
EUMETSAT Satellite Application Facility on
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**Algorithm Theoretical
Baseline Document (ATBD)
ASCAT SSM CDR v8 12.5 km (H121)
ASCAT SSM CDR v8 EXT 12.5 km (H139)**

Metop ASCAT Surface Soil Moisture
Climate Data Record v8 12.5 km sampling (H121)
Climate Data Record v8 Extension 12.5 km sampling (H139)

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1. Executive summary

The Algorithm Theoretical Baseline Document (ATBD) provides a detailed description of the soil moisture retrieval algorithm using backscatter observation from the Advanced Scatterometer (ASCAT) on-board the series of Metop satellites. The concept of the soil moisture retrieval method applicable for the C-band scatterometer is a physically motivated change detection method. The first realization of the concept was based on ERS-1 and ERS-2 scatterometer data [1]–[4] and was later successfully transferred to ASCAT [5]–[7].

2. Introduction

2.1. Purpose of the document

The Algorithm Theoretical Baseline Document (ATBD) is intended to provide a detailed description of the scientific background and theoretical justification behind the algorithm utilized for soil moisture retrieval from the Advanced Scatterometer (ASCAT) instrument aboard the Metop satellite series.

2.2. Targeted audience

This document mainly targets:

1. Remote sensing experts interested in the retrieval and error characterization of satellite soil moisture data sets.
2. Users of remotely sensed soil moisture data sets who want to obtain a more in-depth understanding of the algorithm and sources of error.

3. ASCAT on-board Metop

3.1. Introduction

The European contribution within the framework of the Initial Joint Polar System (IJPS) is the EUMETSAT Polar System (EPS). The space segment of the EPS programme is envisaged to contain three sun-synchronous Meteorological Operational Platforms (Metop-A, -B and -C) jointly developed by ESA and EUMETSAT. Each satellite has a nominal lifetime in orbit of about 5 years, with a planned 6 month overlap between consecutive satellites. The first satellite Metop-A, was launched on 19 October 2006 and ended its mission on 15 November 2021, whereas Metop-B (launched on 17 September 2012) and Metop-C (launched on 7 November 2018) are still operational as of today. The Advanced Scatterometer (ASCAT) is one of the nine primary instruments carried on-board the series of Metop satellites.

3.2. Instrument description

ASCAT is a real aperture radar system operating in C-band (VV polarization) and provides day- and night-time measurement capability, which is almost unaffected by cloud cover. The instrument measures the Normalized Radar Cross Section (NRCS), or so-called backscatter coefficient σ^0 expressed in m^2m^{-2} or dB, from the Earth's surface. The design and performance specification is based on the experience of the Scatterometer flown on the ERS-1 and ERS-2 satellite. It can basically work in two different modes: Measurement or Calibration. The Measurement Mode is the only mode that generates science data for users. The instrument uses a pulse compression method called “chirp”, at which long pulses with linear frequency modulation were generated at a carrier frequency of 5.255 GHz. After receiving and

de-chirping of the ground echoes, a Fourier transform is applied in order to relate different frequencies in the signal to slant range distances. A pre-processing of the noise and echo measurements is done already on board to reduce the data rate to the ground stations, e.g. various averaging takes place reducing the raw data by a factor of approximately 25. Within each pulse repetition interval, after all pulse echoes have been diminished, the contribution of the thermal noise is monitored in order to perform a measurement noise subtraction during the ground processing. A side effect of on board processing is a degree of spatial correlation between different and within received echoes, but this is taken into account later on by the Level 1b processing. The radar pulse repetition frequency (PRF) is approximately 28.26 Hz, which yields 4.71 Hz for the beam pulse repetition frequency in the sequence fore-, mid- and aft beam [8].

The Calibration Mode is used during external calibration campaigns (29 days every 13 months), when the platform passes over three different ground transponders located in central Turkey. The objective of such calibration campaigns is to verify that the backscatter measurements from a target are correct for the whole incidence angle range. In other words, the absolute and relative calibration will be monitored and checked. A stable radar cross section and an accurately known position on the Earth's surface are the basic and important requirements for each transponder. After receiving a pulse from ASCAT, the active transponder sends a delayed pulse back, which in turn can be recorded by ASCAT. A comparison between the localised transponder position and the expected data allows the estimation of three depointing angles and gain correction values for each antenna. An east-west distribution with a displacement of approximately 150 km, will allow to obtain transponder measurements from most of the incidence angles for each antenna beam. This high sampling is necessary in order to reconstruct the characteristics of each antenna gain pattern for the whole incidence angle range and achieve an appropriate relative calibration. Such a calibration set-up allows the establishment of a reference system in order to evaluate and monitor the instrument performance on regular basis [9].

3.3. Geometry and coverage

The Metop satellites are flying in a sun-synchronous orbit (29 day repeat cycle) with an ascending/descending node at 9:30 p.m./a.m. and a minimum orbit height of 822 km. This implies that the satellite will make a little more than 14 orbits per day. The advanced measurement geometry of ASCAT allows twice the coverage, compared to its predecessors flying on ERS-1 and ERS-2. Thus, the daily global coverage increased from 41% to 82%. The spatial resolution was also improved from 50 km to 25-34 km, whilst maintaining the same radiometric accuracy compared to the ERS-1/2 scatterometer.

The advanced global coverage capability is accomplished by two sets of three fan-beam antennas, compared to only one set at the ERS satellites. The fan-beams are arranged broadside and $\pm 45^\circ$ of broadside, thus, allowing to observe three azimuthal directions in each of its two 550 km swaths (see Figure 3.1). The swaths are separated from the satellite ground track by about 360 km for the minimum orbit height.

Each point on the Earth's surface that falls within one of the two swaths, will be seen by all three antennas and a so-called σ^0 triplet can be observed. The incidence angles for those two antennas which are perpendicular to the flight direction intersect the surface between 25° and 53.3° , whereas the other four antennas have an incidence angle range from 33.7° to 64.5° [10]. The multi-angle viewing capability of ASCAT is needed for an effective and precise geophysical retrieval of surface parameters (e.g. wind speed and direction over ocean, vegetation conditions over land). Otherwise remaining ambiguities hamper or render impossible a successful retrieval of such parameters.

3.4. Product processing

Global data products are often classified into different levels according to their processing progress. In case of ASCAT the different product levels can be summarized as follows:

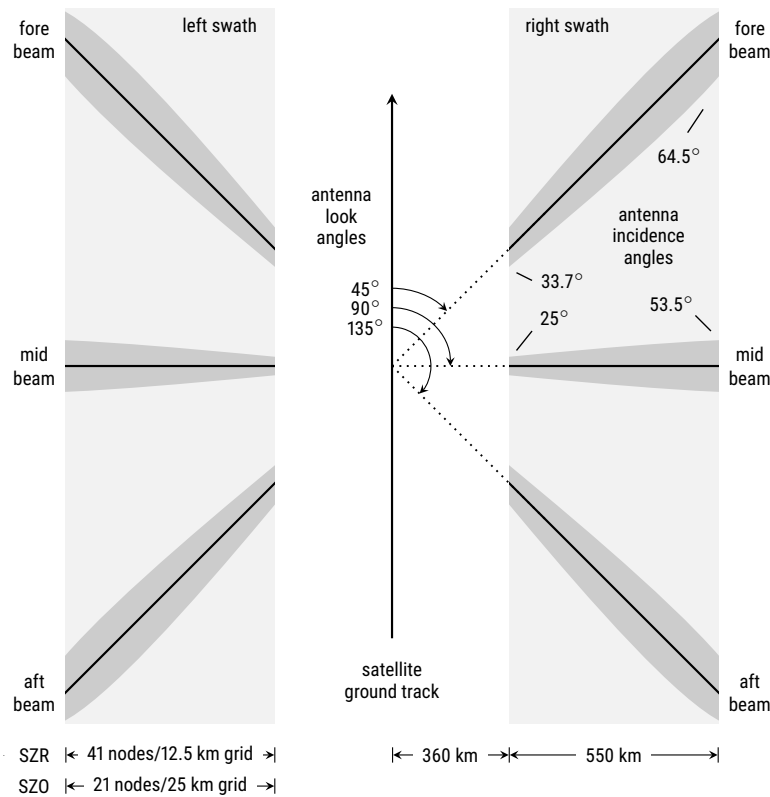


Figure 3.1: ASCAT swath geometry for a Metop minimum orbit height (822 km). The dimensions are symmetric with respect to the satellite ground track [10].

