

		
SO-TN-CBSA-GS-0029 Issue : 3.0 Date : 2019/07/04	CATDS SMOS L3 soil moisture retrieval processor Algorithm Theoretical Baseline Document (ATBD)	Y.H.K, E.J., A.A., F.C., A. M., P.R., A.Q., L.B. Page 1 /61

CATDS SMOS L3 soil moisture retrieval processor Algorithm Theoretical Baseline Document (ATBD)

Project code SO-TN-CBSA-GS-0029

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ACRONYMS

Acronyms	Meaning
ADF	: Auxiliary Data File
AMSR-E	: Advanced Microwave Scanning Radiometer - Earth Observing System
ASL	: Above Surface Layer
ATBD	: Algorithm Theoretical Baseline Document
BREF	: Branch of the decision tree for the day of reference
C-EC	: CATDS Expert Centre
C-PDC	: CATDS Production and Distribution Centre
CATDS	: Centre Aval de Traitement des Données SMOS
CESBIO	: Centre d'Etudes Spatiales de la Biosphère
CDTI	: Spanish bureau for space activities
CFI	: Customer Furnished Items. Collection of multiplatform precompiled C libraries for geolocation computation
CNES	: Centre National d'Etudes Spatiales
DAP	: Data Analysis Product (L2 product)
DFFG	: Discrete Flexible Fine Grid
DFG	: Discrete Fine Grid
DGG	: Discrete Global Grid used for SMOS products : For ESA processors, it is the ISEA grid; for CATDS processors, it is the EASE 25 km gridding system
DPGS	: Data Processing Ground Segment
DQX	: Data Quality Index (posterior theoretical uncertainty)
EASE	: Equal-Area Scalable Earth Grid
ECMWF	: European Centre for Medium-range Weather Forecasting
ESA	: European Space Agency
ESL	: Expert Support Laboratory
FFO	: Forest fraction
FM	: Mean fractions to compute the reference values for the free parameters of the retrieval model(s)
FM0	: Mean fractions to drive the decision tree
FNO	: Nominal soil fraction
FOV	: Field Of View
GQX	: Global Quality Index
HR	: Roughness parameter
ISEA	: Icosahedral Snyder EqualArea Earth fixed grid
L0, L1, L2, L3, L4	: Level 0, 1, 2, 3 and 4 respectively
LAI	: Leaf Area Index
LAI_max	: Maximum value of the LAI over one year for a forest stand
Lat, lon	: Latitude, longitude
LM	: Levenberg-Marquardt
LUT	: Look-Up Table
MIRAS	: Microwave Imaging Radiometer by Aperture Synthesis
MD2, MD3, MD4	: Dielectric index model retrieval options
MN2, MN3, MN4	: Vegetated soil radiative model retrieval options

MW2, MW3, MW4	: Open water radiative model retrieval options
NPE	: Non-Permanent (meteorological conditions)
NSIDC	: National Snow and Ice Data Center
OS	: Ocean Salinity
PROTEUS	: Plate-forme Reconfigurable pour l'Observation les Télécommunications et les Usages Scientifiques
RFI	: Radio Frequency Interference
RSTD	: Theoretical retrieval standard deviation
SM	: Soil volumetric Moisture content
SMOS	: Soil Moisture and Ocean Salinity
Tau	: Vegetation optical thickness (nadir)
TB	: Brightness Temperature
TB(ξ , η)	: Brightness Temperature in the antenna frame (cosdir coordinates, spatial domain)
T \tilde{B} (U, V)	: Discrete Fourier Transform of Brightness Temperature in the antenna frame ((U, V) frequency domain)
TBF	: Modelled TB (from geophysical parameters)
TBH	: Brightness Temperature for Horizontal polarization at the surface of the earth
TBM	: TB measurement
TBV	: Brightness Temperature for Vertical polarization at the surface of the earth
TEC	: Total Electron Content (tecu unit)
TOA	: Top Of Atmosphere
UDP	: User Data Product (L2 product)
WEF	: SMOS pixel Weighting Function

		
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DEFINITIONS

Term	Definition
Apodization function APF	Function applied to TB in Fourier space in order to attenuate the effects of the sharp cut-off at the boundaries of the baseline domain
Auxiliary data	Those data required by the L2 processor which are not part of SMOS data products We differentiate two categories: fixed and evolving (or time varying)
Baseline	Physical distance between any 2 elements of the interferometer
Baseline domain	Star shaped domain covered by every baseline provided by the instrument
Bore sight	Antenna axis: angular direction perpendicular to the antenna best fit plane
Default contribution	Contribution to the radiometric signal computed with physical parameters obtained from auxiliary data only
DFFG working area	Subset of a map on the DFFG grid, which surrounds a given DGG grid node
Director cosines	Natural reference frame at antenna level. Director cosines are $\xi = \sin(\theta) \cos(\phi)$ and $\eta = \sin(\theta) \sin(\phi)$, where θ and ϕ are here respectively the angle to antenna bore-sight and the azimuth in the antenna plane, reference being X polarization direction
DQX	Retrieval error estimate associated to each parameter product with the same unit
Dwell line	The (not quite straight) line along the FOV on which are located views of the same areawhen compounding successive snapshots, for various incidence angles
Fine grid, DFG	Highest resolution grid where auxiliary surface data must be provided
Fixed Parameter Reference value	Geophysical quantity obtained through pre-processing auxiliary data files in order to obtain a view dependant values or initial guesses for a parameter
Flexible Fine grid DFFG	Aggregated DFG to a variable coarser resolution where computation must be done
Forward model fwd	Radiative model to compute TB from physical medium properties
Fraction	Weight to be applied to a surface area when computing the radiometric signal as a sum of contributions
Free Parameter Reference value	quantity obtained through pre-processing auxiliary data files in order Geophysical to apply decision tree and obtain initial guesses for a parameter
Homogeneous pixel	SMOS pixel which consist of a single fraction when considering the surface characteristics (including evolving features such as snow)
L1C node L1C pixel	A given TB data record in the L1C data product. Such a record is defined for an earth location (L1 Auxiliary Earth Grid file DGG) and contains, among others, a collection of SMOS pixels TB and their attached incidences angles and elliptical footprint characteristics
L1C view	Subset of the L1C pixel for identical or quasi identical incidence angles
Local DFG grid	Subset of a map on the DFG grid, which surrounds a given DGG grid node
Mean fraction	Aggregated fraction where the weight is computed using a mean weighting function which does not depend on the incidence angle
Measurement	Brightness temperature measured in one MIRAS polarization mode, along with relevant information (radiometric noise, observation conditions, contributions as computed by the model, flags, polarization direction). A measurement is associated with one Grid point, one Snapshot,

	one WEF and one Footprint.
MEAN_WEF	Weighting function used for carrying out weighted sums over the DFFG independently of incidence angle
MIRAS	<p>Polarization mode MIRAS measures brightness temperatures in four polarization modes:</p> <ul style="list-style-type: none"> -XX along polarization direction X -YY along polarization direction Y -XY one arm set to X, the two others set to Y -YX one arm set to Y, the two others set to X <p>XY and YX mode produce complex brightness temperatures that are complex conjugates. In L1C product, both XY and YX modes feed the XY brightness temperature data field with real and imaginary.</p>
MIRAS operating mode	<p>MIRAS has two operating modes:</p> <p>Dual polarization mode: measurement sequence is :</p> <ul style="list-style-type: none"> - XX - YY - XX - YY - XX - YY ... <p>Full polarization mode: Measurement cycle is</p> <ul style="list-style-type: none"> - XX - XY - YY - YX - XX - XY - YY - YX -XX - ...
Normal soil	Soil which has an upper layer which is able to store liquid water
Prior values	Values of the geophysical parameters, obtained from external sources, that are introduced, with their uncertainties, in the cost function, as reference information of the variability range during the iterative retrieval
Product Confidence Descriptor	Subset of processor outputs that includes indications about the quality of the product. It contains both confidence value and flags.
Product Process Descriptor	Subset of processor outputs that includes information about process options and status. A small subset is given in User Data Product, and the main part is stored in DAP for ESL analysis after launch.
Product Science Flags	Subset of processor outputs that includes information about geophysical external features
Reconstruction	Computation by the L1 processor of brightness temperatures fields from visibilities
Reference value	Value of a physical parameter used in a radiative model, obtained through averaging physical parameters provided as auxiliary parameters for an elementary area, over an aggregated fraction which aggregates the concerned elementary areas.
SMOS Field of view (FOV)	The extent of the snapshot, bounded by both aliased earth images and spatial resolution. The FOV may be defined in the antenna frame of reference or in a geographical system at Earth's surface level.
SMOS fixed grid DGG	Equi-surface grid, defined once and for all, on the nodes of which the soil moisture will be retrieved. The average inter-node distance is close to 15 km in the case of ISEA grid and 25 km in the case of EASE grid. For land surfaces only (including large ice covered areas), the grid should include about 6.5×10^5 nodes for ISEA grid.
SMOS pixel	This expression refers loosely (through its 3dB contours) to the weighting function which characterizes the spatial resolution of the interferometer.
Snapshot	<p>Ensemble of measurements acquired at the same time.</p> <p>The image reconstructed from SMOS interferometric data averaged over the elementary time period.</p>
Uniform pixel	<p>Homogeneous SMOS pixel within which every physical parameter is identical.</p> <p>This is a convenient concept but probably does not exist over land surfaces.</p>
Weighting function (WEF)	Function derived from the apodization function, to be applied to every elementary area inside the SMOS pixel in order to give the proper weight to the corresponding contribution to up-welling radiation.
X_Swath	Distance of the grid node from the satellite track.

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1 INTRODUCTION

The purpose of this ATBD is to describe the algorithms of the daily and time synthesis (Level 3) processors for SMOS (Soil Moisture and Ocean Salinity) satellite produced at CATDS : CNES's level 3 and level 4 production centre for SMOS. The CATDS Soil Moisture Level 3 products include daily ascending and descending multi-orbit soil moisture retrieval products and time synthesis products (3-day, 10-day, monthly products). The document focuses on the scientific motivations behind the selected algorithms, the underlying assumptions and limitations, and the outline of the proposed approach. The purpose of this ATBD is to describe the algorithms behind the daily and time synthesis (Level 3) global products from SMOS (Soil Moisture and Ocean Salinity) satellite produced at CNES's SMOS higher level products centre for SMOS at CATDS. The CATDS Soil Moisture Level 3 products include daily ascending and descending multi-orbit soil moisture retrieval products and time synthesis products (3-day, 10-day, monthly products). The document focuses on the scientific motivations behind the selected algorithms, the underlying assumptions and limitations, and the outline of the proposed approach.

This document provides a short theoretical description for SMOS measurements over land surfaces useful for L3 processing, Detailed scientific explanations on radiative transfer in L-band and retrieval of soil moisture from L-band brightness temperatures for SMOS mission can be found in the L2 SM ATBD [6] and [20]. A detailed description of the retrieval modules specific to the L3 is also given. The algorithms for time synthesis products are also described. L3 processing uses a different gridding system than the L1 and L2 processing, so the inputs of the L3 SM processing are also described in this document, to be able to fully understand the CATDS processing chain for soil moisture.

2 SMOS AND CATDS OVERVIEW

2.1 SMOS CONTEXT

Issues related to the state and evolution of the Earth system are currently considered as a significant problem to be addressed. Global change issues, forecasting of extreme events such as major floods and droughts, improvement of weather forecasts and better management of water resources are consequently under scrutiny. For this purpose it is necessary to achieve a better understanding of the climate system, the water cycle so as to be able to monitor it at a global scale and achieve realistic projection of trends and potential future evolutions, including anthropic effects. To achieve these ambitious goals it is necessary to improve existing models and to have access to observed global data sets of surface variables.

Satellite remote sensing is a key element as it enables to gather repetitively and globally relevant surface variables. However, to be useful, such data must be acquired and processed over relatively long periods of time in a consistent manner. It is also important that data is made available to the science community and leads to innovative approaches as to their use.

SMOS (Soil Moisture and Ocean Salinity), a scientific exploratory mission, has been developed by ESA, CNES and CDTI. The goal of the mission is to estimate soil moisture and sea surface salinity in order to enhance climatologic and meteorological models and forecasts, extreme event prediction (drought, flood) and water resource management.

The SMOS mission is a small satellite (300-500 kg) that uses the generic PROTEUS platform developed by CNES and Thalès Alenia Space. SMOS was successfully launched on the 2nd of November 2009. The mission duration is at least three years including six months for the commissioning. Two additional years of operation have been decided.

2.2 OVERVIEW OF SMOS L0 TO L2 PROCESSING AND PRODUCTS

L0 to L2 processors are developed by the European Space Agency (ESA). The products are divided in half orbits, from pole to pole, ascending or descending, spanning about 50 minutes of acquisition. The processing chain is processed by the Data Processing Ground Segment (DPGS) and is designed with five levels of processing:

- The L0 processor aggregates Source Packets by half orbits after every data dump to the operational ground station. **Level 0 (L0)** products are raw data. They are consolidated (i.e. sorted and grouped by half orbit) with Science Data Packets and Ancillary Data Packets.
- The L1A processor converts all data coming from the spacecraft into engineering units. It produces calibration data and Fringe Wash Function from calibration sequences (noise injection, deep sky observations). Calibrated visibilities are then computed.
Level 1A (L1A) products are calibration data, ancillary data (e.g. telemetry), calibrated visibilities and fringe washing function data.
- The L1B processor converts calibrated visibilities into brightness temperature Fourier components. This is the so-called reconstruction process, which is based on the best approximation of the system response function and its inversion. A foreign source module applies corrections for Sun (direct, reflected and aliases). Aliases of the sky are subtracted to extend the available field of view. Data in the L1B product are sorted by snapshots according to the acquisition sequence.
Level 1B (L1B) products provide the Fourier Components of the snapshots acquired by SMOS.
- The L1C processor provides brightness temperatures in the antenna polarization reference frame, along with geometry of observations, polarization rotation angles to the target polarization frame and footprint size. On a snapshot basis, apodization and inverse Fourier transformation are applied at any DGG (Discrete Global Grid) grid point in the field of view. The DGG is the ISEA grid for ESA processor. Brightness temperatures and associated data are then sorted by ISEA grid points for the land or sea L1C product.
Level 1C (L1C) products provide series of brightness temperatures over a list of known points on Earth defined by the ISEA grid. Two L1C products are generated: one over land with data about 100km out to sea and one over ocean with data about 100km in land.

