtain a continuous measure of land cover heterogeneity, the Shannon diversity index was calculated as part of the SMOS case study on sampling, representativeness, and scale errors (Technical Note on Sampling, Representativeness, and Scale Errors, available at https://earth.esa.int/eogateway/activities/frm4sm-fiducial-reference-measurements-for-soil-moisture/project-deliverables) from the IGBP database.
- CCI auxiliary data (Orange): split up into Water-body fraction, wetland fraction, and topographic complexity. All were adopted from ESA CCI SM.

None of the spatial heterogeneity indicators exhibited statistical associations with the predictive power great enough to be used as a proxy for station representativeness, R^2 values were consistently below about 0.12, explaining a maximum 12% of variations in representativeness. Therefore we can conclude that none of the tested indicators is suited to serve as a new Quality Indicator for soil moisture FRM classification.

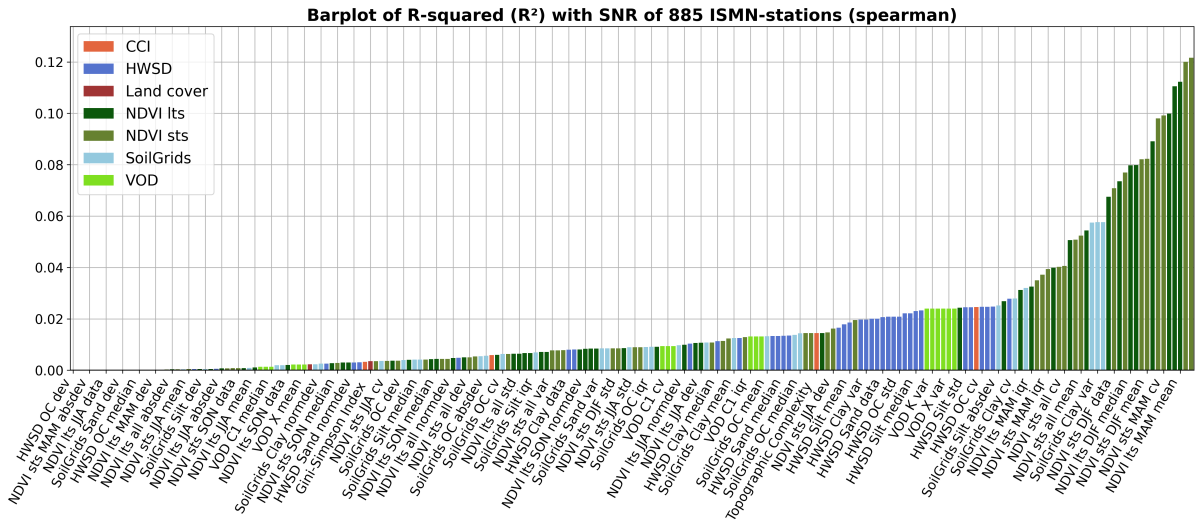


Figure 9: This bar plot depicts the R^2-value between the ISMN station representativeness and the considered heterogeneity proxies. The colors represent the type of indicator (green = Vegetation, blue = Soil texture, red = remaining considered proxies). R^2-values range from near zero to about 0.12 with vegetation parameters exhibiting the greatest association.

Temporal Product Stability

In this task, we demonstrated that instabilities are observed exclusively in L2 soil moisture retrieval products, while L1 brightness temperature measurements remain stable. Given the negligible trends (see Figure 10 observed in brightness temperature, potential instabilities in soil moisture are likely driven primarily by changes on the land surface and limitations in the retrieval process.

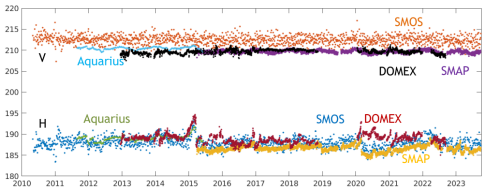


Figure 10: Brightness temperature measurements in V and H polarization of SMOS, SMAP, Aquarius, and DOMEX over an Antarctic ice field (Courtesy: CESBIO).