- Level 0: Unprocessed raw instrument data from the spacecraft. These are transmitted to the ground stations in binary form.
- Level 1a: Reformatted raw data together with already computed supplementary information (radiometric and geometric calibration) for the subsequent processing.
- Level 1b: Calibrated, georeferenced and quality controlled backscatter coefficients in full resolution or spatially averaged. It includes also ancillary engineering and auxiliary data.
- Level 2: Geo-referenced measurements converted to geophysical parameters, at the same spatial and temporal resolution as the Level 1b data.
- Level 3: Geophysical products derived from Level 2 data, which are either re-sampled or gridded points.

The raw data arriving at the ground processing facility are passed into the Level 1 ground processor (see Figure 3.2). This data driven processing chain generates radiometrically calibrated Level 1b backscatter coefficients. It also includes an external calibration processing chain in order to support the localization and normalisation process of the measurement power echoes. Before satellite launch, it is only possible to estimate parameters characterising the expected instrument performance, since some of them depend on in-flight conditions. But once the satellite is in orbit, these parameters can be assessed during a calibration campaign. The first intermediate product generated just before the swath node generation and spatial averaging steps, is called Level 1b full resolution product. The main geophysical parameter in this product

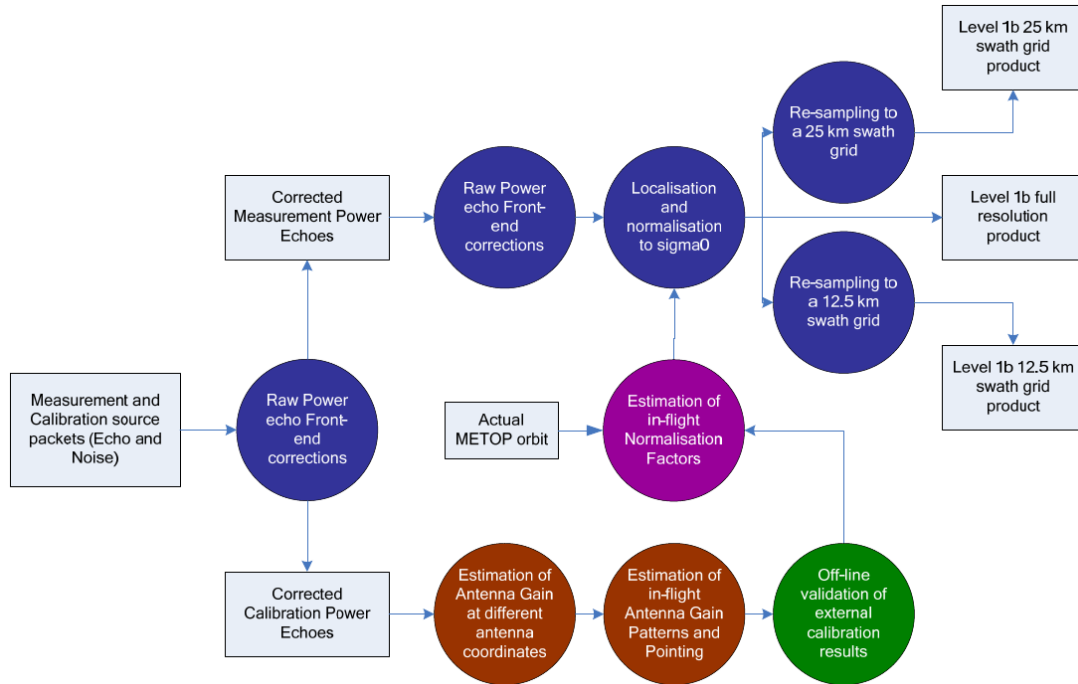


Figure 3.2: Functional overview of the ASCAT Level 1 ground processing chain [12].

is the normalized backscatter coefficient σ^0 . Along each antenna beam 256 σ^0 values are projected on the Earth's surface. The footprint size is about 10×20 km of various shapes and orientations, depending on the Doppler pattern over the surface [11]. The radiometric accuracy and the inter-beam radiometric stability is expected to be less than 0.5 dB peak-to-peak, whereas the georeferencing accuracy is about 4 km. In addition a number of quality flags are computed associated with every individual σ^0 sample along each antenna beam.

The other two products generated within the Level 1b processing are averaged σ^0 values at two different spatial grids. A two-dimensional Hamming window function centered at every grid node is used in both cases for spatial filtering. This weighting function is based on a cosine function, which will basically attenuate the contribution of values with increasing distance. The window width determines which observations will contribute to the weighted result. Observations beyond the window width are disregarded. The spatial resolution is defined as twice the distance from the center to where the window function reaches 50% of its peak intensity (full width at half maximum, FWHM). This spatial averaging is used in the along- and across-track direction, with the objective to generate a set of σ^0 triplets for each grid node of each swath at the desired radiometric resolution. The first product generated with this approach is called the nominal product and has a spatial resolution of 50 km for each grid point. The grid spacing is 25 km with 21 nodes at each swath per line. The higher resolution product has a spatial resolution ranging from 25 to 34 km. This variability is the result of a trade-off between spatial resolution and the desired radiometric accuracy, which lead to an alternating Hamming window width across the swath for the different beams. In this case the grid spacing is only 12.5 km, with 41 nodes at each swath per line.

4. Soil moisture retrieval

The soil moisture retrieval employs a physically motivated change detection method based on C-band backscatter observations. This algorithm leverages backscatter data from multiple incidence angles to

model soil moisture and vegetation dynamics. Semi-empirical model parameters are derived from historical backscatter time series, resampled onto a fixed Earth grid. The SSM retrieval estimates the soil water content in the surface layer (< 5 cm), expressed as a degree of saturation ranging from 0 to 100%.

4.1. Resampling ASCAT Level 1b SZF backscatter

The ASCAT Level 1b SZF backscatter observations are resampled to a fixed Earth grid with a spatial sampling of about 12.5 km using a Hamming window (radius=23688 m). The spatial resampling is performed individually for each of the 6 beams of ASCAT and during this process backscatter observations located in areas not sensitive to soil moisture changes (open water, coastal areas and cities) are excluded. Land cover information (ESA CCI Land Cover 2018 300 m v2.1.1) is used to identify individual full-resolution backscatter echos measured over these areas. The CCI Land Cover data is resampled on a regular lat/lon grid (0.006°), thereby computing the fractional coverage of each land cover class for all pixel with spatial window in the order of the resolution of a full-resolution backscatter echo (10-20 km). This way a threshold can be used for the amount of e.g. urban area (< 25%) or open water (< 50%) fraction that is still acceptable covered by a full-resolution ASCAT backscatter echo.