For more details on the L1 processors, see [2].

- Both L2 processors (land and sea) derive geophysical quantities using an iterative scheme and multi-angular observations of the ISEA grid points. Models that fully simulate SMOS measurements in the antenna reference frame are implemented and certain geophysical parameters are adjusted until the cost function reaches a minimum. Over land, heterogeneity of the surface is accounted for. Quality indices such as theoretical uncertainties of adjusted parameters and flags are also computed by L2 processors.
Level 2 (L2) products, one over land (L2SM), one over sea (L2OS), provide respectively soil moisture or sea surface salinity, along with quality indicators.

For more details on the L2 SM processor, see [6], [20].

3 OVERVIEW OF CATDS SOIL MOISTURE PROCESSING

3.1 LEVEL 3 SOIL MOISTURE OBJECTIVES

Over land, water and energy fluxes at the surface/atmosphere interface are strongly dependent upon soil moisture. We use here the term Soil moisture (SM) to refer to the volumetric soil moisture in the first few centimetres (0-5 cm) of the soil. This is a key variable in numerical weather predictions as well as in surface hydrology and in vegetation monitoring.

The level 3 products are geophysical variables with improved characteristics through temporal and/or spatial re-sampling or processing.

The objectives of the level 3 soil moisture processing are to:

- Retrieve enhanced soil moisture from SMOS brightness temperatures by taking advantage of temporal information,
- Provide global temporal synthesis maps of soil moisture

Level 3 products must be compliant with the SMOS requirements for soil moisture monitoring, i.e. the theoretical uncertainties on the retrieved soil moisture is less than $0.04 \text{ m}^3.\text{m}^{-3}$, a global coverage of 3 days using morning or afternoon orbits independently only and a spatial resolution better than 55 km. Soil moisture is strongly dependent

on the characteristics of the observed surface. In order to prevent any inconsistency resulting from interpolation over highly heterogeneous surfaces no spatial averaging is operated in the algorithms. Soil moisture can show fast temporal dynamics so climatic conditions are taken into consideration to produce temporal averages from daily to monthly basis.

It must also be noted that ascending and descending overpasses are bound to show different values of the retrieved parameters that may not be always comparable. They are thus retrieved separately. Other parameters like surface temperature, dielectric constant, soil roughness, albedo, etc can be processed with soil moisture.

3.2 LEVEL 3 SOIL MOISTURE STRATEGY

1. The level 3 is implemented in a rather unusual way: usually, the level 3 is made from level 2 in a hierarchical logic. However, it has been decided at CATDS to use brightness temperature products in the Fourier domain (L1B) as input for the Level 3 processor and this for the following reasons: At CATDS the Equal-Area Scalable Earth Grid (EASE grid) has been chosen as the product gridding system. It is a more user-friendly, map based, regular global grid. As the brightness temperature products in the spatial domain from DPGS (L1C products) are over the ISEA grid, it was optimal to make the inverse Fourier transform on the EASE grid directly from L1B products. In the process of enhancing the usability of the product the NetCDF format has been selected instead of the BinX used at DPGS.

The choice for EASE is based upon the following reasons: (i) L3 products are global products, they are to be used by a large scientific community, and they will be compared with other sensors products. (ii) Moreover, the EASE grid makes easier the processing of spatial neighbourhoods involved in the L3SM algorithms, and has consequences in the required CPU time. (iii) the sampling rate at 25km is sufficient to comply with the Nyquist- Shannon sampling theorem.

2. The multi-orbit algorithm: Going back to brightness temperatures enabled the implementation of an enhanced soil moisture retrieval algorithm that uses retrievals from several revisits at a time.
3. Producing global maps: At high latitudes SMOS has revisit rates (28.6 daily revisits at the poles) see Figure 9. By using a filtering algorithm, the acquisitions at high latitudes have been reduced to the most accurate ones for each day enabling to produce a map based product.

Figure 1 shows an overview of the soil moisture processing chain at CATDS. The first processor implemented is the L1C processor that allows computing brightness temperatures in the spatial domain L1C from the Fourier components L1B. This is the processor as the operational L1B → L1C processor but applied to the L3 grid (EASE grid instead ISEA grid). L1B products are processed by half-orbits. These L1C products are CATDS internal products; they are not disseminated by CATDS, but are inputs for the next processing steps. The L1C products are then aggregated over one day in a daily L1C separated for ascending and descending orbits (named Super L1C) which are used by the OS and SM processing chains.

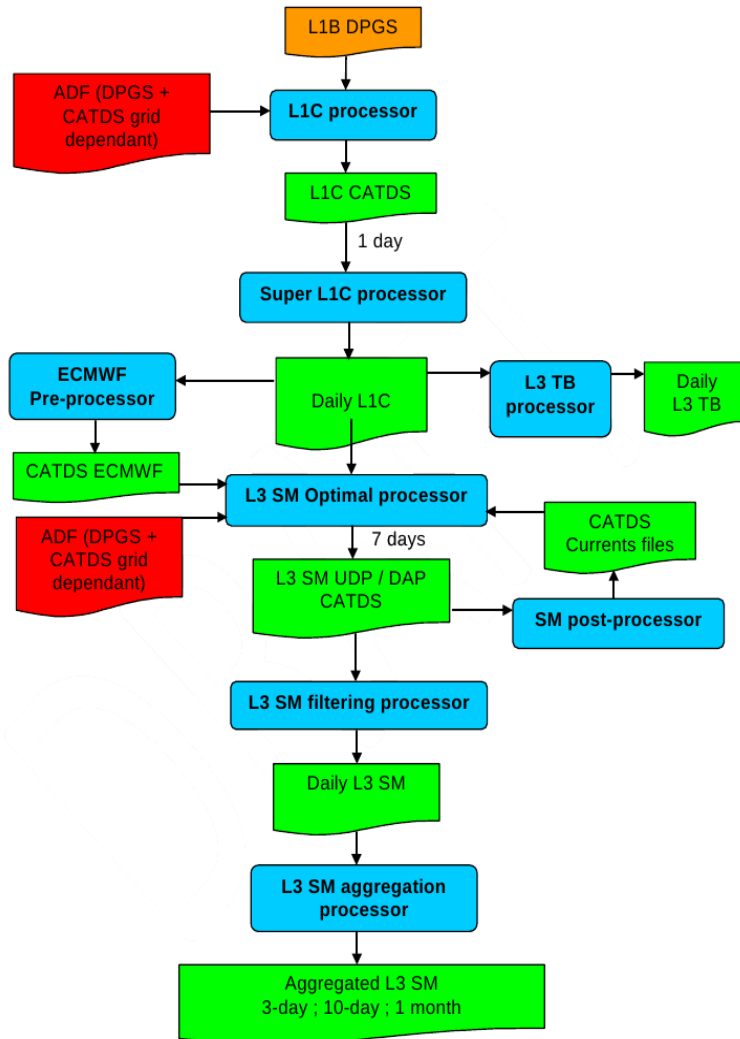


Figure 1: CATDS soil moisture processing chain

The Super L1C are then used by the L3 SM retrieval processor to obtain daily products of geophysical parameters. The L3 SM retrieval processor is based on the Level 2 SM processor adding the ability to make multi-orbit retrieval, which means process several orbits in the same retrieval loop. The L3 SM retrieval processor can also be run in mono-orbit mode; in this case the level 3 SM processor is equivalent to the level 2 SM with only minor differences mainly related to the gridding system. This allows a full coherence between the ESA Level 2 and the CATDS level 3 processors, in order to take advantage of the progress of the 2 developments.

The filtering processor is then used over the level 3 retrievals, to select the best estimation of soil moisture if several retrievals are available for a given day. It also implements an event detection algorithm to flag data for particular events as freezing, dew or snow.. Only the case of freezing is currently implemented in the CATDS. The filtered daily global maps are finally aggregated over different time periods. The SMOS revisit period is 3 days at the equator, so the Earth's surface is covered by SMOS field of view in 3 days. For this reason a 3-day global product with a 3 day moving window is provided by CATDS by aggregating the daily global maps. The CATDS also provides a 10-day product that contains median, minimum and maximum values of soil moisture over 10 days. This product is useful for agronomy and water resource management.

Finally, monthly products provide the mean soil moisture over a month, without taking into account the detected events. This product is useful for climate monitoring.

The next chapters describe each processor in details.

4 L3 SM INPUTS

4.1 THE DISCRETE GLOBAL GRID: EASE

At CATDS, it was preferred a grid format widely used by the community of the potential users of L3 SM products. The Discrete Global Grid (DGG) that is used for all CATDS processing is the Equal-Area Scalable Earth Grid (EASE-Grid) version 2.

The EASE-Grid is intended to be a versatile tool for users of global-scale gridded data, specifically remotely sensed data, although it is gaining popularity as a common gridding scheme for data from other sources as well. It is based on a philosophy of digital mapping and gridding definitions that was developed at the National Snow and Ice Data Center (NSIDC), in Boulder, Colorado (USA). EASE grid documentation can be accessed on the NSIDC website: <http://nsidc.org/data/ease/> This grid is used for several remote sensing data sets like SSM/I, AVHRR, SMMR, TOVS Path-P Polar Pathfinder data sets, or AMSR-E (AQUA) and has been adapted for the SMAP mission. Therefore, EASE-Grid meets the needs to geo-localise SMOS data with other remote sensing data like AMSR-E that also provides soil moisture maps. The EASE-Grid consists of a set of three equal-area projections, combined with an infinite number of possible grid definitions. The three EASE-Grid projections comprise two azimuthal Lambert's equal-area projections, for the Northern or Southern hemisphere, respectively, and a global cylindrical equal-area projection which is the one chosen for the CATDs products, as illustrated in Figure 2. All projections are based on a spherical model of the Earth with radius $R = 6371.228$ km. This radius defines a sphere with the same surface area as the 1924 International Ellipsoid (also known as the International 1924 Authalic Sphere). EASE-Grid users can specify any grid resolution.

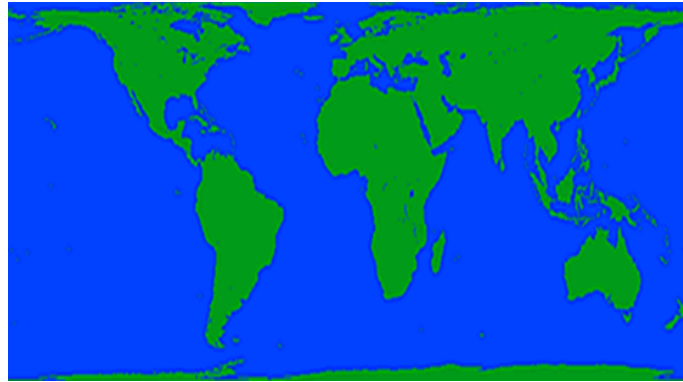


Figure 2: The EASE-Grid global cylindrical projection (NSIDC, http://nsidc.org/data/ease/ease_grid.html)

As stated before to reduce the unnecessary oversampling of the signal **the 25km EASE-Grid is selected for operational products**. This approximately doubles the sensor resolution and respects the Nyquist theorem. Version 2 of the grid is used.

The cylindrical equal-area map is defined as equal-area and equidistant at 30 N/S and by the following equations http://nsidc.org/data/ease/ease_grid2.html:

$$\begin{cases} r = r_0 + R/C * \lambda * \cos(30) \\ s = s_0 - R/C * \sin(\phi) / \cos(30) \\ h = \cos(\phi) / \cos(30) \\ k = \cos(30) / \cos(\phi) \end{cases} \quad (1)$$

Table 3 defines the variables used in the previous equations.

Variable	Definition
R	Column coordinate
S	Row coordinate
H	Particular scale along meridians
K	Particular scale along parallels
λ	Longitude in radians
ϕ	Latitude in radians
R	Radius of the Earth = 6371.228 km
C	Nominal cell size
r0	Map origin column
s0	Map origin row

Table 3: Definitions of Variables in Projection Equations (1)

The values of C, r0, and s0 are determined by the grid that is chosen to overlay the projection. For the global 25km grid, C = 25.02526 km and the grid extents are presented in Table 4

Grid	Dimensions		Map origin		Map origin		Grid extent			
Name	Width	Height	Column (r0)	Row (s0)	Lat.	Long.	Minimum Latitude	Maximum Latitude	Minimum Longitude	Maximum Longitude
ML	1388	584	694.0	292	0.0	0.0	86.72S	86.72N	180.00W	180.00E

Table 4: Grid extent for the global 25km EASE-Grid

Each DGG node is characterized by an identification number, a longitude, latitude and an altitude. This matrix representation is equal-area: each pixel (defined by 4 grid points) has the same surface (626 km²). The distance between the nodes is thus latitude-dependant. Figure 3 shows the distance between 2 grid nodes as a function of latitude, in the direction of the longitude (dx) and the latitude (dy).

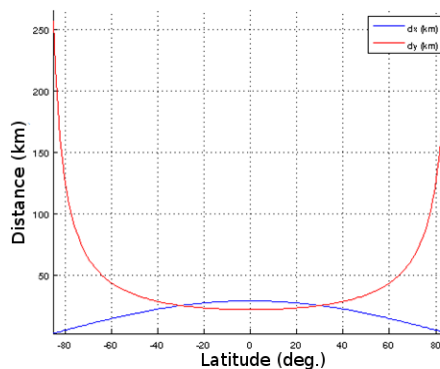


Figure 3: Distance between 2 grid nodes as a function of latitude, in the longitude direction (dx) and latitude direction (dy)

The distance between the nodes is illustrated below for 3 different latitudes:

At 30° N/S latitudes



At the equator



near the poles



For the CATDS processing, the following static auxiliary data files are generated off-line by ESLs with the DGG processor:

- AUX_CDGG , which describes the EASE grid
- AUX_CDGGXYZ, which provides the geocentric coordinates of grid points

The fields contained in AUX_CDGG file are described in Table 5.