These instabilities are thus expected to originate from the retrieval process, for example, when land cover change is not accounted for in the auxiliary data used. Nevertheless, care must be taken in the selection of appropriate reference data. In the context of reference data the relevance of sampling characteristics was also tested when assessing temporal product stability. It was found that product stability should only be calculated against in situ stations that cover at least a 10 year time period and provide at least 1500–2000 temporal matches with the product under investigation. Therefore, we selected only time series that cover at least the period from 2010 to 2020 to ensure a 10-year overlap with all considered satellite products (SMOS, ASCAT, and ESA CCI).

Stability, in general, is defined as the change in uncertainty over time (or, alternatively, as the change in bias over time), and no specific metric to assess it is generally recommended. Here, we adopt the approach used in the Copernicus Climate Change Service (C3S) soil moisture product quality assessment report (*Preimesberger et al.*, 2023) and fit slopes (so called Theil-Sen slopes (*Sen*, 1968)) through annually calculated R and ubRMSD estimates.

Next, we investigated the slopes fitted to annual ubRMSD estimates of SMOS, ASCAT, and ESA CCI SM

(COMBINED v08.1) over the selected ISMN FRM candidates and evaluated them against the GCOS Essential Climate Variable (ECV) requirements for surface soil moisture (goal of 0.005, breakthrough of 0.02, and threshold of 0.01 m^3m^{-3}/decade) (see Figure 11). Results indicate that the products are stable, exhibiting mean slopes close to zero with most stations falling below the GCOS threshold. ESA CCI slopes are centered around non-zero values but largly comply with GCOS limits, reflecting expected quality improvements over time as new satellite data is added (*Gruber et al.*, 2019).

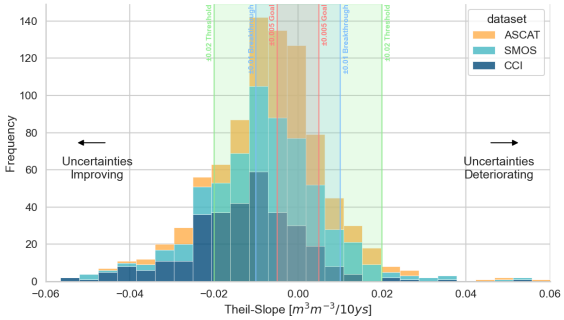
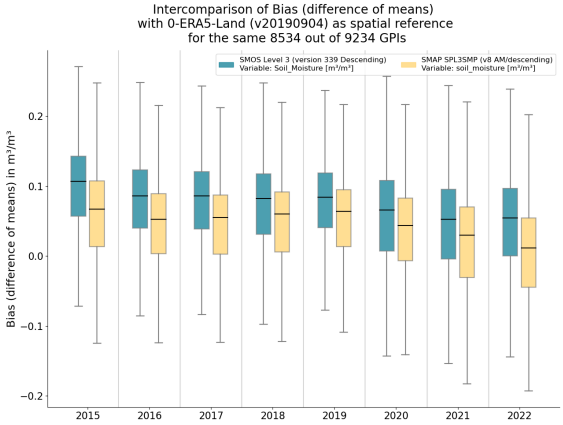


Figure 11: Histogram of slope estimates for annual ubRMSD values across the SMOS, ASCAT, and CCI COMBINED datasets, validated against our in situ selection. Shaded regions denote GCOS stability requirements: the red region represents the goal, the blue region indicates the breakthrough level, and the green region marks the threshold level. Negative slopes reflect decreasing uncertainties, while positive slopes indicate increasing uncertainties.

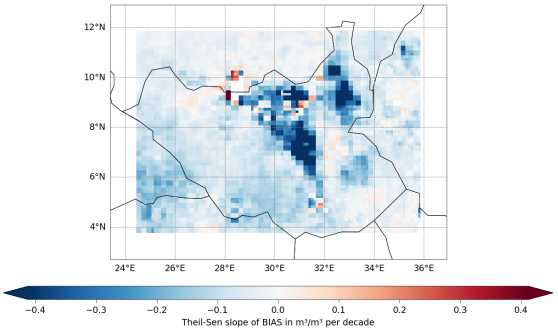
The greatest obstacle in assessing satellite product stability remains the difficulty in distinguishing product instabilities from real geophysical trends due to the lack of reliable reference data. Stability assessments must therefore be conducted using as many independent reference products as possible and rely on the convergence of evidence rather than a single product inter-comparison.