The grid points of the fixed Earth grid are arranged on a Fibonacci grid named after the Fibonacci ratio [13]. The Fibonacci grid differs from other spiral constructed grids on the sphere in that the longitudinal turn between consecutive points along the generative spiral is the golden angle ($360^\circ \cdot (1 - \phi^{-1}) \simeq 137.5^\circ$) or its complementary ($360^\circ \cdot \phi^{-1} \simeq 222.5^\circ$). Since the grid point locations are computed on a spherical Earth, latitude and longitude coordinates are converted to WGS84 ellipsoidal coordinates (EPSG:4326). This transformation introduces deviations of the sampling regularity on a larger scale. However, due to the fact that the Fibonacci grid can only be computed in a closed form on a sphere and deviations are minor considering only the near vicinity of grid points (< 20 km), these irregularities in sampling are deemed acceptable. To visualize this, a small patch on the surface of both the sphere and the ellipsoid can be used as an example. If the patch is small enough, it looks flat, and the distances within this patch are nearly the same for both shapes. But for points across the entire surface, the sphere's uniformity contrasts with the ellipsoid's varied stretching, making the distances diverge more.

4.2. TU Wien soil moisture retrieval algorithm

4.2.1. Introduction

The TU Wien soil moisture retrieval algorithm is a physically based, semi-empirical change detection method. The first version of this approach was developed using ERS-1 and ERS-2 scatterometer data [1]–[4]. Later, this method was successfully applied to ASCAT on the Metop satellite series [5]–[7]. From a mathematical perspective, the retrieval algorithm is simpler than a radiative transfer model and can be solved directly. This allows soil moisture to be estimated directly from scatterometer measurements without the need for repeated adjustments. As a result, it is straightforward to calculate the retrieval error for each location on the land surface [6]. A limitation of this method is that it represents the measurement as a combined value. Unlike radiative transfer models, it does not separate the individual effects of soil, vegetation, and soil-vegetation interactions on the observed backscatter. Therefore, model parameters need to be calibrated using long-term backscatter time series to account for variations in land cover, surface roughness, and other factors.

The basic assumptions of the TU Wien soil moisture retrieval algorithm are:

1. The relationship between the backscatter coefficient σ^0 expressed in decibels (dB) and the surface soil moisture content is linear.

2. The backscatter coefficient σ^0 depends strongly on the incidence angle θ . The exact functional form of the dependency is mainly determined by surface roughness and land cover, but is not affected by changes in the soil moisture content.
3. When vegetation grows, backscatter may decrease or increase, depending on whether the attenuation of the soil contribution is more important than the enhanced contribution from the vegetation canopy, or vice versa. Because the relative magnitude of these effects depends on the incidence angle, the curve $\sigma^0(\theta)$ changes with vegetation phenology over the year. This effect can be exploited to correct for the impact of vegetation phenology in the soil moisture retrieval by assuming that there are distinct incidence angles (θ_d and θ_w) where the backscatter coefficient is stable (in the sense that it is not affected by seasonal changes in above ground vegetation biomass) for dry and wet conditions.
4. Vegetation phenology influences backscatter σ^0 on a seasonal scale. Local short-term fluctuations are suppressed at the scale of the scatterometer measurements.

The following subsections describe the soil moisture retrieval algorithm in more detail.

4.2.2. Correction of azimuth angle dependency

The backscattering coefficient changes as a function of the observed surface properties, most importantly surface dielectric properties, roughness and vegetation. However, the overall magnitude also strongly depends on the measurement geometry, i.e. the incidence angle θ as well as the azimuth angle ϕ .

In some dedicated regions azimuth effects on the backscattering coefficient are very strong (e.g. mountainous areas, sandy desert regions). This target anisotropy is accounted for by applying a polynomial correction term to the backscatter signal as suggested by [14]. The azimuth angle under which a location is seen depends on the beam (Fore, Mid or Aft beam), the swath (left or right) and the orbit direction (ascending or descending), resulting in twelve different azimuth configurations (i.e. ϕ_i with $i \in [1, 12]$) for Metop ASCAT. For each of these configurations the incidence angle dependency of backscatter is modeled as a second-order polynomial.

$$\sigma_i^0(\theta) = A_i \cdot (\theta - 40)^2 + B_i \cdot (\theta - 40) + C_i \quad (1)$$

The coefficients of these twelve polynomials (A_i, B_i, C_i) are determined by fitting the second-order polynomial to all observations falling into the respective configuration category (e.g. fit through all measurements from the left fore beam in ascending direction). Furthermore, an overall model ($i = 13$) is fitted to all observations used as a reference, resulting in a total of $3 \times 13 = 39$ coefficients. A difference of the polynomial coefficients between the twelve individual acquisition geometries and the reference ($i = 13$) using all measurements leads to new polynomial coefficients used to determine the correction for the backscatter measurements. This way, the individual incidence angle dependency of backscatter are adjusted to a mean relationship canceling static azimuth effects.

$$\hat{\sigma}_i^0(\theta) = \sigma_i^0(\theta) + (A_{13} - A_i) \cdot (\theta - 40)^2 + (B_{13} - B_i) \cdot (\theta - 40) + (C_{13} - C_i) \quad (2)$$

where $\hat{\sigma}_i^0$ represents the corrected backscatter for each configuration i . The following step is using the corrected backscatter and formulas are written without the hat nomenclature.

4.2.3. Estimated standard deviation of backscatter

The Estimated Standard Deviation (ESD) describes the backscatter standard deviation (expressed in dB) representing a measure of noise. The ESD computation is the first step in the error propagation. It is

derived from the Fore and Aft beam measurements (σ_f^0, σ_a^0) and based on the following observation: all three beams observe the same target and due to the observation geometry the Fore and Aft beam have the same incidence angle. Thus, as long as there are no azimuth effects, the measurements of the Fore and Aft beam are comparable, i.e. statistically, they are instances of the same distribution. Hence, the expectation of the difference

$$\delta := E[\sigma_f^0 - \sigma_a^0] = 0 \quad (3)$$

should be zero, and its variance should be twice the variance of one of the beams (i.e. $\text{Var}[\delta] = 2 \cdot \text{Var}[\sigma^0]$). This can be derived using error propagation and neglecting higher order terms:

$$\text{Var}[\delta] \approx \text{Var}[\sigma_f^0] \cdot \left(\frac{\partial \delta}{\partial \sigma_f^0}\right)^2 + \text{Var}[\sigma_a^0] \cdot \left(\frac{\partial \delta}{\partial \sigma_a^0}\right)^2 + 2 \cdot \text{Cov}(\sigma_f^0, \sigma_a^0) \cdot \left(\frac{\partial \delta}{\partial \sigma_f^0}\right) \cdot \left(\frac{\partial \delta}{\partial \sigma_a^0}\right) + \dots,$$

whereby the third term is zero under the assumption of i.i.d. (independent and identically distributed random variables).

$$\text{Var}[\delta] \approx \text{Var}[\sigma_f^0] \cdot (1)^2 + \text{Var}[\sigma_a^0] \cdot (-1)^2 + 0 \quad (4)$$

Assuming equal variances for the fore- and aft-beam we have

$$\text{Var}[\delta] \approx \text{Var}[\sigma_f^0] + \text{Var}[\sigma_a^0] = 2 \cdot \text{Var}[\sigma^0] \quad (5)$$

The previous equation can be re-written to find the final formula for the ESD

$$\text{ESD}[\sigma^0] = \sqrt{\frac{\text{Var}[\delta]}{2}} \quad (6)$$

The ESD is computed after strong outliers (defined as $\delta > Q3 + 3 \times \text{IQR}$ or $\delta < Q1 - 3 \times \text{IQR}$) have been removed.