Field	Description
NBND	Number of nodes in the grid
IDENTIFIANT	Unique identification number of a node
LATITUDE	Latitude of the node [-90,90]
LONGITUDE	Longitude of the node [-180,180]
ALTITUDE	Altitude of the node
nlongitude	Number of longitude in the grid
nlatitude	Number of latitude in the grid
resolution	Nominal resolution of the grid (in km)
projection	Projection of the grid (cylindrical)
type	Type of the grid (Ease)
globale	Indication to know if the grid is global or not (yes/no)
ndselig	Number of eligible nodes for a 'list of points' processing
flg_idelig	Flag for the node eligibility (0 not eligible, 1 eligible)

Table 5: Fields in AUX_CDGG file

Customized CATDS processing can be done using a user defined EASE-grid resolution with shifted coordinates if desired. This enables to re-centre the grid on a given location, which is useful to process a calibration/validation area, for example. In this case the user needs to define the new grid and regenerate the following CATDS specific auxiliary data files:

- AUX_CDGG_ and AUX_CDGGXYZ: with the DGG processor
- AUX_CLSMAS, AUX_CMASK and AUX_CRFI

When a grid is chosen as input of the processing chain, it must be kept all through the processing.

4.2 L1C PROCESSING

The L1C processor is in charge of computing SMOS brightness temperature (TB) at antenna reference frame on a given grid from L1B products. The processing is schematized in Figure 4

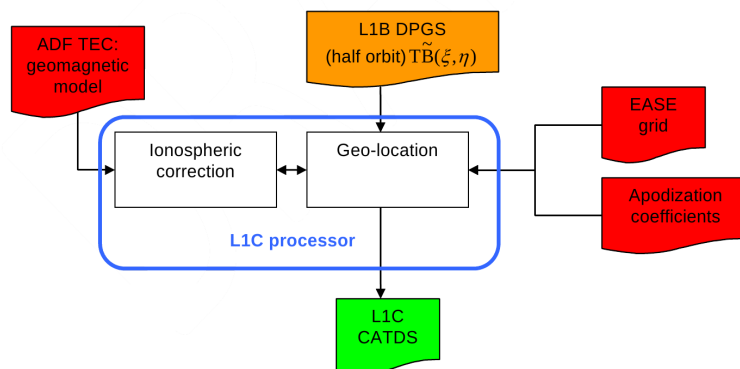


Figure 4: CATDS L1B to L1C processing

The functionalities of the CATDS L1C processor should be exactly the same than those implemented in the ESA operational processing. This processing step will thus not be detailed here (for a detailed description, see L1 ATBD [3]).

This processing allows producing L1C CATDS products on the CATDS DGG (a 25 km EASE grid), starting from operational L1B product. Level 1B are Fourier components of the acquired snapshots and are provided by ESA's ground segment (DPGS) by half-orbits.

Several computations are also carried out to complete the L1c product:

- Computation of the footprint axes approximated by ellipses
- Computation of the geometry (incidence, geometrical angle, coordinates in antenna frame, ...)
- Computation of geophysical parameters (Total Electron Content (TEC) from model IRI2001 or IGS combined TEC map, magnetic field, Faraday, ...)
- Computation of the radiometric noise

The computation of geo-location and geometric data are mainly carried out by Earth Explorer mission CFI functions [1].

4.3 DAILY BRIGHTNESS TEMPERATURE - L1C FILTERING

The CATDS works with time aggregated daily brightness temperatures global maps. These are used by the L3 processing (OS and SM). The Super L1C processor produces two daily products (one for ascending and one for descending orbits) of brightness temperatures, which are daily aggregation of L1C products. Each product contains 14.3 half-orbits per day. The number of revisits increases with the latitude, as illustrated in Figure 5. For any given day, there is no swath overlap below 66° latitude -or even 74° latitude if we consider the narrow swath- which leaves only the north of Greenland, Ellesmere Island and Komsomolets Island. This leaves little grid nodes where soil moisture retrieval is relevant. So, for each DGG located in high latitudes where there is a swath overlap, we select the half-orbit where measured brightness temperatures are nearest to the centre of the swath (parameter X_Swath minimized). The radiometric accuracy of brightness temperatures is generally higher at the centre of the swath than on the edges.

As mentioned above the distinction between ascending and descending orbits is preserved. For one day, two daily global super L1C (SL1C) products are generated: one for ascending, one for descending orbits. SL1C product contains the same scientific fields than the L1C product, but the file is organised in a different way. L1C is organised snapshot by snapshot, and SL1C is organised by latitude bands with several snapshots, illustrated in Figure 6. The bands are still stored by temporal layers. Time is not considered here as an absolute datation of each snapshot but with respect to acquisition sequence within each orbit.

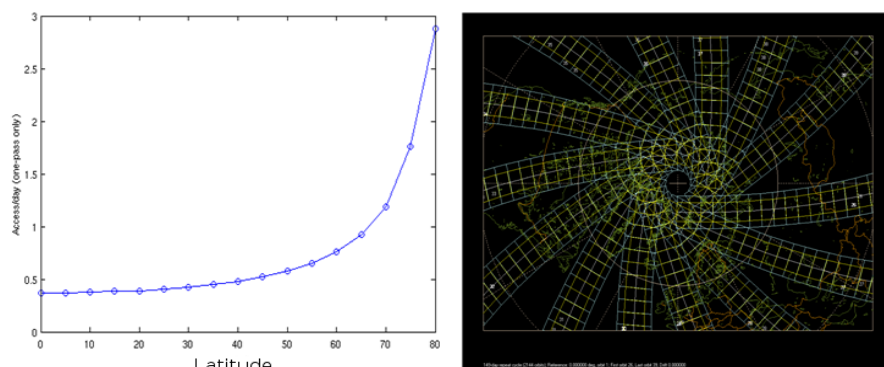


Figure 5: Spacecraft revisits over one day for ascending orbits: revisits per day according to the latitude (left) swath earth projection over North Pole (right).

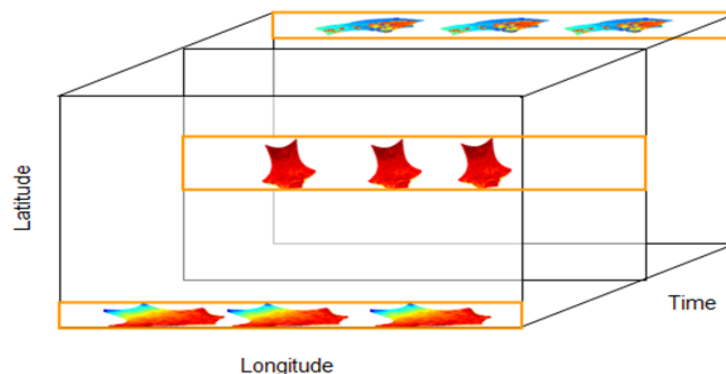


Figure 6: Daily SL1C CATDS format organisation: bands of latitudes

5 L3 SM OPTIMAL PROCESSING

5.1 MOTIVATIONS AND CONCEPT

The main goal of L3 SM Optimal processor is to retrieve soil moisture from observed SMOS multi- angular brightness temperatures that come from one or several daily SL1C products.

The algorithm is based on the level 2 soil moisture retrieval which is done by iteratively minimizing a cost function in a bayesian context. The cost function is constructed from quadratic difference between the observed TB and the modelled ones, and the quadratic difference between the retrieved parameter and their a-priori value, all scaled by their uncertainty. The main difference with the L2 processing is to take **into account several revisits simultaneously** (dwell line aggregation) in a multi-orbit retrieval. For each daily product and each grid node, three **multi-angular** acquisitions at maximum are considered during the synthesis period. One for the product date (reference day or «JREF »), one before and one after selected from a search period of 7 days centred around the reference day ($JREF \pm 3$ days). These acquisitions are used to derive soil moisture and vegetation optical thickness and other geophysical parameters.

Several reasons have motivated the multi-orbit retrieval choice:

- Increase the number of acquisitions over a given node: taking into account several revisits (multi-orbit) increases the number of views available for a node, improving the soil moisture retrieval. As the number of views increases, more nodes are considered for the retrieval resulting in a larger coverage. This is mostly significant at the edge of the swath for which a single overpass does not provide enough brightness temperatures for a complete retrieval. Moreover, having more views increases the number of geophysical parameters that can be derived.
- Take advantage of the temporal correlation of vegetation optical thickness: the vegetation optical thickness is mainly related to vegetation water content which can be considered as highly correlated over a period of 3 days. So considering that the vegetation optical thickness is correlated over a given period of time the number of degrees of freedom in the multi-revisits cost function optimization is decreased. The system is thus more constrained and the robustness of the retrieval is improved. As it will be detailed later the soil moisture values are considered as uncorrelated
- Enhance the approximation behind the mean antenna weighting function: A mean theoretical antenna weighting function is used for the retrieval of geophysical parameters. This function has been computed taking into consideration all possible acquisition configurations (incidence angle, azimuth angles). But in many cases in the mono-orbit retrievals a small set of incidence angles is used, rendering the real and theoretical mean antenna weighting functions quite different. By using multi-orbit retrievals the acquisition configurations are increased and the real and theoretical mean antenna weighting functions are closer.

The L3, physical model to retrieve the soil moisture is the same as the L2 processor. Therefore, the ESA Level 2 SM processor is used and adapted in the L3 SM retrieval processor, to allow multi- orbit retrieval, i.e. processing several orbits in the same retrieval loop.

The L3 SM retrieval processor can also be run in mono-orbit mode, to process only one day, in this case the level 3 SM core processor is exactly the ESA level 2 SM algorithmic core but running on an EASE based gridding system.

The L3 SM Optimal processor produces daily global maps of soil moisture and other geophysical parameters (albedo, dielectric constant, surface temperature for example). There are 3 multi-orbit products: one for the reference day, and 2 others: one for the revisits before the reference day and one for the revisits after the reference day.

Ascending and descending orbits are processed separately. The reasons for this separation is that for ascending orbits (early morning, local time around 06:00 am), ionospheric effects is expected to be minimal. Surface conditions are also close to thermal equilibrium. The retrievals will then be more accurate, but dew and morning frost can sometimes affect the measurements. Furthermore, surface temperature changes affect the retrievals. During the descending orbits (local solar time around 06:00 pm) the temperature gradients are high. Also the radio frequency interference probability is different between ascending and descending orbits.

The inputs and outputs of L3 SM processor are schematized in Figure 7. The L3 SM multi-orbit processor uses 7 SL1C and 7 SMOS-ECMWF products as inputs (dynamic inputs). For the static inputs, only one file is used for each type. Prior values of free parameters come from auxiliary data such as ECMWF, or from previous retrievals using «current files ». The L3 SM optimal processor selects the more recent current files from those available (one for each

type). The nominal processing works only with current RFI maps; Tau, flood and HR current maps are deactivated. The user can choose to add other current maps.

Only one auxiliary Leaf Area Index file (AUX_DFFLAI) is used for the processing period in the multi-orbit retrieval. It is the one which contains the reference day and whose start time is the closer to the reference day.

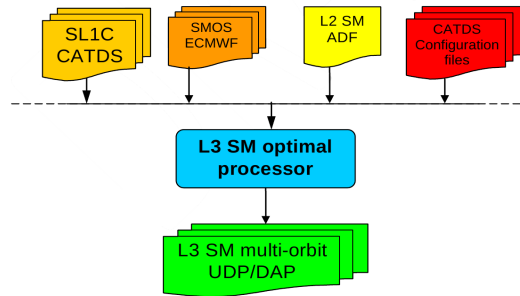


Figure 7: CATDS L3 SM optimal processor inputs and outputs

5.2 DETAILED DESCRIPTION OF THE ALGORITHMS

The L3 SM processor works on a daily SL1C product, considered as the reference day. For each node, it selects two other SL1C, picked from a time period of 7 days centred on the reference day: 1 revisit before (in the 3 days before the reference day) and 1 revisit after (in the 3 days after the reference day). The mono-orbit mode (L2 SM case) processes only the reference day.

L3 SM Optimal processor is divided in 7 processing steps, as presented in Figure 8 and listed below. Several are similar to L2 SM processing steps and 2 more steps are specific to the multi-orbit processing (number 1 and 2). They are listed as follow:

1. Revisit selection
2. Dwell lines reconstruction
3. Pre-processing
4. Decision tree
5. Retrieval of free parameters
6. Post-retrieval
7. Output generation

The next paragraphs are dedicated to each step. In order to understand every step, it is strongly recommended to read the L2 SM ATBD [6] before. Note that the algorithmic core that works DGG by DGG is kept from the L2 SM processor, and is not affected by the different gridding system.

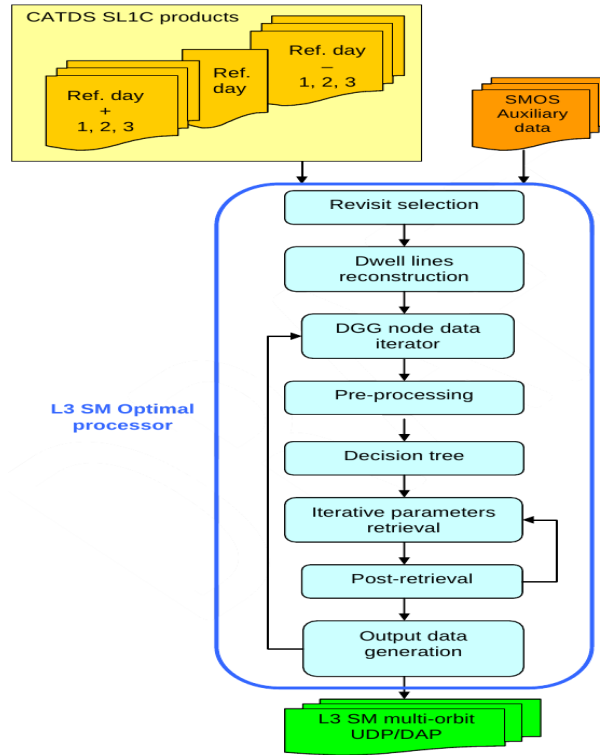


Figure 8: L3 SM Optimal processing steps

5.2.1 REVISIT SELECTION

For each DGG node of the reference day, we need to identify the revisit products that will be processed at the same time as the reference day (JREF). The number of available views differs from one day to another for a given DGG. Thus selecting revisits increases the angular sampling of brightness temperatures available for the retrieval. The processing works on a 7 days period centred on the reference day (JREF +/- 3 days, see Figure 9). This can be changed in the configuration file (multi-orbit mode only), that sets:

- The number of days taken into account in this time interval: TEMP_SYNTH, which is set to 7 days as default value
- The maximum number of dwell lines: N_ORB_VOIS, which is set to 3 as default value (reference product + 2 revisits products). The 2 revisit products are selected from both sides of the reference day: one before and one after the reference day.