To track "instability," the slopes concept was extended beyond unbiased root mean square difference (ubRMSD) to also include the correlation coefficient (R) and bias, involving the fitting of slopes to the mean annual estimates of these metrics. In this context, the bias slope offered the most accurate depiction of the increasing soil moisture trends in a case study over South Sudan.

Our study showed that real geophysical changes, such as an increase in recent flooding events, are correctly observed in satellite products but are missing in the ERA5-Land model simulations that are often used as a supposedly stable regional reference. Consequently, using ERA5-Land as a reference in this region would cause these missing geophysical signals to be wrongly interpreted as satellite product instability. Subsequently, a preliminary trend analysis framework was included in QA4SM release 3 to assess annual trends of different skill metrics over time between two or more data sets (cf. Figure 12).



(a) Annual Intercomparison bias plot



(b) Annual bias Theil-Sen slope between ERA5-Land and SMOS L3

Figure 12: New visualizations for stability metrics in QA4SM release 3: The boxplot illustrates a decreasing bias trend in SMOS L3 and SMAP L3 compared to ERA5-Land especially pronounced from 2020 onward, while the mapplot highlights the corresponding area in South Sudan. It illustrates bias slope estimates for SMOS L3 relative to ERA5-Land, highlighting a pronounced decline in the northeastern region of South Sudan.

FRM Protocols and Procedures

To date, no standardized guidelines exist for the installation, operation, and maintenance of in situ soil moisture sensors, and barely any existing ground measurement networks can be considered "fiducial". Three important activities were carried out to work towards such guidelines.

- A joint proposal for the EURAMET Green Deal 2024 call was submitted together with the SoMMet consortium and a host of other trans-disciplinary partners to establish a first set of metrologically-secured, fully-traceable FRM super-sites in compliance with the QA4EO and CEOS-FRM guidelines, and to demonstrate their merit in some case studies. Unfortunately, the proposal was not selected for funding, but the consortium is exploring alternative funding possibilities
- A collaboration was established with the U.S. National Coordinated Soil Moisture Monitoring Network (NCSMMN), which is currently compiling comprehensive guidelines for wide-scale standardized soil moisture monitoring (including sensor selection, installation, calibration, maintanance, etc.). These guidelines, which are soon to be released, will be incorporated into the FRM Protocols and Procedures for Soil Moisture (FPP-SM, available at https://earth.esa.int/eogateway/activities/frm4sm-fiducial-reference-measurements-for-soil-moisture/project-deliverables) document and integrated with the FRM requirements and guidelines developed in QA4EO and FRM4SM to provide the first complete guide for the installation, operation, and maintenance of fully CEOS compliant FRM networks.
- A field campaign is currently in preparation, to be carried out by the FRM4SM consortium together with MeteoSwiss, to conduct experiments for assessing the uncertainties associated with different soil moisture sensor calibration methodologies, and to develop best practice guidelines accordingly which are to be implemented into the WMO-No. 8 "Guide to Instruments and Methods of Observation".

4.2 QA4SM Evolution and Maintenance

The evolution activities for QA4SM went through a third major development cycle, consisting of design and implementation, testing and verification, and deployment and maintenance activities as described in Section 3.4. This resulted in QA4SM release 3, which was accepted and deployed at the end of the extended project phase. Results from other project activities, in particular from Evolution of FRM Methodologies and SMOS Case Studies were incrementally integrated into the ongoing evolution of the QA4SM online service. Several points described in Section 3.7 in the conclusions of the initial project phase were picked up and addressed in the extension phase. Some were fully implemented in QA4SM release 3, while others

are continued as new results emerge from R&D activities (e.g., implementation of new quality indicators and metrics). In particular, the automation of integration and verification of operational products was implemented in an initial version for first products in release 3 and will be continued in future projects. Figure 13 shows the redesigned QA4SM landing page and Figure 14 shows the validation types which are supported in QA4SM release 3.