4.2.4. Estimation of slope and curvature

In general, backscatter measurements over land show a strong dependence on the incidence angle and a linear function (defined in the dB domain) is usually deemed sufficient to describe this relationship. The backscatter coefficient at an arbitrary incidence angle σ^0 (in dB) can be modelled as

$$\sigma^0(\theta) = \sigma^0(40) + \sigma' \cdot (\theta - 40), \quad (7)$$

where the reference incidence angle is chosen to be 40° , $\sigma^0(40)$ representing the backscatter at the reference incidence angle (in dB) and σ' the slope (in dB/degree). For almost all land cover types this situation is valid, because of the steep decrease of backscatter with increasing incidence angle. However, in case of a considerable amount of volume scattering effects, the signal can also flatten out towards the higher end of incidence angles. In order to account for these effects, a second-order polynomial is used to describe the incidence angle dependency of backscatter adding the curvature σ'' term.

$$\sigma^0(\theta) = \sigma^0(40) + \sigma' \cdot (\theta - 40) + \frac{1}{2} \cdot \sigma'' \cdot (\theta - 40)^2 \quad (8)$$

From a mathematical point of view, Eqn. 8 represents a Taylor polynomial, since the function is based on the finite sum of values of the function's derivatives at a single point. Therefore, the reference incidence

angle at 40° can be regarded as expansion point and the first σ' (dB/degree) and second derivative σ'' (dB/degree²) of $\sigma^0(40)$ are referred to as slope and curvature, respectively. Once these parameters are known, the Taylor polynomial can be used to estimate backscatter in the proximity. Rearranging Eqn. 8 allows the computation of $\sigma^0(40)$ from backscatter taken at an arbitrary incidence angle σ^0 .

The methodology to estimate σ' and σ'' has evolved over time, but each approach is based on the local slope computation [15]. A local slope represents an instantaneous characterization of the incidence angle dependency of backscatter, which can be estimated from the differences $\sigma_f^0 - \sigma_m^0$ and $\sigma_a^0 - \sigma_m^0$. This is possible because for a given measurement triplet, the Fore and Aft beam share the same incidence angle (i.e. $\theta_f = \theta_a$):

$$\sigma'_{fm} = \frac{\sigma_m^0 - \sigma_f^0}{\theta_m - \theta_f}, \quad \sigma'_{am} = \frac{\sigma_m^0 - \sigma_a^0}{\theta_m - \theta_a} \quad (9)$$

σ'_{fm} and σ'_{am} are estimates of the slope value at the midpoint local incidence angles

$$\theta_{fm} = \frac{\theta_m + \theta_f}{2}, \quad \theta_{am} = \frac{\theta_m + \theta_a}{2} \quad (10)$$

If it is possible to generate a large sample of local slope values evenly distributed over the entire incidence angle range, a first order approximation of $\sigma'(\theta)$ can be used to determine σ' and σ'' at 40° derived from a linear regression model.

$$\sigma'(\theta) = \sigma' + \sigma'' \cdot (\theta - 40) \quad (11)$$

The selection and weighting of the local slope values in the regression model has changed over time. Data density constraints and computational considerations have lead to alternative implementations. An overview of these methods can be found in [15]. The most recent method of estimating σ' and σ'' is based on a Kernel Smoother (KS) [16]. The KS approach offers the possibility to estimate σ' and σ'' either as a climatology (i.e. 366 values, similar to previous methods) or as a time series (i.e. daily values). However, for the moment the computation of σ' and σ'' is based on the climatology and the time series approach is still under investigation.

In case of the climatology, the regression coefficients are estimated for each day of year d by selecting local slope values from all available years in close proximity (i.e. ± 21 days or $\lambda = 42$ days) for the day under question d_0 . Within the time window, the local slope values are weighted according to their temporal distance using the Epanechnikov kernel (see [17] and Figure 4.1, chapter 6)):

$$k(d_0, d) = D \left(\frac{d - d_0}{\lambda} \right) \quad (12)$$

with

$$D(t) = \begin{cases} \frac{3}{4} \cdot (1 - t^2) & \text{if } |t| \leq 1 \\ 0 & \text{else} \end{cases} \quad (13)$$

The Epanechnikov kernel integrates to one and has finite support in range $[-\lambda, \lambda]$. The kernel width λ is a crucial parameter that determines how strongly neighboring measurements influence the final estimate: an increase in λ decreases the variance, but, at the same time, increases the bias of the estimate.

Normally, the kernel is a function of the independent variable (in our case θ), but since it is the goal to find the coefficients of the linear approximation (Eqn. 11) over the whole incidence angle range at a given day d_0 , the kernel is a function of the day of the year. All local slope values in-between the interval $|(d - d_0)/\lambda| \leq 1$ are weighted according to their distance to the current day of year d_0 and take part in the linear regression (Eqn. 14).

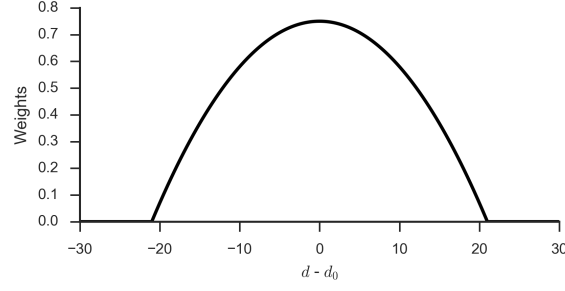


Figure 4.1: Example of the Epanechnikov kernel ($\lambda = 21$).

Let $\mathbf{x} \in \mathbb{R}^N$ and $\mathbf{y} \in \mathbb{R}^N$ denote the vectors containing θ_l and σ'_l , respectively, within the support of the kernel for day d_0 . Let further $\mathbf{A} \in \mathbb{R}^{N \times 2}$ be the design matrix, whose first column is all 1, and whose second column is given by $\mathbf{x}$, and $\mathbf{W}(d_0) \in \mathbb{R}^{N \times N}$ a diagonal weight matrix, whose i -th diagonal entry is given by the value of the kernel for the i -th local slope, i.e. $\mathbf{W}(d_0)[i, i] = k(d_0, d_i)$. Then, the estimates for σ' and σ'' at day d_0 are obtained as

$$\begin{pmatrix} \sigma'(d_0) \\ \sigma''(d_0) \end{pmatrix} = (\mathbf{A}^T \mathbf{W}(d_0) \mathbf{A})^{-1} \mathbf{A}^T \mathbf{W}(d_0) \mathbf{y} = \mathbf{B} \mathbf{y} \quad (14)$$

If the error covariance of the local slope values used in the fit is given by Σ_1 , then the error covariance of the parameters is given by

$$\Sigma_{\sigma', \sigma''} = \mathbf{B} \Sigma_1 \mathbf{B}^T \quad (15)$$

At the moment, it is assumed that Σ_1 is homoscedastic (i.e., the errors for all local slope values have the same variance s_l^2) and the errors are uncorrelated: $\Sigma_1 = \mathbf{I} s_l^2$, and estimate s_l^2 from the residuals of the fit (in order to avoid confusion with σ for the representation of backscatter, the variance notation is s^2).

4.2.5. Interpolation to reference incidence angle

Once $\sigma'(d)$ and $\sigma''(d)$ have been computed on a daily basis d , the incidence angle interpolation can be applied to the backscatter measurements of each beam b (Fore, Mid, Aft) using

$$\sigma_b^0(40) = \sigma_b^0(\theta_b) - \sigma'(d) \cdot \Delta\theta_b - \frac{1}{2} \cdot \sigma''(d) \cdot \Delta\theta_b^2 \quad (16)$$

with $\Delta\theta_b = \theta_b - 40$. The backscatter observations of the three beams interpolated to a common reference angle are averaged:

$$\bar{\sigma}^0(40) = \frac{1}{3} \cdot \sum_{b \in \{f, m, a\}} \sigma_b^0(40) \quad (17)$$

which gives the final backscatter $\bar{\sigma}^0(40)$ interpolated at the reference incidence angle. The noise variance of the interpolated backscatter at the reference incidence angle for each beam b is given by:

$$\text{Var}[\sigma_b^0(40)] = \text{ESD}[\sigma^0]^2 + \text{Var}[\sigma'(d)] \cdot \Delta\theta_b^2 + \frac{1}{4} \cdot \text{Var}[\sigma''(d)] \cdot \Delta\theta_b^4 \quad (18)$$

and after averaging, the noise variance reduces to:

$$\text{Var} [\bar{\sigma}^0(40)] = \frac{1}{9} \cdot \sum_{b \in \{f, m, a\}} \text{Var} [\sigma_b^0(40)] \quad (19)$$

The following step is using the averaged backscatter at the common reference incidence angle of the three beams and formulas are written without the bar-nomenclature.