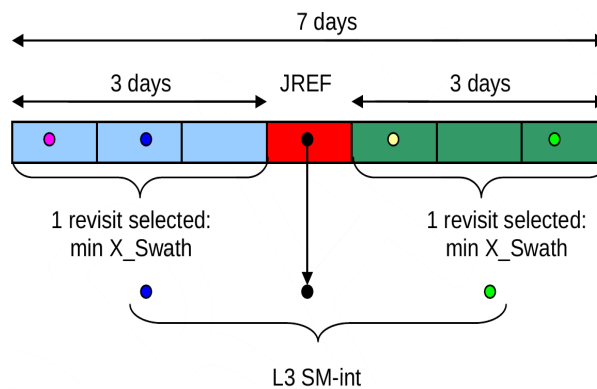


Figure 9: Example of a revisit selection around the reference day

Seven super L1c (SL1C) products are given as input of the revisit selection processing. Only DGG nodes seen on the reference day are processed. For each DGG node, the SL1C containing measurements for the node are identified. Among them, 2 revisit products at a maximum are selected for each DGG node: one (and only one) before and one (and only one) after the reference day. If several revisits are available on a 3 days period (before or after JREF), the

orbit for which the node is closer to the centre of the swath is selected. It maximizes the number of TB views and enhances the retrieval reliability.

If no revisits are available on the 3 days before and after the reference day, only the reference day is processed.

5.2.2 DWELL LINES RECONSTRUCTION

The SL1C products are organised snapshot by snapshot (c.f. §4.3). For the L3 SM retrieval, the TBs for different incidence angles need to be gathered by DGG node, as dwell lines.

First, dwell lines are reconstructed for the DGG nodes of the reference day, for all the products selected in the previous step. They are stored in the L3 SM int temporary file.

The dwell lines reconstruction follows these processing steps, node by node:

- Available TB at different incidence angles are selected in the temporal layers in SL1C product (a TB in a snapshot tally with one incidence angle)
- The selected TB are extracted and stored in the L3 SM int temporary file

For full polarization, the brightness temperature sequence in the snapshots is as follow:

Cross-pol TB (Real and imaginary part)	-	XY	-	XY
Pure TB	XX	XX	YY	YY
Snapshot Id	1	2	3	4

Table 6: Brightness Temperature sequence in full polarisation mode

SMOS is acquiring full polarization brightness temperatures as operational nominal mode. During commission phase the dual polarisation mode was tested on a 2 weekly basis from January 2010 to April 2010. The brightness temperature sequence for those acquisitions was XX, YY.

Only available TB fill up the dwell line, the polarization flag is used to determine the polarization of each TB. At the end of this step, all DGG nodes «seen »by the reference day have been processed; the L3 SM int temporary file is produced and is ready for the next steps.

5.2.3 PRE-PROCESSING

The pre-processing steps are kept as there are implemented in the L2 SM operational processor, see [6], section 3.2.2 for the complete explanations. It is performed on each dwell line, separately, for the reference day (the day at the middle of the seven day period) and for the revisits, if they are available.

The objective of the pre-processing is to **filter brightness temperatures** for identified RFI pollutions and aliasing effects, to **quantify radiometric uncertainties** and to prepare the retrieval by **determining observation conditions**.

The first pre-processing step consists in checking the SL1C TB for the seven days, with the following operations:

1. Spatial resolution filtering
2. RFI detection
3. Rejection of grid nodes where sun specular reflection occurs (from L1c flag)
4. Computation of CRFI (radiometric noise correction factor)
5. Computation of the initial validation index MVAL0

At the end of this process, some TBs or some grid nodes are discarded.

The second pre-processing step consists in the following operations from auxiliary data:

1. Definition of the working area on the DFFG grid. The working area is a 123 x 123 km box centred on the DGG node that is being processed. It ensures that all the contributions to the signal are considered in the retrieval. The DFFG grid is a higher resolution grid (4 km in current configuration) on which parameters will be defined and surface contributions will be computed
2. Generate DFFG LUTs: projection and resampling of auxiliary data on the DFFG grid (ECMWF data, soil properties, snow cover, sea ice). Note that seven SMOS-ECMWF products are given as input of the processing for the multi-orbit mode
3. Compute atmospheric and sky contribution
4. Compute weighting functions: angular dependent synthetic antenna weighting function (WEF) and mean synthetic antenna weighting function (MEAN_WEF) over the working area on the DFFG grid
5. Compute the geometric surface fractions and the radiometric surface fractions for the seven days

In order to optimize the pre-processing, only products in the temporary file L3 SM int are processed for L1C pre-processing, computation of atmospheric and galactic contributions, weighting functions, and fractions FM and FM0.

For the generation of the LUT over the DFFG fine grid, all the products over the 7 days period are used because the reference values from climate data (AUX_ECMWF) need to be interpolated over a 123 x 123 km area and thus needs information from neighbouring nodes.

The pre-processing differs from the L2 operational processor in the number of calls and in the processing conditions on DGG nodes.

5.2.4 DECISION TREE

Optimization of geophysical parameters is done over a given fraction of the surface. All other fractions are considered as default contributions to the signal following the same philosophy as in the Level 2 processor. The decision tree procedure determines the **models associated to the retrieved parameters and default models according to the type of observed surface. It also determines the free and fixed parameters according to observation conditions.**

The decision tree is the same than the one described in the ATBD of the L2 SM processor [6]. This one includes these main steps:

1. Update of the static fractions according to the ECMWF dynamic data (characterization of the possible presence of frozen soil, ice, snow, flood)
2. Selection of a tree branch according to the radiometric fractions
3. Selection of the retrieval model and the fraction(s) on which the parameters are retrieved
4. Selection of the subset of parameter to be retrieved
5. Selection of prior values for each parameter (or default values), with their associated standard deviations.

The decision tree is applied independently on each revisit of each reference day grid node.

5.2.4.1 Selection of the decision tree branch and the associated model

After step 2), a decision tree branch is selected for the reference day and for each revisit. For each grid node, only revisits that have the same decision tree branch of the reference day, named **BREF**, are identified and selected to be retrieved at the same time as the reference day. The BREF determines the model and the fraction(s) on which the parameters are retrieved in step 3. This approach allows us to select 3-days that have consistent conditions of observations.

5.2.4.2 Selection of the retrieval conditions

Step 4 defines the retrieval conditions applied to the TB: number and nature of the free parameters, their initial values and their uncertainties. The retrieval conditions are defined by testing the MVAL parameters, proportional to the number and the quality of available TBs on a grid node. The retrieval conditions are «none », «minimum », «full »or «maximum »according to the MVAL value compared to thresholds. This step is adapted to the multi-orbit case. A unique MVAL parameter is taken into account in the multi-orbit case, it is the maximum of the MVAL computed for each selected revisits (with BREF parameter). Thus, the same set of parameters is retrieved on each revisit.

The maximum of MVAL has been privileged because it allows to increase the number of free parameters for some DGG nodes, especially those at the edges of the swath, for which one overpass does not provide enough TB angular samples to retrieve soil moisture.

5.2.4.3 Computation of prior and reference values of parameters

In step 5, initial values of the free (retrieved) parameters and reference (default contributions) values are computed, from auxiliary data. The parameters are initialized using static and dynamic files. Only one AUX_DFFLAI is used throughout the seven days period and seven AUX_ECMWF files. The user can choose to initialise some parameters (Tau or HR) with the current files (but they are not activated by default in the actual operational mode). In this case, the same current file value is allocated to the initial values of all the revisits. For example, for 3 overpasses, tau1, tau2 and tau3 are initialised with the same current tau.

5.2.4.4 Prior values for free parameters

Prior values (i.e. initial values) are computed for the selected free parameters P_i , cf Table 23 of the L2 ATBD [6] Free parameters prior values are computed in the same way as in the L2 SM processor, their computation is reminded here.

This computation is done on the working area, defined on the DFFG grid, centred on each DGG node. The prior values of the free parameters are computed from the parameter values in the DFFG LUT, at DFFG cells within the retrieval fractions. The selected free parameters are shared by all the retrieval fractions. Therefore, the prior values for the free parameters are also shared by all the retrieval fractions, i.e. the prior values are independent of fractions and incidence angles. They are thus computed by averaging the prior values over the DFFG cells in the retrieval fractions using the mean weighting function. The prior value $P_{i,0}$ of a parameter on a DGG node is expressed as follow:

$$P_{i,0} = \frac{\sum_{(i,j)} [P(i,j) \cdot \text{MeanWef}(i,j) \cdot \sum_{(s)} F(i,j)]}{\sum_{(i,j)} [\text{MeanWef}(i,j) \cdot \sum_{(s)} F(i,j)]} \quad (2)$$

where

- i,j : the indexes of a cell in the working area on the DFFG grid
- $P(i,j)$: the prior value on a DFFG cell
- MeanWef : mean value of the WEF on a DFFG cell
- F : percentage of the free fraction F_s on a DFFG cell
- S : set of the free fractions on which the free parameters are retrieved

In the L3 SM processing, the prior vegetation optical thickness spatial variability is also computed for every reference grid node. It is a vegetation optical thickness standard deviation for every reference grid node, derived from ADF LAI_MAX and LAI, on the working area and weighted by the MEAN_WEF function. It is computed as follow:

$$\text{StdTau} = \frac{\sqrt{\sum_{(i,j)} ((\text{TauC}(i,j) - \text{TauM})^2 \cdot \text{MeanWef}(i,j))}}{\sum_{(i,j)} \text{MeanWef}(i,j)} \quad (3)$$

Where:

- $\text{TauC}(i,j)$ the Tau for a DFFG cell (i,j) in the working area
- TauM the mean Tau computed on a grid point, weighted by the mean wef

It is computed separately for nominal and forest fractions. It is why that always equal $\sum_{(i,j)} \text{MeanWef}(i,j)$ is not always equal to 1.

5.2.4.5 Reference values for fixed parameters

Reference values for fixed parameters are computed in the same way as the prior values of the free parameters. The only difference is that their values are computed using the actual position dependent antenna weighting function, while the prior values for free parameters are computed using the mean antenna weighting function. The idea is that depending on acquisition configuration (view angle and azimuth angle) the surface fractions might vary in a non-negligible way, due to presence of water for instance.

For each parameter whose values are available on the DFFG scale, its reference values are computed by averaging the DFFG values using the incidence-angle-dependent weighting function. Thus, each fixed parameter has an array of reference values corresponding to all incidence angles. The reference value $P_{i,r}$ of a parameter on a DGG node is expressed as follow:

$$P_{i,r} = \frac{\sum_{(i,j)} [P(i,j) \cdot \text{MeanWef}(i,j) \cdot \sum_{(s)} F(i,j)]}{\sum_{(i,j)} [\text{MeanWef}(i,j) \cdot \sum_{(s)} F(i,j)]} \quad (4)$$

where

- i,j : the indexes of a cell in the working area on the DFFG grid
- $P(i,j)$: the prior value on a DFFG cell
- MeanWef : mean value of the WEF on a DFFG cell
- F : percentage of the free fraction F_s on a DFFG cell
- S : set of the free fractions on which the free parameters are retrieved

5.2.5 RETRIEVAL OF THE FREE PARAMETERS

This step retrieves the identified free parameters, from SMOS brightness temperatures acquired on a DGG node. In the multi-orbit retrieval scheme, the objectives are to enhance the retrieval reliability and to extend the soil moisture retrieval areas, by taking into account a period of 7 days for the retrieval and by correlating the vegetation optical thickness over the 7 days period. This approach reduces the number of degrees of freedom in the cost function minimization, the system is more constrained and the robustness of the retrieval is improved. For each free parameter, there are as many estimated values as there are SL1C products to retrieve on each DGG node.

The main modifications of L2 SM processor concern the data format and the computation of the vegetation optical thickness covariance matrix.

5.2.5.1 Organizing the multi-orbit information

The following expressions are adapted from the L2 SM ATBD to the Level 3 multi-orbit approach. There are two main differences compared to the Level 2:

- retrievals are performed using brightness temperatures profiles coming from up to three orbits, T, U and V observing the same SMOS grid-points and produce a set of triplet of retrieved parameters $p_i^{TUV} = [p_i^T, p_i^U, p_i^V]^t$
- when Tau is a retrieved parameter, a constraint on the retrieved triplet $[Tau^T, Tau^U, Tau^V]$ values is applied
 - In the current version of the algorithms (i.e. version 310 and previous ones of the processor) the constraint on these retrieved Tau values is based on a correlation binding principle
 - **For future release (i.e. > version 310), the constraint on these retrieved values is based on a minimum variance principle**

Before describing this new approach, we will first review the approach used in versions ≤ 310 . Notation:

- the upper script «t» denotes the transpose operator to not mix up with upper script capital «T» which denotes the orbit T.
- I_N is the square $N \times N$ identity matrix
- Z_N is the square $N \times N$ zero matrix
- Sometimes $[]$ are used over quantities, just to remind their matrix or vector nature.