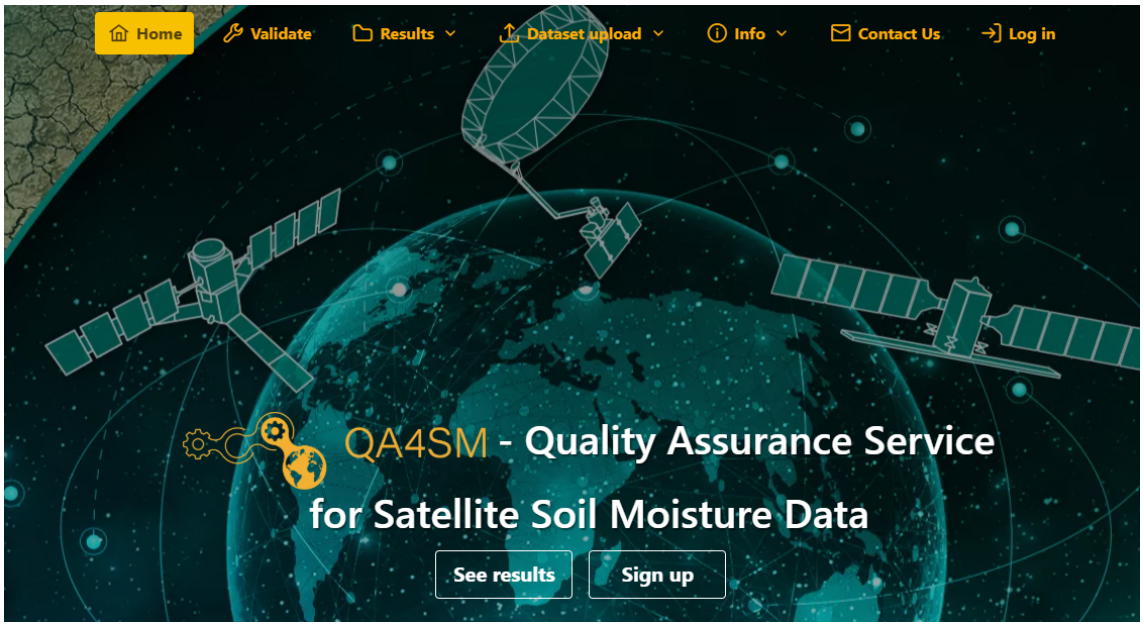


Figure 13: Redesigned QA4SM landing page

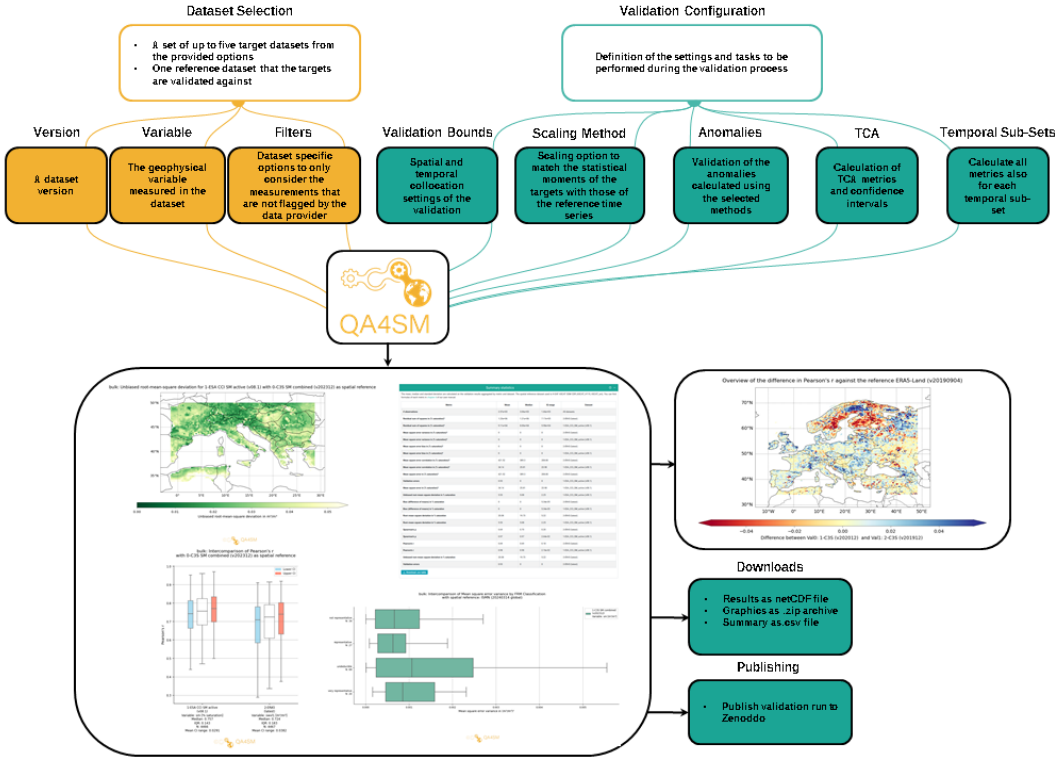


Figure 14: QA4SM validation types

The following features and enhancements were implemented in QA4SM release 3:

- **Intra-Annual Metrics:** Users are enabled to include monthly or seasonal intra-annual metrics in their data validations with QA4SM. Metrics are calculated for each temporal subwindow and intercomparison plots are generated by QA4SM to allow for an assessment of intra-annual variations in product performance.
- **Inter-annual stability metrics:** Users can select inter-annual stability metrics instead of the intra-annual metrics described above. In this case, QA4SM provides annual estimates for all regular metrics in the selected validation period, and Theil-Sen slopes for R, ubRMSD and bias to assess the temporal stability of validated data products. Example plots for both intra-annual and stability metrics are shown in Figure 15.
- **Automated data record extensions:** Selected datasets are automatically extended where a suitable API is made available by the data provider. Automatic scheduling and update pipelines are implemented based on Apache Airflow. In a further step, the downloaded datasets are automatically validated and a validation report is generated by QA4SM. This validation step is currently experimental and is initially implemented for SMOS L2 data products. It will be extended to other datasets in a future project.