4.2.6. Estimation of dry and wet backscatter reference

The estimation of the dry and wet references is based on the 2nd and 98th percentiles of the $\sigma^0(40)$ time series, calculated monthly with a time window of ± 3.5 years. These reference values are used to translate backscatter variations into changes in relative soil surface moisture (SSM) and to correct for various signal disturbances, such as vegetation, soil roughness, and land cover.

Traditionally, the dry and wet backscatter references have been estimated using the entire backscatter time series, which has performed well over time spans of 3–10 years. However, as the backscatter record now extends beyond 15 years, long-term land cover changes have become a significant source of trends in backscatter. Recent analyses have shown that ASCAT SSM trends exhibit pronounced anomalies in specific regions worldwide. These anomalies are particularly evident in areas with gradually changing ground conditions, such as urban expansion or deforestation. The annual estimation of the dry and wet backscatter references is intended to remove non-climatic effects from the backscatter time series, thereby enabling accurate detection and monitoring of climate extremes within the SSM record.

The vegetation correction is derived from temporal variations in the incidence angle dependency of backscatter, based on the following physical principles: Generally, the backscattering coefficient decreases rapidly with increasing incidence angle, except for very rough surfaces [18]. The main scattering mechanisms in vegetated areas are volume scattering within the vegetation canopy and surface scattering from the underlying soil [19]. These two mechanisms exhibit distinct behaviors, allowing differentiation between volume and surface scattering. As a result, backscatter curves with identical soil moisture levels but different vegetation states intersect at a specific incidence angle. At this cross-over angle, vegetation effects are minimized. Figure 4.2 illustrates this scenario for the two extreme cases of completely dry and fully saturated soil. This "cross-over angle" concept defines the dry and wet cross-over angles, denoted as θ_d and θ_w , respectively.

In the beginning, these angles were globally set to $\theta_d = 25^\circ$ and $\theta_w = 40^\circ$ and have been experimentally derived from previous studies [2], [3]. However, a recent study [20] showed that spatially-variable cross-over angle outperform static angles. The computation of the spatially-variable cross-over angle is based on Vegetation Continuous Field (VCF) data set [21] containing three bands describing percent of tree cover (tc), non-tree vegetation (v), and bare ground (bg). The three bands are used as weights assuming that no vegetation correction is required in case of bare ground ($\theta_d = \theta_w = 40^\circ$), while tree and non-tree vegetated surfaces tend to have lower cross-over angle ($\theta_d = 10^\circ$, $\theta_w = 30^\circ$).

$$\theta_d = 10 \cdot v + 10 \cdot tc + 40 \cdot bg \quad (20)$$

$$\theta_w = 30 \cdot v + 30 \cdot tc + 40 \cdot bg \quad (21)$$

The global maps shown in Figure 4.3 and Figure 4.4 illustrate the spatial distribution of θ_d and θ_w derived from the VCF5KYR 2016 data set using Equation 20 and Equation 21.

In order to determine the lowest and highest backscatter irrespective of vegetation conditions, σ_{40}^0 is interpolated to the dry/wet crossover angle using Equation 8, i.e.

$$\sigma^0(\theta_d) = \sigma^0(40) + \sigma'(d) \cdot \Delta\theta_d + \frac{1}{2} \cdot \sigma''(d) \cdot \Delta\theta_d^2 \quad (22)$$

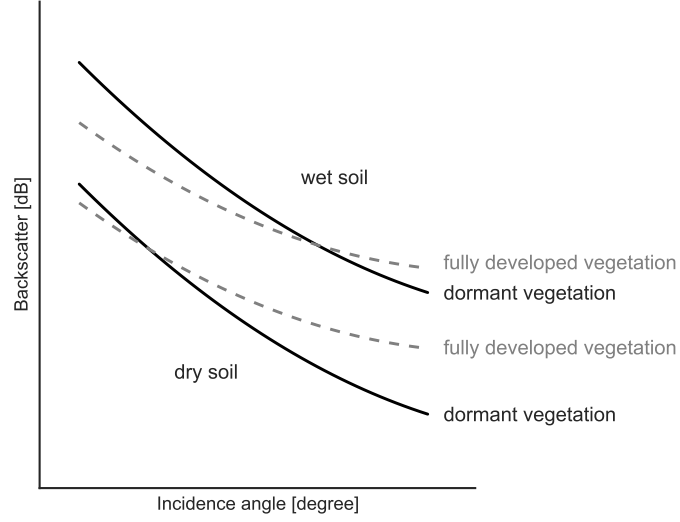


Figure 4.2: Crossover angle concept.

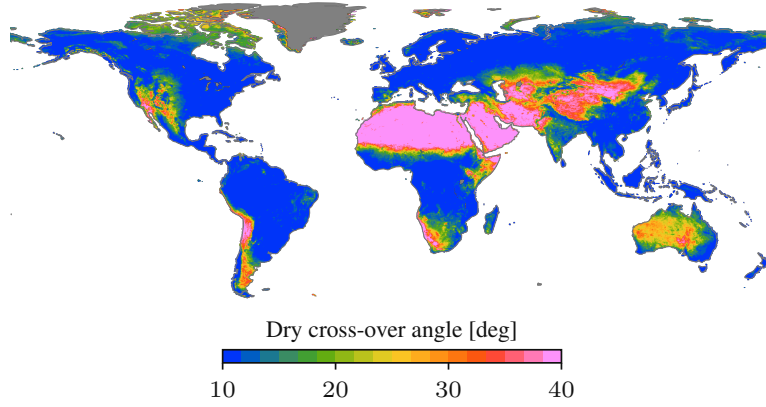


Figure 4.3: Dry cross-over angle map.

$$\sigma^0(\theta_w) = \sigma^0(40) + \sigma'(d) \cdot \Delta\theta_w + \frac{1}{2} \cdot \sigma''(d) \cdot \Delta\theta_w^2 \quad (23)$$

with $\Delta\theta_d = (\theta_d - 40)$ and $\Delta\theta_w = (\theta_w - 40)$. The noise of $\sigma^0(\theta_d)$ and $\sigma^0(\theta_w)$ can be computed using error propagation.

$$\text{Var}[\sigma^0(\theta_d)] = \text{Var}[\sigma^0(40)] + \text{Var}[\sigma'(d)] \cdot \Delta\theta_d^2 + \frac{1}{4} \cdot \text{Var}[\sigma''(d)] \cdot \Delta\theta_d^4 \quad (24)$$

$$\text{Var}[\sigma^0(\theta_w)] = \text{Var}[\sigma^0(40)] + \text{Var}[\sigma'(d)] \cdot \Delta\theta_w^2 + \frac{1}{4} \cdot \text{Var}[\sigma''(d)] \cdot \Delta\theta_w^4 \quad (25)$$

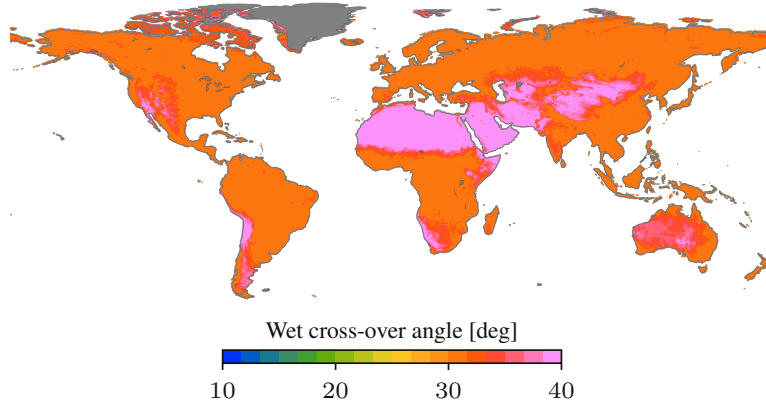


Figure 4.4: Wet cross-over angle map.