TB_{Mn} of the NV overpasses are gathered in TBM, to be used in the same cost function. As an example, for a DGG node with 3 overpasses ($NV = 3$): the product of reference and 2 revisits to be used, the measured brightness temperatures vector TBM is expressed as follow:

$$TB = (|TB_{M1}|_{t1}|TB_{M2}|_{t2}|TB_{M3}|_{t3}) \quad (5)$$

Where:

- t1: product of reference (overpass n = 1)
- t2: revisit product before reference day (overpass n = 2)
- t3: revisit product after reference day (overpass n = 3)

$$\begin{aligned} TB_{M1} &= |TB_M(geom_{1,1}, t1) \dots TB_M(geom_{1,NT_1}, t1)|_{t1} \\ TB_{M2} &= |TB_M(geom_{2,1}, t2) \dots TB_M(geom_{2,NT_2}, t2)|_{t2} \\ TB_{M3} &= |TB_M(geom_{3,1}, t3) \dots TB_M(geom_{3,NT_3}, t3)|_{t3} \end{aligned} \quad (6)$$

The size of TB_M depends on the number of selected revisit products and on the number of views for each overpass. It is thus variable for one DGG node to another.

5.2.5.2 Simulated Brightness Temperatures

The same direct models as for the level 2 are used during the level 3 retrieval phase. They simulate SMOS measurements in the antenna reference frame (see [6]).

TB_{Fn} correspond to the brightness temperatures computed from the parameters and the forward models, for a DGG node and at a time t_n . It depends on the set of geophysical parameters $P_1, P_2 \dots P_{NP}$ and the geometry $geom_{n,k}$. We consider the set of NP free parameters to be retrieved to be the same for each T, U and V orbits leading to the NP^{TUV} total number of parameters to be retrieved equals to $3*NP$ -the so called free parameters- P^{TUV} .

$$TB_{Fn} = TB_{Fn}(geom_{n,k}, P_1(t_n), P_2(t_n), \dots, P_{NP}(t_n)) \quad (7)$$

To simplify the notation, the equation above is written as follow: $TB_{Fn} = TB_{Fn}(geom_{n,k}, P_i(t_n))$

The contribution of each fraction in the working area is simulated from fixed and free parameters that are being optimised. The global modelling of SMOS brightness temperatures on each DGG node includes:

- A variable part computed by the models where free parameters are optimized on the main fractions
- A fixed part simulated with the default models on the other fractions

The simulated brightness temperatures for a node are modelled for each incidence angle and each polarization (X and Y polarizations).

In the same way as above, let TBF corresponds to the modelled brightness temperatures from the different overpasses selected for the retrieval. It is also gathered, in the same order than TBM:

$$TB_F = (|TB_{F1}|_{t1}|TB_{F2}|_{t2}|TB_{F3}|_{t3}) \quad (8)$$

where

- t1: reference product (overpass n = 1)
- t2: revisit product before reference day (overpass n = 2)
- t3: revisit product after reference day (overpass n = 3)

5.2.5.3 Computation of the cost function

The retrieval loop consists in optimizing geophysical parameters to minimize a cost function, which is proportional to:

- The quadratic difference between the measured brightness temperatures and the modelled ones for every incidence angles selected in the previous steps. This quadratic difference is weighted by the inverse of TB covariance matrix (i.e. uncertainties if there is no covariance between TBs),
- The quadratic difference between the free parameters and their initial values, weighted by the inverse of parameter covariance matrix (i.e. uncertainties if there is no covariance between parameters)

Then, the retrieved parameter P^{TUV} is the overall triplets of values expressed under the form or a column vector of NP^{TUV} lines:

$P^{TUV} = [P_i^{TUV}]$ is the overall free parameters column vector of NP^{TUV} lines, which minimize the cost function COST:

$$COST = \Delta_{TB}^{TUVt} \cdot [COV_{TB}^{TUV}]^{-1} \cdot \Delta_{TB}^{TUV} + \Delta_P^{TUVt} \cdot [COV_P^{TUV}]^{-1} \cdot \Delta_P^{TUV} \quad (9)$$

with :

$$\begin{aligned} \Delta_{TB}^{TUV} &= TBF^{TUV}(\theta_m^{TUV}, p_i^{TUV}, \dots) - TBM^{TUV}(\theta_m^{TUV}) \\ \Delta_P^{TUV} &= P^{TUV} - P_0^{TUV} \end{aligned} \quad (10)$$

$TBM^{TUV}(\theta_m^{TUV})$ is the overall concatenated column vector of NT^{TUV} measured values taken from the three orbits T, U and V.

$$TBM^{TUV}(\theta_m^{TUV}) = \begin{bmatrix} TBM^T(\theta_m^T) \\ TBM^U(\theta_m^U) \\ TBM^V(\theta_m^V) \end{bmatrix} \quad (11)$$

The specific vector of measurements $[TBM^T(\theta_m^T)]$, taken from the orbit T has NT^T values, the one taken from the orbit U, $[TBM^U(\theta_m^U)]$, has NT^U values and the one from the orbit V, $[TBM^V(\theta_m^V)]$, has NT^V values. NT^{TUV} is equal to $NT^T + NT^U + NT^V$.

It is associated to the overall forward model vector $[TBF^{TUV}(\theta_m^{TUV}, p_i^{TUV}, \dots)]$ of NT^{TUV} modelled values built following the same organization:

$$TBF^{TUV}(\theta_m^{TUV}, p_i^{TUV}, \dots) = \begin{bmatrix} TBM^T(\theta_m^T, p_i^T, \dots) \\ TBM^U(\theta_m^U, p_i^U, \dots) \\ TBM^V(\theta_m^V, p_i^V, \dots) \end{bmatrix} \quad (12)$$

$[COV_{TB}^{TUV}]$ is the error covariance matrix for the overall observed TBM^{TUV} . The P_0^{TUV} are the prior estimates of the NP^{TUV} free physical parameters, with prior error covariance matrix $[COV_P^{TUV}]$. COST can thus be written under the general and very classical quadratic form:

$$COST = \Delta_Z^t \cdot [COV_Z]^{-1} \cdot \Delta_Z$$

where the $NT^{TUV} + NP^{TUV}$ ranked $[COV_Z]$ matrix is the block diagonal matrix built from the matrices $[COV_{TB}^{TUV}]$ and $[COV_P^{TUV}]$ and the $(NT^{TUV} + NP^{TUV})$ length column vector Δ_Z consists of the concatenation of Δ_{TB}^{TUV} and Δ_P^{TUV} .

Jacobian matrix

The partial derivatives of the cost function with respect to the vector of the free parameters, P, are required for the minimization process and to compute the standard deviation of post retrieval parameters uncertainties RSTD. Considering that $[COV_Z]$ is a symmetric matrix independent of P then the vector of partial derivatives of the cost function is:

$$\frac{\partial COST}{\partial P} = 2\Delta_Z^t \cdot [COV_Z]^{-1} \cdot \frac{\partial \Delta_Z}{\partial P} \quad (13)$$

Let's call $[DRV_Z]$ the Jacobian matrix of Δ_Z with respect to P which is $\frac{\partial \Delta_Z}{\partial P}$, it is a matrix of $NT^{TUV} + NP^{TUV}$ lines x NP^{TUV} columns.

The first NT^{TUV} lines of $[DRV_Z]$ is the Jacobian of the forward model $TBF^{TUV}(\theta_m^{TUV}, p_i^{TUV}, \dots)$. It is estimated using finite differences. The last NP^{TUV} is the Jacobian of the prior constraints is very simple in this case, it is $I_{NP^{TUV}}$ the $NP^{TUV} \times NP^{TUV}$ identity matrix.

The theoretical covariance matrix of the retrieved parameters uncertainty, $[COV_{post}]$, under the linear tangent model approximation provided by the Jacobin matrix $[DRV_Z]$ is hence:

$$[COV_{post}] = [[DRV_Z]^t \cdot [COV_Z]^{-1} \cdot [DRV_Z]]^{(-1)} \quad (14)$$

$[COV_{post}]$ is a $NP^{TUV} \times NP^{TUV}$ holding its diagonal the theoretical retrieval variances vector. It is used to compute the vector of estimated standard deviation of the retrieved parameters values, RSTD:

$$RSTD = \sqrt{diag([COV_{post}])} \quad (15)$$

BUILDING COV_{TB} MATRICES AND Δ_{TB} vectors

The uncertainty on the observation system is defined from one part containing the antenna radiometric uncertainties, for a L1C pixel, which are provided as standard deviation for each view of this node [and a second part that accounting for other sources of errors coming from the image reconstruction]. The first part is formed by the vector, [DTBa] having M_{AVA} components and is provided by L1 files and since algorithms uses variances, the terms must be squared. [The second part is provided as the extra variance σ_{IR}^2 which is configurable and provided in the TGRD UPF]

For any orbit $orb \in T, U, V$, the total contribution is given by a diagonal matrix written as follows:

$$COV_{TB}^{orb} = \begin{bmatrix} (DTB_{a1}^{orb})^2 & 0 & 0 \\ 0 & \cdots & 0 \\ 0 & 0 & (DTB_{aNT^{orb}}^{orb})^2 \end{bmatrix} + \sigma_{IR}^2 \cdot I_{NT^{orb}} \quad (16)$$

Where the subscript a refers to the antenna [and $I_{NT^{orb}}$ is the identity $NT^{orb} \times NT^{orb}$ matrix. It is associated with the Δ_{TB}^{orb} contribution to the overall Δ vector:

$$\Delta_{TB}^{orb} = \begin{bmatrix} TBF^{orb}(\theta_1^{orb}, p_i^{orb}, \dots - TBM^{orb}(\theta_1^{orb}) \\ TBF^{orb}(\theta_{NT}^{orb}, p_i^{orb}, \dots - TBM^{orb}(\theta_{NT^{orb}}^{orb}) \end{bmatrix} \quad (17)$$

The overall contribution from the three orbits T, U and V is obtained by the block diagonal matrix concatenation:

$$COV_{TB}^{orb} = \begin{bmatrix} [COV_{TB}^T] & 0 & 0 \\ 0 & [COV_{TB}^U] & 0 \\ 0 & 0 & [COV_{TB}^V] \end{bmatrix} \quad (18)$$

in association to the column vector concatenation

$$\Delta_{TB}^{TUV} = \begin{bmatrix} [\Delta_{TB}^T] \\ [\Delta_{TB}^U] \\ [\Delta_{TB}^V] \end{bmatrix} \quad (19)$$

COV_{TB}^{TUV} is a $NT^{TUV} \times NT^{TUV}$ square matrix and Δ_{TB}^{TUV} is a column vector of NT^{TUV} elements. We remind that $NT^{TUV} = NT^T + NT^U + NT^V$.

NATURAL BAYESIAN CONSTRAINT TO PRIOR VALUES

The Bayesian *a priori* constraints COV_P^{TUV} on retrieved parameters is the second block diagonal part of COV_Z . It is built from the variances, $\sigma_{0_i}^2$, of the prior values, p_{0_i} of all the retrieved parameters p_i .

For a given parameter p_i , $\sigma_{0_i}^2$ are assumed to be the same for all the T,U and V components:

$$COV_{p_i}^{TUV} = \begin{bmatrix} \sigma_{0_i}^2 & 0 & 0 \\ 0 & \sigma_{0_i}^2 & 0 \\ 0 & 0 & \sigma_{0_i}^2 \end{bmatrix} \quad (20)$$

It is the contribution for the retrieved parameter p_i to the COV_P^{TUV} matrix. It is associated with :

$$\Delta_{p_i}^{TUV} = \begin{bmatrix} p_i^T - p_{0_i}^T \\ p_i^U - p_{0_i}^U \\ p_i^V - p_{0_i}^V \end{bmatrix} \quad (21)$$

which is the contribution for the retrieved parameter p_i to the Δ_P^{TUV} vector. Then for the whole list of retrieved parameters COV_P^{TUV} is the block diagonal matrix built from the $COV_{p_i}^{TUV}$ matrices and associated to the Δ_P^{TUV} column vector built from the concatenation of $\Delta_{p_i}^{TUV}$ vectors.

$$COV_P^{TUV} = \begin{bmatrix} [COV_{p_1}^{TUV}] & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & [COV_{p_{NP}}^{TUV}] \end{bmatrix} \quad (22)$$

to be associated with

$$\Delta_P^{TUV} = \begin{bmatrix} [\Delta_{p_1}^{TUV}] \\ \vdots \\ [\Delta_{p_{NP}}^{TUV}] \end{bmatrix} \quad (23)$$

COV_P^{TUV} is a $NP^{TUV} \times NP^{TUV}$ square matrix and Δ_P^{TUV} is column vector of NP^{TUV} . We remind that $NP^{TUV} = 3 \times NP$.

Adding constraints on the retrieved Tau values

The cost function will behave exactly as the Level 2 but using three orbits instead of one which is the first difference between the Level 3 and the Level 2. The second difference adds specific constraints on the retrieved triplet Tau^T , Tau^U and Tau^V . The next section presents the constrain used in version 310 and previous ones. Then, we present a new version of the constraint to be applied for the future release of the processor (higher than version 310). Adding constraints on the retrieved Tau values is applicable only if at least two Tau values are retrieved (see section 1.6 on degraded cases).

5.2.5.4 Constraint on Tau, version 310 and previous ones

Its size is fixed by the number of selected revisit products NV; it is thus variable for one DGG node to another (between 1 and 3). The CovPi matrix dimension is NV x NV. It is written:

$$COV_{P_i} = \begin{pmatrix} \sigma_{i0}^2(t_1) & \sigma_{i0}(t_1) \cdot \sigma_{i0}(t_2) \cdot \rho(t_1, t_2) & \cdots & \sigma_{i0}(t_1) \cdot \sigma_{i0}(t_{NV}) \cdot \rho(t_1, t_{NV}) \\ \sigma_{i0}(t_2) \cdot \sigma_{i0}(t_1) \cdot \rho(t_2, t_1) & \sigma_{i0}^2(t_2) & \vdots & \vdots \\ \vdots & \vdots & \sigma_{i0}^2(t_n) & \vdots \\ \sigma_{i0}(t_{NV}) \cdot \sigma_{i0}(t_1) \cdot \rho(t_{NV}, t_1) & \cdots & \cdots & \sigma_{i0}^2(t_{NV}) \end{pmatrix} \quad (24)$$

where

- Its diagonal terms are prior standard deviation (ASTD):
 $\sigma_{i0}(t_n)$ is the ASTD of the parameter P_i at the time t_n
They are supposed constant on the period of 7 days, for all the products and for one parameter: $\sigma_{i0}(t_1) = \sigma_{i0}(t_2) = \sigma_{i0}(t_n)$
- The non-diagonal terms are the covariance of the parameter P_i between the products at 2 different times.
 $\rho_i(t_1, t_2)$ is the auto-correlation of the parameter P_i between the times t_1 and t_2 , it is the correlation function Correl.
As mentioned above all cross-correlation terms are neglected.