- **Sharing of data and results:** Users are enabled to share their validation results with other users, so that others can perform independent validations with the same data. Upon request, uploaded datasets can be shared with user groups, which are set up by the QA4SM administrators. Users, who uploaded datasets, can see on the "My datasets" page which user groups have access to their datasets.
- **Automatic clean up of aged validation results:** Old validations are automatically removed from QA4SM after their owners have been notified. User have the option to archive results if they want to preserve them. In this case, their validations will not be removed from the system.
- **Redesigned user interface and technical consolidation:** The QA4SM landing page and user interface were redesigned to modernise the look and feel of the QA4SM service and to sreamline the user interaction with QA4SM. Less visible for users, the code structure of QA4SM was consolidated to update all external software dependencies including Angular and Python versions, to optimise the interaction between the frontend and backend layers of the software architecture and to improved the maintainability of the system.

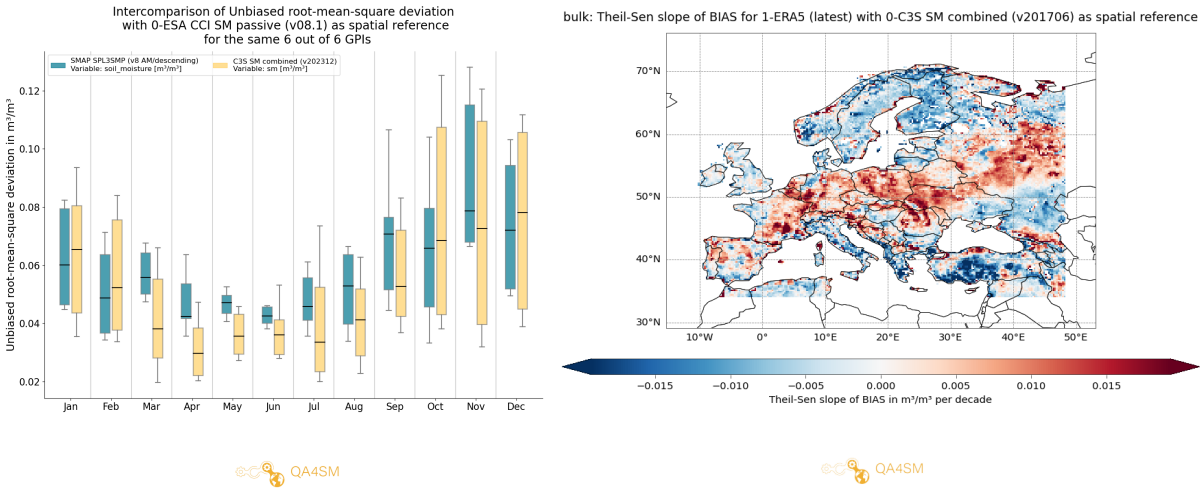


Figure 15: QA4SM plots for monthy intra-annual metrics and stability metrics

An up-to-date description of all QA4SM features and validation options in release 3 is available in the QA4SM Software User Manual v3.0.