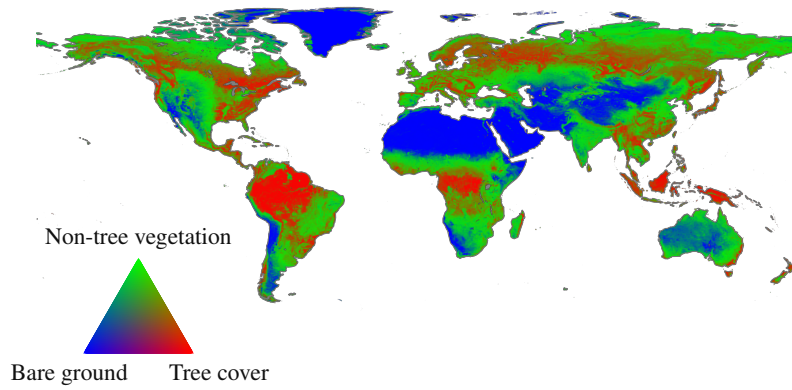


Figure 4.5: VCF5KYR 2016 data set [21].

The 2nd and 98th percentile are used as a robust estimate to determine the lowest and highest backscatter on a yearly (y) basis, using a time window of ± 2 years. This approach allows mitigating long-term land cover changes in backscatter observations. The yearly dry and wet backscatter reference at their cross-over angles ($\sigma_d^0(\theta_d, y)$, $\sigma_w^0(\theta_w, y)$) can only be compared to backscatter measurements under the same incidence angle. Thus, an interpolation to the reference incidence angle of 40° is required.

$$\sigma_d^0(40) = \sigma_d^0(\theta_d, y) - \sigma'(d) \cdot \Delta\theta_d - \frac{1}{2} \cdot \sigma''(d) \cdot \Delta\theta_d^2 \quad (26)$$

$$\sigma_w^0(40) = \sigma_w^0(\theta_w, y) - \sigma'(d) \cdot \Delta\theta_w - \frac{1}{2} \cdot \sigma''(d) \cdot \Delta\theta_w^2 \quad (27)$$

The noise is given by

$$\text{Var}[\sigma_d^0(40)] = \text{Var}[\sigma_d^0(\theta_d, y)] - \text{Var}[\sigma'(d)] \cdot \Delta\theta_d^2 - \frac{1}{4} \cdot \text{Var}[\sigma''(d)] \cdot \Delta\theta_d^4 \quad (28)$$

$$\text{Var}[\sigma_w^0(40)] = \text{Var}[\sigma_w^0(\theta_w, y)] - \text{Var}[\sigma'(d)] \cdot \Delta\theta_w^2 - \frac{1}{4} \cdot \text{Var}[\sigma''(d)] \cdot \Delta\theta_w^4 \quad (29)$$

Dry correction

In its current formulation, the soil moisture retrieval does not include a dry backscatter correction

Wet correction

In some regions truly saturated conditions are never captured simply due to the prevailing climate. Hence, a correction needs to be applied simulating wet conditions, allowing to estimate a real or better wet reference. The application of wet correction is based on an external climate data set [22], since scatterometer measurements alone are not sufficient to locate these regions. The wet correction is done in two steps: first the lowest level of the wet reference is set to -10 dB and subsequently, in regions with rarely saturated soil moisture conditions, $\sigma_w^0(40)$ values are raised until a sensitivity (defined as $\sigma_w^0(40) - \sigma_d^0(40)$) of at least 5 dB has been reached [7].

4.2.7. Surface soil moisture computation

The surface soil moisture computation is based on the assumption of a linear relationship between backscatter and surface soil moisture. Therefore, the normalized backscatter measurements are scaled between the dry and wet reference to obtain relative surface soil moisture expressed in degree of saturation, ranging from 0 % (dry soil) and 100 % (saturated soil). The topsoil layer is directly exposed to rain, wind, sunlight, etc. which can cause rapid changes in the topsoil moisture conditions. Furthermore, the penetration depth of the C-band microwave signal into the soil (depending on soil surface conditions) is just a few centimeter (1-2 cm), but could also be deeper in very dry soil regimes. Thus, dry or saturated soil refers to the very top surface soil moisture conditions. From a hydrological perspective, soil will never be absolutely dry and reach a minimum moisture level, however the exact amount of residual water content is usually unknown. In order to account for this uncertainty and the robust estimation of the dry and wet backscatter reference using percentiles, the backscatter observations are scaled between $a = 5$ and $b = 95$. This approach also avoids many consecutive low or high backscatter observations scaled to extreme values.

$$sm = a + \frac{\sigma^0(40) - \sigma_d^0(40)}{\sigma_w^0(40) - \sigma_d^0(40)} \cdot (b - a) \quad (30)$$

In Equation 30, sm is the estimated surface soil moisture that represents the topmost soil layer (< 5 cm) and can be converted into (absolute) volumetric units (m^3m^{-3}) with the help of soil porosity information.

$$\Theta = \Theta_r + p \cdot \frac{sm}{100} \quad (31)$$

where Θ is absolute soil moisture in m^3m^{-3} , p is porosity in m^3m^{-3} . If the exact amount of residual water content Θ_r in m^3m^{-3} is known, it can be used to adjust the absolute soil moisture content.

By proceeding with the error propagation, the following noise estimate of surface soil moisture and absolute surface soil moisture can be obtained:

$$\begin{aligned} \text{Var}[sm] = & \text{Var}[\sigma^0(40)] \cdot \left(\frac{b - a}{\sigma_w^0(40) - \sigma_d^0(40)} \right)^2 \\ & + \text{Var}[\sigma_d^0(40)] \cdot \left((b - a) \cdot \frac{\sigma^0(40) - \sigma_d^0(40)}{(\sigma_w^0(40) - \sigma_d^0(40))^2} - \frac{b - a}{\sigma_w^0(40) - \sigma_d^0(40)} \right)^2 \\ & + \text{Var}[\sigma_w^0(40)] \cdot \left((b - a) \cdot \frac{\sigma^0(40) - \sigma_d^0(40)}{(\sigma_w^0(40) - \sigma_d^0(40))^2} \right)^2 \end{aligned} \quad (32)$$

$$\text{Var}[\Theta] = \text{Var}[p] \cdot \frac{sm}{100} + \text{Var}[sm] \cdot \frac{p}{100} \quad (33)$$

4.3. Side note on error propagation

Let $\mathbf{x} = [x_1, \dots, x_p]$ be a p -dimensional observation vector. $\mathbf{x}$ is assumed to be an instance of p -dimensional random variable, with known covariance matrix $\Sigma_{\mathbf{x}}$. We are interested in how the covariance transforms under a mapping: $\mathbb{R}^p \rightarrow \mathbb{R}^q$, $\mathbf{y} = f(\mathbf{x})$, i.e., given $\mathbf{x}$ and f , we would like to know the covariance of $\mathbf{y}$, $\Sigma_{\mathbf{y}}$. If f is a linear mapping of the form $\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{b}$, $\mathbf{A} \in \mathbb{R}^{q \times p}$, $\mathbf{b} \in \mathbb{R}^q$, then the covariance transforms like

$$\Sigma_{\mathbf{y}} = \mathbf{A}\Sigma_{\mathbf{x}}\mathbf{A}^T \quad (34)$$

whereby $\mathbf{A}^T$ denotes the transpose of $\mathbf{A}$.