Taking into account the hypothesis below, the expression of Cov_{P_i} can be simplified:

$$COV_{P_i} = \sigma_{i0}^2(t_A) \cdot \begin{pmatrix} 1 & \rho_i(t_1, t_2) & \cdots & \rho_i(t_1, t_{NV}) \\ \rho_i(t_2, t_1) & 1 & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ \rho_i(t_{NV}, t_1) & \cdots & \cdots & 1 \end{pmatrix} \quad (25)$$

Temporal correlation function for vegetation optical thickness.

Two types of vegetation surfaces are considered in the processor: optically thin vegetation (crops, fields, savannah, etc.) which can undergo strong seasonal variations and optically thick vegetation (forest) whose signal is more linked to branch water content and more stable in time. Note that specific phenomena can skew the estimator of the vegetation opacity:

- Freezing event: in the case of persistent freezing, water of the vegetation can freeze and the vegetation can thus become almost transparent in L band.
- Important rain falls: in the case of a rain interception, the vegetation can become very opaque in L-band.
- Snow cover on the vegetation: a snow cover not taken into account during the retrieval will produce a bias on the estimator of the vegetation opacity. This bias depends on the parameters of snow (thickness, snow density, snow moisture, etc ...).

In the L3 SM multi-orbit processing, **the vegetation optical thickness is correlated in time on a 7-days period. It is assumed that the vegetation varies slowly during this short period.**

A step in the processing is thus added to define and parameterize a temporal correlation function for the vegetation optical thickness that takes into account the impact of climatic events to avoid the specific events listed above. This step is activated only if vegetation optical thickness Tau is a free parameter, for the products selected in the previous steps.

The vegetation optical thickness correlation is modelled with a Gaussian auto-correlation function:

$$Correl_{Tau}(t_1, t_2) = Corr_{max}(t_1, t_2) \cdot \exp\left(-\frac{(t_1 - t_2)^2}{T_c^2}\right) \quad (26)$$

Where

- t_1 et t_2 are the time (expressed in days) of the $Tau(t_1)$ and $Tau(t_2)$ retrievals
- $Corr_{max}(t_1, t_2)$ is the maximum amplitude of the correlation function between t_1 et t_2
- T_c is the characteristic correlation time for the vegetation optical thickness Tau
 T_c depends on the selected tree branch (BREF):

- For forest surface (BREF=11): $T_c = TCMAX2$, with $TCMAX2 = 30$ days
- For low vegetation (BREF=12): $T_c = TCMAX1$, with $TCMAX1=10$ days

Figure 10 illustrates the values of the correlation function Correl for different values of T_c .

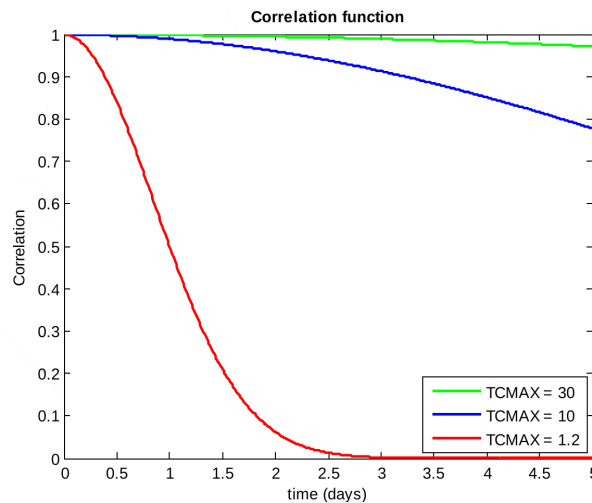


Figure 10: Evolution of the correlation function Correl for different values of TC

This correlation function is convenient. For example, in order to have a constant optical thickness a high value of T_c should be considered in combination of $Corr_{max}(t_1, t_2) = 1$. For uncorrelated optical thickness $Corr_{max}(t_1, t_2) = 0$

should be chosen. These 2 parameters can be set in the configuration file.

The fractions on which the parameters are retrieved can vary from one revisit to the other due to climatic events, without changing the decision tree branch chosen for the retrieval. The vegetation optical thickness temporal correlation is modified in order to take into account such variations, particularly if the vegetation optical thickness is spatially variable.

$Corr_{max}(t_1, t_2)$ is thus dependent of the prior vegetation optical thickness spatial variability over the working area, and also dependent on the retrieval surface fraction change. It is computed as follow:

The working area is considered as homogenous if the mean standard deviation of prior vegetation optical thickness is strictly lower than a threshold. The vegetation optical thickness taken into account depends on the decision tree branch:

- If the retrieval is performed over the forest fraction FFO (tree branch = 11), it is the vegetation optical thickness of the forest, derived from LAI_MAX
- If the retrieval is performed on a non-forest fraction, it is the vegetation optical thickness of low vegetation, derived from LAI

TH_STD_TAU1 and TH_STD_TAU2 are customizable and are equal to 0.05 by default in the L3 SM operational processor. If the mean standard deviation is higher than the threshold then the surface is considered as heterogeneous

1. for homogenous surfaces:

$Corr_{max}(t_1, t_2) = C0$, where C0 is a processing parameter and is equal to 0.999 by default.

2. for heterogeneous surfaces, the correlation amplitude is linearly scaled with the main surface fraction variation:

$$Corr_{max}(t_1, t_2) = \max \left(C0, \left(1 - \frac{(FM0_{Pri}(t_1) - FM0_{Pri}(t_2))}{\max(FM0_{Pri}(t_1), FM0_{Pri}(t_2))} \cdot \frac{1}{TH_{DFM0_{Pri}}} \right), 0 \right) \quad (27)$$

Where:

- $FM0_{Pri}(t)$ is the main fraction that has activated the decision tree branch BREF for the date t
- $TH_{DFM0_{Pri}}$ is a processing parameter that fixes for each FM0 the maximum of the relative variation of $FM0_{Pri}$, $DFM0_{Pri}/FM0_{Pri}$. Beyond this threshold, the temporal correlation is supposed to be null

The value of $Corr_{max}$ as a function of the relative variation of $FM0_{Pri}$ is illustrated on Figure 11.

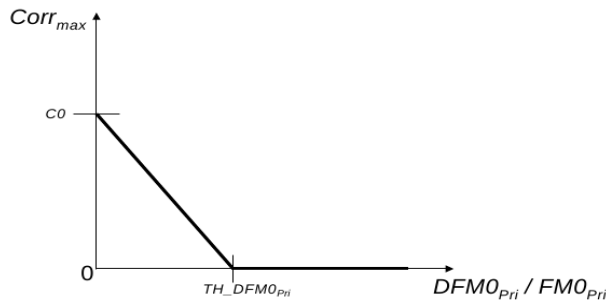


Figure 11: Value of $Corr_{max}$ deduced from the relative variation of $FM0_{Pri}$

For the heterogeneous decision tree branch (17), there is no main fraction, $Corr_{max}$ is null:
 $Corr_{max}(t_1, t_2) = 0$ if BREF=17

The parameters of the correlation function can be modified in the processor configuration file.

5.2.5.5 Case versions L3SMOPT>310

We present in the section the modified constraint applied on Tau, based on minimum variance.

Whenever Tau is a retrieved parameter, in this approach we want the triplet TauTUV to have a minimum variance within a tolerance. This constraint can naturally be introduced at the [eq] level by adding the variance as a penalty term weighted by an efficiency coefficient $1/(var_{ref}^{Tau})$ expressing the tolerance required for the minimum variance Tau^{TUV} goal.

Two values for var_{ref}^{Tau} are used depending on the decision tree branch of the reference orbit. One specific value is used for forest surfaces (S_Tree_1 = 11) and one specific value for all other surfaces than forest, including the nominal case (S_Tree_1 = 12) but also any other retrieval case provided that Tau is a retrieved parameter.

$$COST = \Delta_Z^t \cdot [COV_Z]^{-1} \cdot \Delta_Z + \frac{var(Tau^{TUV})}{var_{ref}^{Tau}} \quad (28)$$

With the traditional sample variance:

$$var(Tau^{TUV}) = \frac{1}{N_0 - 1} \cdot \underbrace{\sum_{orb \in \{TUV\}} (Tau^{orb} - \overline{Tau^{TUV}})^2}_{orb \in \{TUV\}} \quad (29)$$

And the sample mean:

$$\overline{Tau^{TUV}} = \frac{1}{N_0} \cdot \underbrace{\sum_{orb \in \{TUV\}} Tau^{orb}}_{orb \in \{TUV\}} \quad (30)$$

N₀ is the number of orbits available, nominally it is equal to 3 when the three orbits, T, U and V are in use. It is more appropriate to rewrite the above expression into matrix vector product. By doing so, we just need to extend COV_p^{TUV} and Δ_p^{TUV} unchanging the general formulation. We assume a nominal orbit case i.e. N₀ = 3, though in the following expressions we left N₀ for genericity.

$$\frac{var(Tau^{TUV})}{var_{ref}^{Tau}} = \Delta_{CT}^t \cdot [M_{CT}]^{-1} \cdot \Delta_{CT} \quad (31)$$

with M_{CT} = (N₀ - 1) · var_{ref}^{Tau} · I_{N₀} and

$$\Delta_{CT} = \begin{bmatrix} Tau^T - \overline{Tau^{TUV}} \\ Tau^U - \overline{Tau^{TUV}} \\ Tau^V - \overline{Tau^{TUV}} \end{bmatrix} \quad (32)$$

By building the matrix COV_{Z'} by block diagonal extension of the matrix COV_Z with the matrix M_{CT} and building the column vector Δ_{Z'} by concatenating Δ_{CT} to the end of Δ_Z:

$$COV_{Z'} = \begin{bmatrix} [COV_Z] & 0 \\ 0 & [M_{CT}] \end{bmatrix} \quad (33)$$

and

$$\Delta_{Z'} = \begin{bmatrix} [\Delta_Z] \\ [\Delta_{CT}] \end{bmatrix} \quad (34)$$

Then the form of the equation can be kept, just substituting COV_Z by COV_{Z'} and Δ_Z by Δ_{Z'}.

The DRV_Z Jacobian matrix is to be extended accordingly by three line with the block Jacobian 3x3 matrix, DRV_{CT}, of Δ_{CT} set for the columns where Tau^{TUV} are located. All the other columns of these three added lines are set to 0.

$$DRV_{CT} = \frac{\partial \Delta_{CT}}{\partial Tau^{TUV}} = \begin{bmatrix} +\frac{N_0-1}{N_0} & -\frac{1}{N_0} & -\frac{1}{N_0} \\ -\frac{1}{N_0} & +\frac{N_0-1}{N_0} & -\frac{1}{N_0} \\ -\frac{1}{N_0} & -\frac{1}{N_0} & +\frac{N_0-1}{N_0} \end{bmatrix} \quad (35)$$

5.2.5.6 Degraded cases

Although the most frequent L3 retrievals are achieved nominally using three orbits, it will happen that only two or one orbits can be used for some grid-point retrieval. The most frequent degraded case would probably be two with one of the three orbits discarded due to not enough observations in brightness temperatures profiles. It is typically the case when the observed grid point is located within a band of ~ 100 km at the outer edges of an orbit swath. The presence of RFI and the associated TB screening can lead to a similar situation but occurring at any location within the swath and potentially more eliminated orbits. Finally, frequent degraded cases will happen during season transition when the surface changes (snow, frost, ...) during the period of time covered by the three orbits. Potentially different decision tree branches for each orbit may be selected. When it happens, the decision tree branch of the reference day serves as the reference for the two others orbits decision tree branches. Those that do not match the reference are eliminated. In such situations the nominal $\{T, U, V\}$ set shrinks to any subset of two or one elements. The case with no orbit remaining at all is also possible but in that case the retrievals are not attempted. As a consequence all the expressions presented in the previous subsections shall adapt to the various possible situations. Mainly it consists in not including rows and columns associated with the eliminated orbit(s). When Tau it is a retrieved parameters, the number of orbits; N_0 , used for the regularization by minimum variance shall be set appropriately to compute the M_{CT} and DRV_{CT} terms. When only one orbit remains and whatever the regularization used for Tau, it has no more meaning as only a single Tau is retrieved is this case. The section 5.2.5.5 is thus applicable if and only if the number of orbit is > 1 .

5.2.6 RETRIEVAL OF THE FREE PARAMETERS

This step retrieves the identified free parameters, from SMOS brightness temperatures acquired on a DGG node. In the multi-orbit retrieval scheme, the objectives are to enhance the retrieval reliability and to extend the soil moisture retrieval areas, by taking into account a period of 7 days for the retrieval and by correlating the vegetation optical thickness over the 7 days period. This approach reduces the number of degrees of freedom in the cost function minimization, the system is more constrained and the robustness of the retrieval is improved. For each free parameter, there are as many estimated values as there are SL1C products to retrieve on each DGG node. The main modifications of L2 SM processor concern the data format and the computation of the vegetation optical thickness covariance matrix.

5.2.7 THE MINIMIZATION SCHEME

The minimization algorithm of the cost function is the same as the one used in L2 operational processor: **the Levenberg-Marquardt iterative scheme**. The Levenberg-Marquardt (LM) algorithm is an iterative technique that locates the minimum of a function that is expressed as the sum of squares of nonlinear functions. It has become a standard technique for nonlinear least-squares problems and can be thought of as a combination of steepest descent and the Gauss-Newton method. When the current solution is far from the correct one, the algorithm behaves like a steepest descent method: slow, but guaranteed to converge. When the current solution is close to the correct solution, it becomes a Gauss-Newton method. For each iteration loop, some convergence criterions are evaluated to decide if the retrieval is successful or not. If the convergence criterions are not adequate, the loop continues with a new iteration, with updated estimations for free parameters. If the maximum number of iterations is reached without a successful retrieval, or if the loop did not converge for other reasons, the appropriated flags are raised. If the convergence criterions are adequate, the retrieval loop ends and the current values are considered optimal values of the free parameters.