4.3 SMOS Case Studies

Based on the activities (Section 3.5) and outcomes ("SMOS validation studies" in Section 3.7) of SMOS FRM4SM Phase 1, focus was put on improving the understanding of the uncertainty budget, and the following activities were further developed: 1) the refinement of the methodology to represent SMOS uncertainty at global scale, and 2) the impact of the validation methodology on the results. Here are the main points that were developed during the CCN phase:

- **Map of predicted SMOS uncertainty (ubRMSD) at global scale:** During FMR4SM Phase 1, SMOS Case Studies 1 and 2 investigated the sensitivity of the SMOS performance to the content of the footprint. Relationships between the SMOS SM ubRMSD (ISMN as reference) and the presence of vegetation, topography, open water and characteristics of the soil texture, within the SMOS footprint, were found and defined. Based on these first results, the methodology was revised and those regressions were extrapolated at global scale. These activities resulted in the publication *Gibon et al.* (2024) in Science of Remote Sensing, from which the graphical abstract is given below in Figure 16. The resulting map should be interpreted as the upper bound of the SMOS uncertainty due to multiple contributions independent of SMOS (reference scale mismatch, uncertainty on the in situ measurements...).

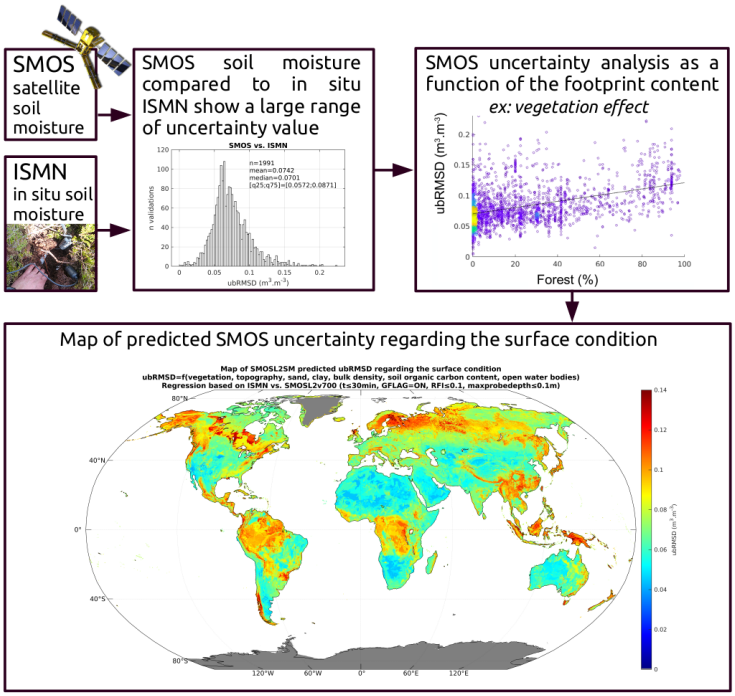


Figure 16: Graphical abstract of the article *Gibon et al.* (2024)

- **Investigation on the multiple effects of the heterogeneity within the footprint on the assessment:** The spatial distribution of the different surface conditions within the footprint, called heterogeneity, impacts SMOS performances in multiple ways. Two main effects are expected with increasing heterogeneity: i) increase of the retrieval modelling complexity and ii) increase of the representativeness scale mismatch with the in situ measurements. The first point was assessed by quantifying the level of heterogeneity with different methods, such as the number of classes within the footprint or the Shannon/Gini indices. The analysis did not show clear signal of SMOS performances worsening with the increasing of diversity within the footprint. The second point was assessed by continuing the analysis started in Case Study 3 and found that the similarity of surface condition between the probe and the SMOS footprint could have a significant impact on the SMOS performances. A new indicator was then created for each probe, that classifies the in situ sites as not similar, similar and very similar.
- **List of relevant sites (with probes) for validation of coarse scale SM satellite product:** An

indicator was then defined for each probe, to state the degree of similarity of surface condition with the SMOS footprint. Merging the indicator based on heterogeneity, with TUWIEN indice based on SNR analyses (not representative, representative and very representative), a list of probes was defined. It is recommended to use the identified probes, to perform validation of coarse scale soil moisture (CCI, SMOS, SMAP or CIMR...).