If, on the other hand, f is a non-linear mapping, we first linearize it by replacing its first order Taylor approximation about the operation point $\mathbf{x}_0$:

$$\mathbf{y} = f(\mathbf{x}) \approx f(\mathbf{x}_0) + \left(\frac{\delta f}{\delta \mathbf{x}}\right)(\mathbf{x} - \mathbf{x}_0) \quad (35)$$

whereby $\left(\frac{\delta f}{\delta \mathbf{x}}\right)$ is the Jacobian J of f . Putting everything together, we finally obtain

$$\Sigma_{\mathbf{y}} = \left(\frac{\delta f}{\delta \mathbf{x}}\right) \Sigma_{\mathbf{x}} \left(\frac{\delta f}{\delta \mathbf{x}}\right)^T \quad (36)$$

for the variance of $\mathbf{y}$ under the mapping f . Equation 36 serves as the cornerstone of the error propagation scheme.

4.4. Limitations and caveats

The soil moisture retrieval is applied on a global basis over land, but in certain situations (dense forest, snow cover, frozen soil, open water, topographic complex or urban area dominating the satellite footprint), the retrieval of reliable soil moisture is not always possible. Nonetheless, soil moisture is computed, and additional information is provided to mask invalid soil moisture measurements. Users are advised to use the best auxiliary data available to improve the flagging of snow, frozen soil and (temporally) standing water. A processing flag, correction flag, subsurface scattering probability flag and noise estimation are provided in the soil moisture product. It is crucial to recognize that the error model employed cannot account for all sources of error, notably frozen soil, snow, subsurface scattering, and wetland effects. Consequently, noise estimation may not accurately capture uncertainties in these scenarios.

Under the following conditions, the soil moisture retrieval should be most suited:

- low to moderate vegetation regimes,
- unfrozen and no snow,
- no subsurface scattering,
- low to moderate topographic variations,
- no wetlands and coastal areas,
- no soil sealing,
- no radio frequency interference.

4.4.1. Vegetation

The influence of vegetation on the backscatter signal is currently accounted for using a seasonal correction. The so-called cross-over angle concept (see section 4.2.6) allows the determination of the dry and wet backscatter reference at incidence angles where the backscattering coefficient is stable despite seasonal changes in the above ground biomass. The assumption that a climatology is sufficient to represent the inter-annual cycle of vegetation phenology no longer holds true in areas with a high level of variation in seasonal vegetation patterns. Semi-arid regions or areas with large scale disruptions (e.g. fires) can therefore have a decreased quality in the representation of the seasonal cycle of soil moisture. However, short-term anomalies in soil moisture are not affected by a misinterpretation of the seasonal vegetation cycle. The impact of strongly varying inter-annual vegetation cycles has not been quantified and needs to be recognized as a limitation in the current representation of the vegetation correction.

In densely vegetated areas (such as Tropical rainforests) the C-band microwaves are not able to penetrate to the ground. Hence, a soil moisture signal from the soil surface is not contained in the backscatter measurements, which is typically characterized by a very low signal variation (signal sensitivity). However, such cases lead to an increase in the error of the soil moisture estimate (according to Eq. 32, the root mean square error is proportional to the inverse of the squared sensitivity) and can thus be identified.

4.4.2. Desert areas

Desert areas exhibit challenging conditions for the retrieval of surface soil moisture information from radar scatterometry. The backscatter signal strength and dynamics in combination with different scattering mechanisms are the main challenges. These effects can be attributed to the climate and surface conditions leading to different implications (e.g. lack of saturated soil conditions, azimuth anisotropy, high noise, volume scattering, subsurface scattering).

Desert environments are characterized by a shortage of soil moisture due to a limited amount of annual precipitation. As pointed out in section 4.2.6, this leads to the application of the wet correction, since saturated soil conditions are never captured by the scatterometer. In addition, the overall backscatter signal strength and dynamics are very low, especially sandy deserts can have a backscatter below -20 dB. Such areas are prone to be affected by azimuth anisotropy and Bragg scattering [23]. Latter is related to small scale ripples on dunes enhancing the backscatter signal for a specific range of incidence angles.

4.4.3. Subsurface scattering

In very dry environments, soil volume scattering can play an import role. The penetration depth of microwaves can be large (i.e. up to several meters), causing volume scattering and increasing the chance of hitting a subsurface bedrock. The latter can be observed especially in some parts of North Africa, leading to an inverse relationship between backscatter and soil moisture. During dry-down, the soil moisture retrieval algorithm shows an increase of soil moisture even though the real soil surface is completely dry. The reason is that the backscatter signal is coming from the subsurface when it is completely dry, and during wet conditions the penetration depth is too shallow to reach this layer.

4.4.4. Snow

Depending on the physical parameters of the snow layer (i.e. liquid water content, roughness of the air-snow interface, depth and layering of the snow pack, grain size and shape) different scattering mechanisms characterize the overall backscatter signal. Snow scattering phenomena are not treated in the soil moisture retrieval algorithm and snow covered periods needs to be masked based on auxiliary information, e.g. using snow cover information from land surface models.

4.4.5. Frozen soil

At temperatures below 0°C microwave backscatter drops, because of the inability of the soil water molecules to align themselves to the external electromagnetic field. The effect of freezing is more complex in case of vegetation, because plants have adaptive mechanisms to withstand the cold weather. Like for snow, handling backscatter from soil freezing periods is not covered by the soil moisture retrieval algorithm and affected time periods needs to be masked based on auxiliary information, e.g. using soil temperature information from land surface models.

4.4.6. Surface water and wetlands

Backscatter characteristics are primarily controlled by the roughness of the water surface, which is related to the short penetration depth of C-band microwaves (< 1-2 mm). A calm water surface acts like a mirror, scattering almost the complete signal into the forward direction. Waves caused by near surface winds increase the backscatter looking at up- and downwind direction, and reduces the signal normal to the wind direction. As a result, open water can have a disturbing influence on the retrieval of soil moisture, if the area covered is large compared to the overall footprint size. Locations with (temporary) standing water needs to be treated carefully.

4.4.7. Topographic complexity

A high variability of backscatter can be observed in mountainous areas, which is not necessarily coupled with soil moisture changes. Hence, the surface topography directly influences the scattering behaviour, which is not considered in the soil moisture retrieval algorithm. A reduced soil moisture retrieval performance can be expected in topographically complex areas.

4.4.8. Urban areas

In (sub-)urban regions, the presence of bare ground is typically limited to small patches of parkland and grassland, presenting challenges for the meaningful retrieval of surface soil moisture. As outlined in section 4.1, major cities are masked within the resampling process of ASCAT Level 1b SZF backscatter by identifying the predominant land cover type (ESA CCI Land Cover 2018 300 m v2.1.1). However, in the remaining unmasked (sub-)urban areas with possibly mixed land cover, the backscatter signal can be influenced by the slopes of aligned scattering targets such as buildings, which can lead to double or multiple bounces of the radar signal. Backscatter from a few point-like targets in certain viewing directions can become significantly high, potentially affecting the overall response within the footprint, even at the coarse resolution of ASCAT backscatter observations [14].

4.4.9. Radio frequency interference

The increasing occurrence of radio frequency interference (RFI) events in recent years, particularly near urban areas, poses another challenge as ASCAT's frequency range is now being shared with mobile telecommunication services. Although information gathered in the ASCAT noise reception window generally allows for the masking of RFI-affected measurements during raw data processing, this may in turn compromise the consistency and continuity of surface soil moisture data. The backscatter40 flag contains information on whether backscatter noise is out of limits and possibly affected by RFI (see [24]).