5.2.8 THE POST-RETRIEVAL

The objective of the post-retrieval is to analyse the results after convergence in order to validate the retrieval or to try a new one by simplifying the initial conditions (i.e. with less free parameters). It also does a retrieval using the cardioid model if it has not been done yet. The same tests as those presented in the post-processing section of the ATBD L2 SM [6] are applied. The post-retrieval is integrated in the previous retrieval loop; it is applied on every reference DGG with a retrieval. The distinction is kept between the parameters of each day taken into account in the retrieval. The main processing steps are:

1. Control of the retrieved parameters reliability using the parameter errors computed from pseudo-Hessian matrix at the end of the iterative scheme: they are called "theoretical uncertainties" or RSTD,

2. Outliers detection by comparing measured and modelled brightness temperatures
3. Retrieval analysis to decide if a new retrieval is necessary,
4. Computation of Chi2 and Chi2 probability (CHI2_P) retrieval performances parameters (quality indexes)
5. Update of the flags and counters
6. Computation of TB_TOA_DQX and TB_ASX_DQX
7. Computation of the polarization ratio
8. Start additional cardioid retrieval

Some steps are adapted for the multi-orbit retrieval. For step 3), the parameter of the validation are derived from RSTD computed with the parameters of the reference day. This avoids filtering the retrievals of the reference day because of a lower reliability of the parameters retrieved on the days of revisits.

If the multi-orbit retrieval is not validated in R2, the retrieval is tried again only on the reference day (i.e. a mono-orbit case) in R2. For step 4), the Chi2 and Chi2P parameters are computed on the TB vector used by the cost function that comes from the aggregation of several TB vector from several overpasses. Chi2 and Chi2P are computed one time per DGG node and are thus common to every retrieved day. These parameters are duplicated when the products are written.

5.2.9 OUTPUT DATA GENERATION

The information is formatted in order to be stored in the output products of the L3 SM optimal processor. There are 2 types of output products: User Data Product (UDP) and Data Analysis Product (DAP). Each type of product is split in 3 categories, depending on the days processed in the retrieval, as illustrated on Figure 12:

- 1 UDP and 1 DAP for the "3 days before" the reference day
- 1 UDP and 1 DAP for the reference day
- 1 UDP and 1 DAP for the "3 days after" the reference day

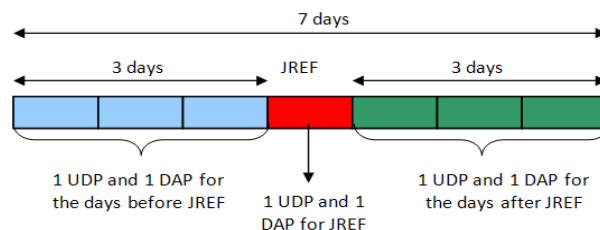


Figure 12: Products outputs for the processing of one reference day

During the retrieval loop, the variables are vectored and the information on the day they belong to is kept. The retrieved parameters on the NV products and their uncertainties are stored, and the global quality index GQX is computed independently for the NV retrievals. These variables are redistributed in the 3 categories of output products after the processing, depending on their date (before reference day, reference day, after reference day).

About the GQX:

The GQX is a Global Quality Index that takes into account all the sources of error, unlike the DQX that characterizes uncertainties related to radiometric uncertainty and those on the constrained parameters. The GQX is a number from 1 to 20 indicating to the user the overall quality of a given SMOS data, the lower the number the better the quality. The index is a weighted coefficient from 20 terms (see ATBD L2 SM [6]), which qualitatively should be considered in an overall quality index. It is normalized so that its value can be understood as a % of soil moisture. For example if it is 4, this is the specification of SMOS. If it is 10 or more, we can consider that the information provided by SMOS is very low (= not accurate ?, low quality ?).

The meaning of this index is to give an overall quality index of a SMOS data, but its numerical value will be only reliable for the current version of the products the GQX is not fully validated so the user is recommended to neglect its value and base his analysis and filtering on the DQX.

6 SM POST-PROCESSING

6.1 OBJECTIVE

For each DGG node, a parameter value is updated regularly from the retrievals of a day in a global map called current maps. The current maps are internal products of the CATDS. When activated, the current maps are used as initial value of some parameters in the next L3 SM optimal processing.

The SM post-processor reads UDP products, checks quality and eventually resets or updates the maps according to a procedure described in the next paragraph. The inputs and outputs of the SM processor are schematized in Figure 13. The following parameters current maps are available:

- Radio frequencies interferences RFI: implemented / activated
- Low vegetation optical thickness Tau_Nad_LV: implemented / not activated
- Forest optical thickness Tau_Nad_FO: implemented / not activated
- Optical thickness current
- Roughness ROU: implemented / not activated can be used by a choice of the user
- Flood FLOOD: not implemented / not activated

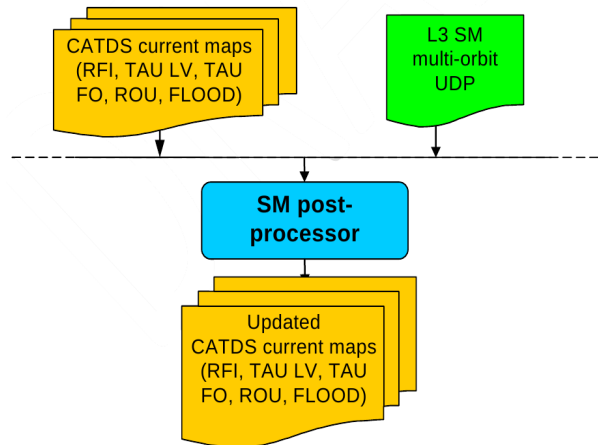


Figure 13: CATDS SM post-processor inputs and outputs

6.2 DETAILED DESCRIPTION OF THE ALGORITHMS

The post-processor first selects the most recent current map available (one for each type). Only UDP products from the reference day are used by the post-processor to process the reference day and update the current maps.

The post-processor gives to the L3 SM optimal processor some **a priori values**. A-priori values are in fact always computed from default parameters. For a DGG node, when an a-priori value is available in the current map, this value replaces the default one in order to be used as input of the retrieval.

6.2.1 VEGETATION OPTICAL THICKNESS CURRENT MAPS FOR LOW VEGETATION

The basic concept is when the retrieval of optical thickness is possible and successful, this optical thickness updates the current map. The idea is that the new optical thickness at nadir will be more accurate and/or up to date than the LAI derived one and remains valid for at least 3 days (DGG in swath maximum revisit time at the equator). However, it might also be affected by spurious events such as a heavy rainfall. The new optical thickness at nadir is for a whole node but actually only for the class for which the retrieval process was carried out (e.g. low vegetation or forest). Therefore, when the retrieval of optical thickness is possible and successful, the TAU map class to be updated is the fraction for which Optical_Thickness_Nad is retrieved (low vegetation or forest).

	Parameter	Description	Units
1	lat	Latitude	degree
2	lon	Longitude	degree
3	Optical_Thickness_Nad_Lv	Nadir optical thickness value of low vegetation	neper
4	Optical_Thickness_Nad_Lv_Dqx	Special DQX of nadir optical thickness value of low vegetation	neper
5	Date_Stamp	Date of the parameters , expressed as a number of days since 1st January 2000, 00:00:00	
6	DT_Branch	Decision tree branch fraction code of DGG cell	

Table 7: AUX_CFTLV* file content

The vegetation optical thickness current map for low vegetation, named AUX_CFTLV*, and stored in the NetCDF format, contains the following fields, Table 7:

A period of validity is introduced: each update has a shelf life limited of some days; a parameter and its uncertainty are reinitialized beyond this period of validity. The temporal validity of the current maps is also tested in the L3 SM optimal processing. For the vegetation optical thickness current map for low vegetation, the period of validity is $\text{Temp_Tau_Lv} = 3$ days. This parameter is configurable in the configuration file of the post-processor. When the post-processor updates the current map, the date of the last acquisition is checked. If the lag is larger than the allowed Temps_Tau_Lv , a missing value is put.

A quality check is performed on the retrieved parameters before updating a current map: the retrieved parameters must be in physical intervals to be considered valid for the update, and the flag $\text{FL_Current_Tau_Nadir_LV}$ in UDP must be activated. The ranges of the retrieved parameters for the quality check (minimum, maximum values) are in the post-processor configuration file, and can be changed if needed. The vegetation optical thickness current map for low vegetation is only updated following LV class retrievals: Current $\text{Optical_Thickness_Nad_Lv}$ is updated with the retrieved $\text{Optical_Thickness_Nad}$ value (UDP).

Current $\text{Optical_Thickness_Nad_Lv_Dqx}$ is updated with a specific RSTD, the $\text{Optical_Thickness_Cur_Dqx}$ (in UDP), obtained like a classical RSTD, but with a matrix COVZ_CURRENT computed assuming that $\text{Optical_Thickness_Nad}$ is completely free (that is, practically, a very high ASTD). This RSTD is lower than the DQX, which leads to constrain more the next retrieval of tau to be closer to this initial value, because the confidence in this value is better. Current date is updated with swath acquisition date.

If there is a valid value in the current map, the value is updated only if the DQX of the new estimation is better and if the decision tree branch number is the same. This algorithm is activated or deactivated by the parameter Maj_Tau_Lv in the post-processor configuration file. It is performed at the end of each day (period of the processing = $\text{Periode_Tau_Lv} = 1$ day), with all the UDP of the day.

The current maps can be also reset before use (all the file set to missing value) by activating the parameter Init_Cur_Tau_Lv in the post-processor configuration file. The use of the vegetation optical thickness current map for low vegetation in the retrieval is activated or deactivated by the parameter $\text{USE_CURRENT_TAU_NAD_LV}$ in the L3 SM optimal processor configuration file. By default in the CATDS operational chain, it is not activated (=0).

6.2.2 VEGETATION OPTICAL THICKNESS CURRENT MAPS FOR FOREST

The principle is the same that for vegetation optical thickness current map for low vegetation. It is also considered that for forests we will only update for fine tuning as the relevant variable is linked to the branch volume and thus should remain fairly constant. Any variation should be linked to changes in other variables (interception, litter water content ...).

The vegetation optical thickness current map for forest, named AUX_CFTFO*, and stored in the NetCDF format, contains the following fields, Table 8:

The temporal validity of the vegetation optical thickness current map for forest is very long, it is set to one year: $\text{Temp_Tau_Fo} = 365$ days. A quality check is performed on the retrieved parameters before updating a cur-

	Parameter	Description	Units
1	lat	Latitude	degree
2	lon	Longitude	degree
3	Optical_Thickness_Nad_Fo	Nadir Optical thickness value of forest	neper
4	Optical_Thickness_Nad_Fo_Dqx	Special DQX of Optical thickness value of forest	neper
5	Date_Stamp	Date of the parameters, expressed as a number of days since 1st January 2000, 00:00:00	
6	DT_Branch	Decision tree branch fraction code of DGG cell	

Table 8: AUX_CFTFO* file content

	Parameter	Description	Units
1	lat	Latitude	degree
2	lon	Longitude	degree
3	NSnap	Accumulated valid snapshots from the UDPs (sum of M_AVA0)	
4	N_RFI_X	Number of FOVs considered significantly affected by RFI in X polarization on specified DGG cell	
5	N_RFI_Y	Number of FOVs considered significantly affected by RFI in Y polarization on specified DGG cell	

Table 9: AUX_RFI file content

rent map: the retrieved parameters must be in physical intervals to be considered valid for the update, and the flag FL_Current_Tau_Nadir_FO in UDP must be activated. The ranges of the retrieved parameters for the quality check (minimum, maximum values) are in the post-processor configuration file, and can be changed if needed. The vegetation optical thickness current map for forest is only updated following FO class retrievals:

Current Optical_Thickness_Nad_Fo is updated with the retrieved Optical_Thickness_Nad value (UDP)

Current Optical_Thickness_Nad_Fo_Dqx is updated with a specific RSTD, the Optical_Thickness_Cur_Dqx (in UDP)

Current date is updated with swath acquisition date.

If there is a valid value in the current map, the value is updated only if the DQX of the new estimation is better and if the decision tree branch number is the same. This algorithm is activated or deactivated by the parameter Maj_Tau_Fo in the post-processor configuration file. It is performed at the end of each day (period of the processing = Periode_Tau_Fo = 1 day), with all the UDP of the day. The current maps can be also reset before use (all the file set to missing value) by activating the parameter Init_Cur_Tau_Fo in the post-processor configuration file. The use of the vegetation optical thickness current map for forest in the retrieval is activated or deactivated by the parameter USE_CURRENT_TAU_NAD_FO in the L3 SM optimal processor configuration file. By default in the CATDS operational chain, it is not activated (=0).

6.2.3 RFI CURRENT MAPS

The RFI current map includes both the total number of times views have observed the DGG node: NSnap, and the total number of cases NRFIp where an anomalously high TB has been unambiguously detected for polarization p (X and Y) in the L3 SM Optimal processor. Over any node, if the **RFI current map indicates potential RFI**, the brightness temperatures radiometric sensitivity is degraded by a factor depending upon the ratio $RRFI = NRFI / NSNAP$. The polarization information may be more relevant at the Earth surface as RFI signal may be polarized and thus affect only one polarization while, at antenna level, RFI may be distributed on both X and Y component. However, though the information is used as if they were one ($NRFI = NRFI-X + NRFI-Y$), the statistics are established for each through individual tracking.