- **Improvement on the understanding of the different SMOS uncertainty budget components:** FMR4SM Phase 1 initiated the definition of the uncertainty budget of SMOS when using in situ measurement as reference, see Figure 7. In the CCN extension phase, the uncertainty budget was developed to approximate ranges for each component, as shown below in Figure 17. First, global uncertainty, u_{total}, from the ubRMSD range of values of SMOS vs. ISMN. The lowest boundary of the SMOS uncertainty component, u_{SMOS}, is estimated using a climatology of the SMOS SM DQX (Data Quality Index). The reference uncertainty u_{insitu}, and u_{scale} are estimated from literature review. The contribution of the heterogeneity can affect the other components. One should interpret those values with care, as there are first approximations, but they highlight that each component is in the same order of magnitude. Setting the uncertainty budget is essential to better assess the mission requirement of 0.04 $m^3.m^{-3}$.

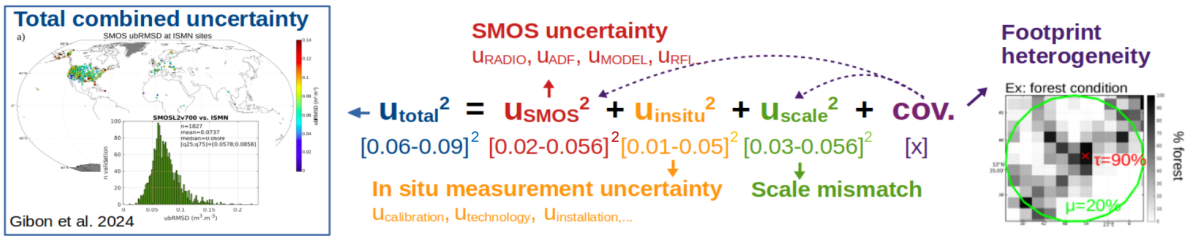


Figure 17: Estimation of the SMOS uncertainty budget

- **Colocation strategies influence (spatial and temporal):** Soil moisture is highly variable in time and space, consequently, the choice of the colocation parameters between SMOS and the in situ probe can impact strongly the result. Focusing on dense networks, analysis shows that the various probes present within the same SMOS footprint, depict a significant range of ubRMSD that is greater than the mission requirement of 0.04 $m^3.m^{-3}$.
- **SMOS product assessment (L2/L2 data test/L3) using QA4SM:** The SMOS data were implemented in the QA4SM platform, and is used to assess the performances of different versions of SMOS data.

4.4 FRM4SM Dissemination and Outreach

SAG and QA4SM user engagement

In the second phase, Keith Bellingham joined the Scientific Advisory Group (SAG). The SAG was regularly informed about project activities through newsletters and invited to participate in a questionnaire. The FRM4SM questionnaire was distributed to SAG members and selected additional scientific stakeholders, to obtain input from their respective areas of expertise. The questionnaire was evaluated and compiled into a road map to guide future FRM4SM activities.

Websites

- Contents of the ESA FRM4SM website were updated (https://earth.esa.int/eogateway/activities/frm4sm-fiducial-reference-measurements-for-soil-moisture)
- A web story about the QA4SM workshop was published on the ESA webpage. (https://earth.esa.int/eogateway/news/workshop-demonstrates-benefits-of-soil-moisture-data-validation-tool)

Journal publications:

Gibon et al. (2024): Gibon, F., A. Mialon, P. Richaume, N. Rodriguez-Fernaandez, D. Aberer, A. Boresch, R. Crapolicchio, W. Dorigo, A. Gruber, I. Himmelbauer, W. Preimesberger, R. Sabia, P. Stradiotti, M. Tercjak, and Y. H. Kerr (2024), Estimating the uncertainties of satellite derived soil moisture at global scale, Science of Remote Sensing, 10, p. 100,147, doi:https://doi.org/10.1016/j.srs.2024.100147

Gruber et al. (2024) Gruber, A., Formanek, M., Pöppl, F., Dorigo, W., Wagner, W., Povey, A., Muñoz-Sabater, J., Embury, O., Bulgin, C., and Merchant, C. (submitted). Making sense of uncertainties: Ask the right question. Surveys of Geophysics.