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List of Acronyms

ASAR	Advanced Synthetic Aperture Radar (on Envisat)
ASAR GM	ASAR Global Monitoring
ASCAT	Advanced Scatterometer
ATBD	Algorithm Theoretical Baseline Document
BUFR	Binary Universal Form for the Representation of meteorological data
DORIS	Doppler Orbitography and Radiopositioning Integrated by Satellite (on Envisat)
ECMWF	European Centre for Medium-range Weather Forecasts
Envisat	Environmental Satellite
ERS	European Remote-sensing Satellite (1 and 2)
ESA	European Space Agency
EUM	Short for EUMETSAT
EUMETCast	EUMETSAT's Broadcast System for Environment Data
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FTP	File Transfer Protocol
H SAF	SAF on Support to Operational Hydrology and Water Management
Météo France	National Meteorological Service of France
Metop	Meteorological Operational Platform
NRT	Near Real-Time
NWP	Near Weather Prediction
PRD	Product Requirements Document
PUM	Product User Manual
PVR	Product Validation Report
SAF	Satellite Application Facility
SAR	Synthetic Aperture Radar
SRTM	Shuttle Radar Topography Mission
SZF	Sigma Zero Full resolution
SZO	Sigma Zero Operational (25 km spatial sampling)
SZR	Sigma Zero Research (12.5 km spatial sampling)
TU Wien	Technische Universität Wien (Vienna University of Technology)

WARP Soil Water Retrieval Package

WARP H WARP Hydrology

WARP NRT WARP Near Real-Time

ZAMG Zentralanstalt für Meteorologie und Geodynamik (National Meteorological Service of Austria)

Appendices

A. Introduction to H SAF

H SAF is part of the distributed application ground segment of the “European Organization for the Exploitation of Meteorological Satellites (EUMETSAT)”. The application ground segment consists of a Central Application Facilities located at EUMETSAT Headquarters, and a network of eight “Satellite Application Facilities (SAFs)”, located and managed by EUMETSAT Member States and dedicated to development and operational activities to provide satellite-derived data to support specific user communities (see Figure A.1):

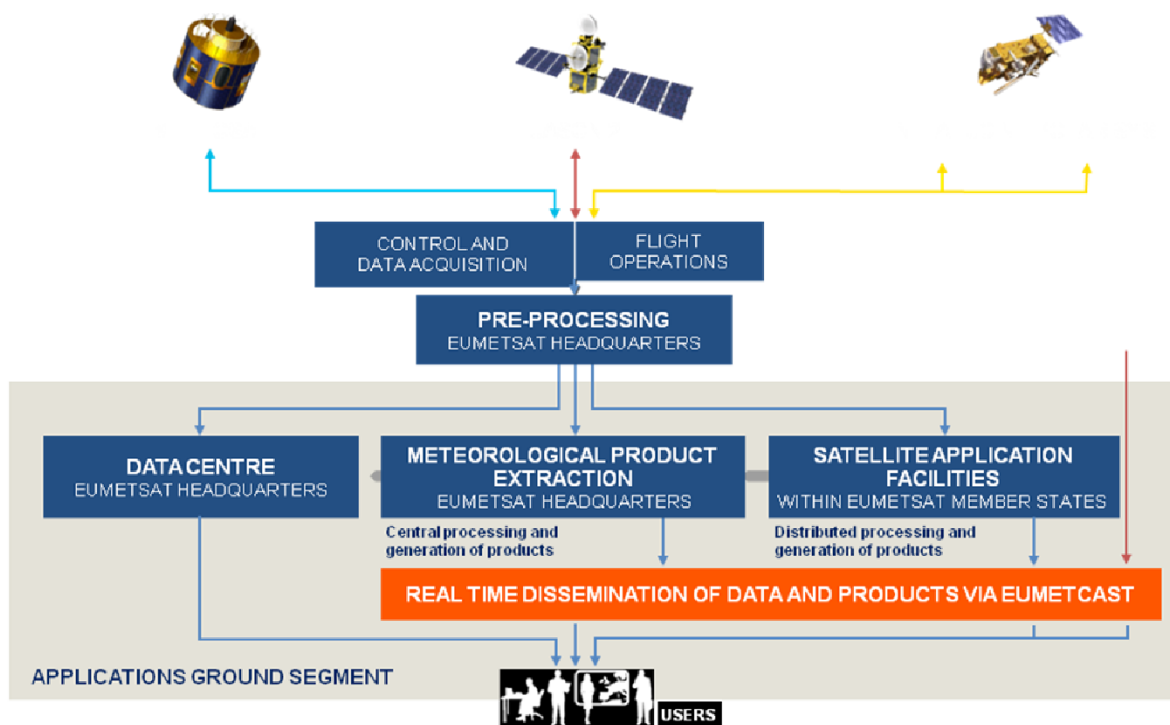


Figure A.1: Conceptual scheme of the EUMETSAT Application Ground Segment.

Figure A.2, shown below, depicts the composition of the EUMETSAT SAF network, with the indication of each SAF’s specific theme and Leading Entity.

B. Purpose of the H SAF

The main objectives of H SAF are:

a) to provide new satellite-derived products from existing and future satellites with sufficient time and space resolution to satisfy the needs of operational hydrology, by generating, centralizing, archiving and disseminating the following products:

- precipitation (liquid, solid, rate, accumulated);
- soil moisture (at large-scale, at local-scale, at surface, in the roots region);
- snow parameters (detection, cover, melting conditions, water equivalent);



Figure A.2: Current composition of the EUMETSAT SAF Network.

b) to perform independent validation of the usefulness of the products for fighting against floods, landslides, avalanches, and evaluating water resources; the activity includes:

- downscaling/upscaling modelling from observed/predicted fields to basin level;
- fusion of satellite-derived measurements with data from radar and raingauge networks;
- assimilation of satellite-derived products in hydrological models;
- assessment of the impact of the new satellite-derived products on hydrological applications.

C. Products / Deliveries of the H SAF

For the full list of the Operational products delivered by H SAF, and for details on their characteristics, please see H SAF website <http://h-saf.eumetsat.int>. All products are available via EUMETSAT data delivery service (EUMETCast¹), or via ftp download; they are also published in the H SAF website².

All intellectual property rights of the H SAF products belong to EUMETSAT. The use of these products is granted to every interested user, free of charge. If you wish to use these products, EUMETSAT's copyright credit must be shown by displaying the words "copyright (year) EUMETSAT" on each of the products used.

D. System Overview

H SAF is lead by the Italian Air Force Meteorological Service (ITAF MET) and carried on by a consortium of 21 members from 11 countries (see website: <http://h-saf.eumetsat.int/> for details)

Following major areas can be distinguished within the H SAF system context:

¹<http://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/index.html>

²<http://h-saf.eumetsat.int/>

- Product generation area
- Central Services area (for data archiving, dissemination, catalogue and any other centralized services)
- Validation services area which includes Quality Monitoring/Assessment and Hydrological Impact Validation.

Products generation area is composed of 5 processing centres physically deployed in 5 different countries; these are:

- for precipitation products: ITAF CNMCA (Italy)
- for soil moisture products: GeoSphere (Austria), ECMWF (UK)
- for snow products: TSMS (Turkey), FMI (Finland)

Central area provides systems for archiving and dissemination; located at ITAF CNMCA (Italy), it is interfaced with the production area through a front-end, in charge of product collecting. A central archive is aimed to the maintenance of the H SAF products; it is also located at ITAF CNMCA.

Validation services provided by H SAF consists of:

- Hydrovalidation of the products using models (hydrological impact assessment);
- Product validation (Quality Assessment and Monitoring).

Both services are based on country-specific activities such as impact studies (for hydrological study) or product validation and value assessment. Hydrovalidation service is coordinated by IMWM (Poland), whilst Quality Assessment and Monitoring service is coordinated by DPC (Italy): The Services activities are performed by experts from the national meteorological and hydrological Institutes of Austria, Belgium, Bulgaria, Finland, France, Germany, Hungary, Italy, Poland, Slovakia, Turkey, and from ECMWF.