Conference and workshop contributions

- Alexander Gruber presented FRM4SM at the ISSI workshop "Remote Sensing in Climatology – ECVs and their uncertainty" in Bern, held from 13-17 November 2023 in Bern.
- FRM4SM was presented at the 7th Soil Moisture Validation and Application Workshop in June 2024 in the USA.
- A QA4SM User Workshop was held as part of the 7th Satellite Validation and Application Workshop. Feedback from the QA4SM user workshop was evaluated and integrated into the future planning of QA4SM activities.
- An FRM4SM poster was presented at 1st Stakeholder meeting of the CIPM Sectorial Task Group on Climate Change and Environment (16 to 18 September 2024).
- FRM4SM and QA4SM have been presented at the SMOS Science Conference 2024.
- FRM4SM status updates with a focus on the SMOS activities have been presented at the SMOS Level 2 Progress meeting 30 (October 2023), 31 (Januray 2024) and 32 (May 2024).

European Geoscience Union (EGU) - General Assembly

- Four different contributions were presented at EGU 2024 in a joint Soil Moisture Remote Sensing / Soil Moisture Error Characterization session:
  - Irene (oral): FRM4SM project overview (https://meetingorganizer.copernicus.org/EGU24/EGU24-11186.html)
  - Nico (oral): QA4SM (https://meetingorganizer.copernicus.org/EGU24/EGU24-2102.html)
  - Daniel (poster): Temporal product stability assessment (https://meetingorganizer.copernicus.org/EGU24/EGU24-16136.html)
  - François (poster): SMOS case studies (https://meetingorganizer.copernicus.org/EGU24/EGU24-5023.html)
- An EGU splinter meeting with discussions on calibration and uncertainty was held successfully and led to a new collaboration with Paul Vandôme from CIRAD, France.
- A joint Soil Moisture Remote Sensing / Soil Moisture Error Characterization session was prepared and accepted again for EGU 2025.

ESA Living Planet Symposium

- A Soil Moisture Error Characterization session was proposed for the ESA Living Planet Symposium 2025 and integrated into the wider-scope "Soil Moisture" session.
- Several abstracts have been submitted to the ESA Living Planet Symposium 2025 and are currently awaiting acceptance.

- Arnaud (oral): FRM4SM project overview
- François (poster): SMOS case studies
- Daniel (poster): QA4SM feature update

CEOS LPV

- Soil moisture has been upgraded to Validation Stage 4 (https://lpvs.gsfc.nasa.gov/index.html).
- Alexander Gruber was appointed as the new soil moisture focus area lead.
- QA4SM is now officially endorsed on the CEOS LPV website (https://lpvs.gsfc.nasa.gov/SM/SM_home.html).

Collaborative Efforts During Phase 2

- Joaquín Muñoz Sabater, Scientific Officer of the Copernicus Climate Change Services (C3S), expressed his support to join forces between QA4SM and C3S quality assurance (EQC) activities.
- Andre Obregon, manager of the Copernicus EQC program, has expressed interest and is currently exploring avenues to strengthen synergies/collaborations between FRM4SM/QA4SM and the Copernicus EQC in the next project phase.
- Maria Piles has agreed to provide CIMR simulation data once available next year, and to consider QA4SM for CIMR validation in close collaboration.
- The ESA CCI SM and C3S SM validation will, from the next phase starting Fall 2024, be done officially using QA4SM.
- A joint project proposal with the SoMMet consortium and other partners for exploring and utilizing soil moisture FRM sites has been submitted to the EURAMET 2024 Green Deal call, but got rejected. Alternative funding routes are currently being explored.
- A field campaign together with MeteoSwiss is currently in planning and will be carried out early 2025.
- Close collaboration with ESA SMOS ESL and NASA JPL SMAP team (Andreas Colliander).

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