The RFI current map, named AUX_CFRFI*, and stored in the NetCDF format, contains the following fields, Table 9:

There is **no temporal validity** for this current file. A DGG node is updated when the flag FL_Current_RFI in

	Parameter	Description	Units
1	lat	Latitude	degree
2	lon	Longitude	degree
3	Hr	Maximal roughness	
4	Hr_Dqx	Special DQX of Maximal roughness	
5	Date_Stamp	Number of days since reference day	
6	Dt_Branch	Decision tree branch fraction code of DGG cell	

Table 10: AUX_CFROU file content

the UDP is activated. For each DGG node, the RFI current map is updated as followed: the counter NSNAP is incremented by M_AVA0, while the NRFI-X, NRFI-Y counters are updated as well when RFI are detected for the X and/or Y polarized views among the M_AVA0 checked.

This algorithm is activated or deactivated by the parameter Maj_Rfi in the post-processor configuration file. It is **performed at the end of each day** (period of the processing = Periode_Rfi_Default = 1 day), with all the UDP of the day.

The current maps can be also reset before use (all the file set to missing value) by activating the parameter Init_Cur_Rfi in the post-processor configuration file.

The use of the RFI current map by L3 SM Optimal processor to flag the input TB is activated or deactivated by the parameter USE_CURRENT_RFI in the L3 SM optimal processor configuration file. By default in the CATDS operational chain, it is activated (=1).

6.2.4 ROUGHNESS CURRENT MAPS

The basic concept is when the retrieval of HR parameter is possible and successful the retrieved HR is used to update the evolving HR map or helps improving the current value used for HR. The current HR map will then be used in the next swath processes rather than the HR parameter derived from the surface auxiliary file.

The roughness current map, named AUX_CFROU*, and stored in the NetCDF format, and contains the following fields, Table 10:

The **temporal validity** of the roughness current map is around one month: Temp_Rou = **30 days**. A **quality check** is performed on the retrieved parameters before updating a current map: the retrieved parameters must be within an interval of realistic values to be considered valid for the update, and the flag FL_Current_HR in UDP must be activated. The ranges of the retrieved parameters for the quality check (minimum, maximum values) are in the post-processor configuration file, and can be changed if needed.

The roughness current map is only updated following LV class retrievals: Current Hr is updated with the retrieved Hr value (UDP). Current Hr_Dqx is updated with a specific RSTD, the Hr_Cur_Dqx (in UDP). Current date is updated with swath acquisition date.

If there is a valid value in the current map, the value is updated only if the DQX of the new estimation is better and if the decision tree branch number is the same. This algorithm is activated or deactivated by the parameter Maj_Rfi in the post-processor configuration file. It is performed at the end of each day (period of the processing = Periode_Rou = 1 day), with all the UDP of the day. The current maps can be also reset before use (all the file set to missing value) by activating the parameter Init_Cur_Rou in the post-processor configuration file.

The use of the roughness current map in the retrieval is activated or deactivated by the parameter USE_CURRENT_HR in the L3 SM optimal processor configuration file. By default in the CATDS operational chain, it is not activated (=0).

6.2.5 FLOOD CURRENT MAPS

In the future, a flood current map will contain some accumulated SMOS retrieved information associated with ex-

	Parameter	Description	Units
1	lat	Latitude	degree
2	lon	Longitude	degree
3	Fl_Flood_Prob	Appearance Probability of flood flag	

Table 11: AUX_CFFLO file content

ternal risk information to provide a more accurate flag on flooding risk. The flood current map, named AUX_CFFLO*, and stored in the NetCDF format, contains the following fields, Table 11:

For the moment, it is not activated. This algorithm is activated or deactivated by the parameter Maj_Flo in the post-processor configuration file. It is set to 0 for the moment.

7 L3 SM FILTERING

7.1 OBJECTIVE

This step of filtering allows to select soil moisture and optical thickness data. It aggregates all the available values for a day and selects one per nodes. It corresponds to a first aggregation of the soil moisture and optical thickness product over a period of 1 day which considers separately the ascending orbits from the descending ones. These L3 SM intermediate daily products includes event detection flags ((see paragraph §7.2.2) obtained from time series analysis of SMOS data and ancillary data. Event detection consists in detecting a particular state of the observed surface by using temporal information. An "event" can be a case of freezing, dew, snow or flood for example. They can be detected only if the characteristic time of the event is longer than revisit time of SMOS. For the moment, only freezing events are implemented (soil and/or vegetation). These flags are also used to filter data in the monthly products aggregation.

The inputs and outputs of L3 SM filtering processor are schematized in Figure 14. Several L3 SM UDP products are used as inputs: all the UDP that can contain the day to process, i.e. the 2 L3 SM UDP for reference day (ascending and descending), and for the multi-orbit case: 6 UDP for the 3 days before reference day and 6 UDP for the 3 days after reference day. If time series analysis is enabled, the processor also needs some other dilay products generated during the analysis period defined in a configuration file (7 days by default). The SMOS ECMWF file associated with the reference day is used in order to provide some meteorological parameters such as the temperature, useful for the time series analysis.

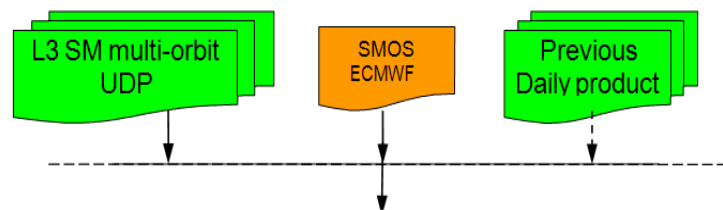


Figure 14: CATDS L3 SM filtering processor inputs and outputs

7.2 DETAILED DESCRIPTION OF THE ALGORITHMS

The processing steps are the following ones:

1. A daily data aggregation, if several daily revisits are available (see Figure 18). Ascending and descending orbits are processed separately.
2. Event detection (see paragraph §7.2.2): development in time series (ascending and descending orbits together) and analysis of the time series to diagnose a particular behavior of the parameter evolution

The processing chain is presented in Figure 15. The first step is always processed, while event detection should be activated or deactivated by the parameter ANALYSE_SERIE in the L3 SM filtering processor configuration file. By default in the CATDS operational chain, it is activated (=1).

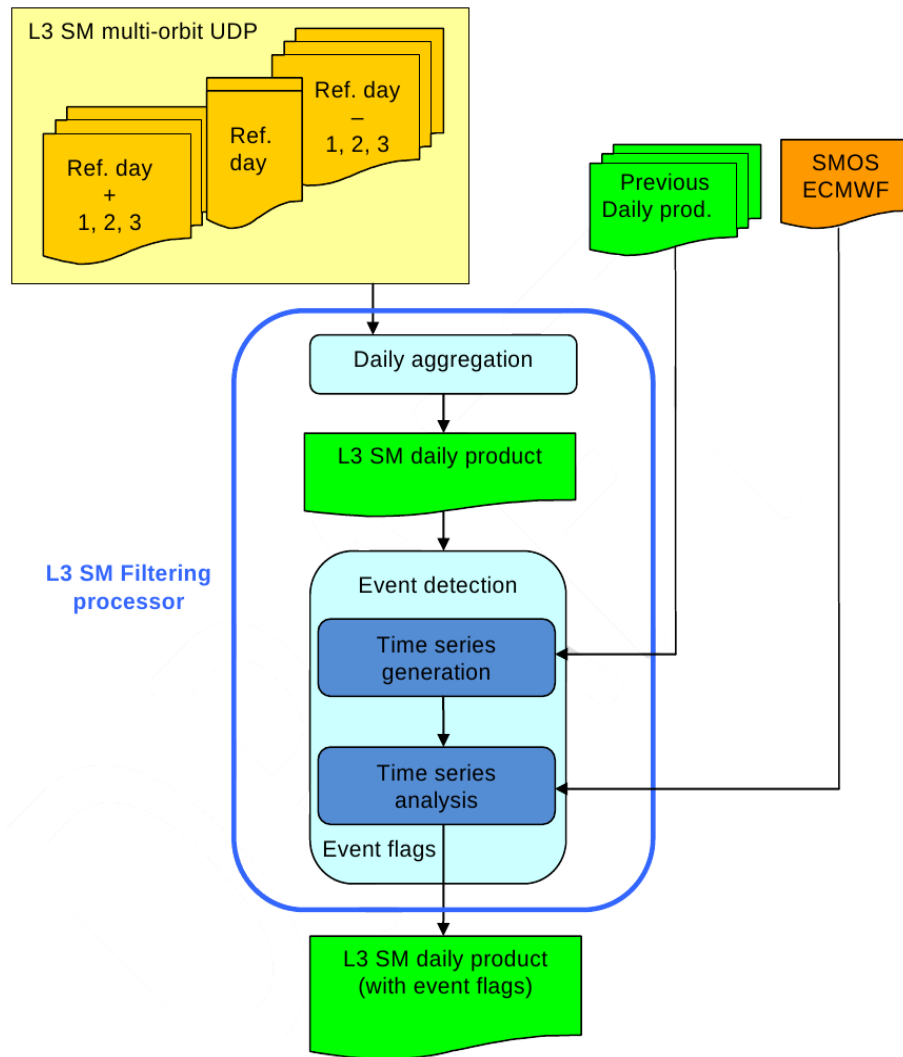


Figure 15: L3 SM Filtering processing steps

7.2.1 DAILY AGGREGATION

This step is a reorganization of the data for obtaining a daily composite. The inputs of this step are the L3 SM UDP products that can contain an estimation of some parameters for the reference day. Ascending and descending orbits are processed separately. The algorithm consists in selecting a particular SM value for a day among all the SM values available the same day in L3 SM UDP products. It works around a reference day JREF, on a period of 7 days (JREF +/- 3 days), as presented on Figure 16. Note that this algorithm is only necessary for the multi-orbit mode.

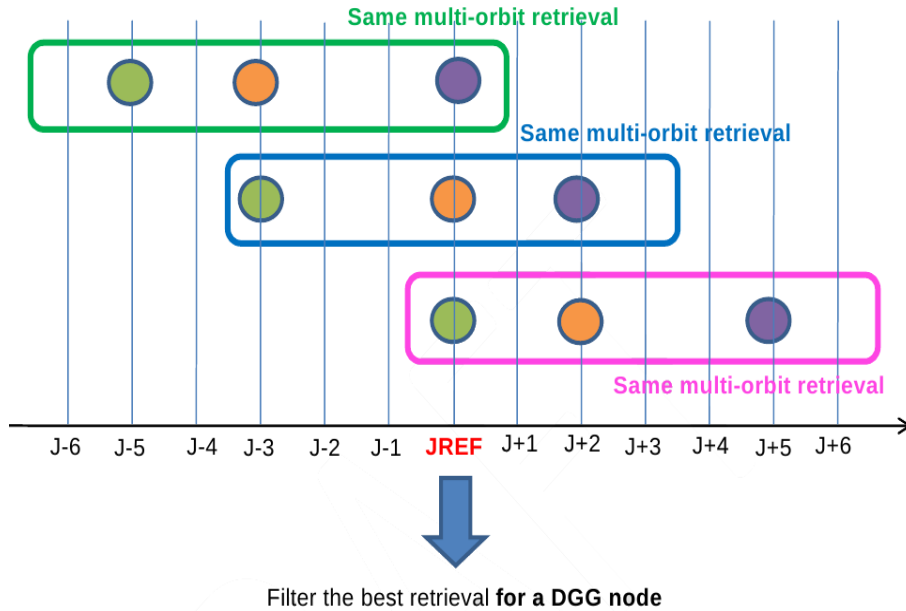


Figure 16: SM values available for a reference day in L3 SM UDP products

The daily aggregation algorithm processes for each DGG node all the L3 SM UDP products that contain an estimation of the soil moisture on the reference day. **The soil moisture values with the associated lowest data quality index SM_DQX (highest accuracy) is selected.** The minimum and maximum of available SM and their associated SM DQX are stored in the daily product in order to check the coherence of the several estimations of soil moisture for the reference day. The selected **dielectric constant value is the one that minimizes the module of the dielectric constant** $DQX(\sqrt{\Re(Dielect_Const_Dqx)^2 + \Im(Dielect_Const_Dqx)^2})$

Note that the dielectric constant used for the daily aggregation is the one from the cardioid model retrieval, Dielectric_Const_MD in the UDP product. The selection is different for the dielectric constant because there is a dedicated 3 days aggregated product for it. The vegetation optical thickness and GQX that are associated to the dielectric constant selected are also integrated in the daily product. The output of this step are 2 daily products (ascending and descending orbits) on a reference day.

7.2.2 EVENT DETECTION

The L3 SM processing gives access to temporal information that can be used to detect some particular meteorological events. The event detection algorithm consists in detecting a particular state of the observed surface by using temporal information [2bis]. This is a change detection algorithm. Event flags are updated in the daily products from a time series analysis. Time series of 7 days (configurable with the parameter TEMP_SERIE) are thus generated and analyzed.

In the L2 processing, climate data from auxiliary ECMWF product yield the Non Permanent Event (like snow) fractions. However, it is possible that, on a grid node, this information is partially erroneous so that contributions to the simulated brightness temperatures will be inaccurate and/or biased. In this case, one could possibly detect such inaccuracies by analyzing the evolution of the geophysical parameters which will be over or underestimated. Also the information given by weather prediction model can be partially erroneous with a given uncertainty in this case the observation from SMOS can be useful to enhance the event flagging.

The signature of these events on the estimation of soil moisture and other retrieved parameters is analysed which can allow us to detect them. This kind of diagnostic should be done from time series analysis when geophysical parameters estimators behave in an unexpected way. To help the diagnostic, additional information (temperature of surface, precipitations, etc ...) coming from external data, such as ECMWF data, are taken into consideration.

The following events are potentially detectable by SMOS:

- freezing of soil and/or vegetation
- dew or morning freezing
- snow
- ice
- flood
- interception of rain by vegetation (canopy, litter)

For the time being, the event detection algorithm in the CATDS chain is configured to detect the following the soil freezing and thawing.

Differentiation of the vegetation freezing from soil freezing is implemented but not activated because the optical thickness change is not accurate enough to get to this level of detail. From our actual knowledge of the SMOS signal it seems that the use of angular signature and polarization signature essential to differentiate the event. This is being inspected.

7.2.2.1 Time series generation

For a reference day, a time series is made to be analyzed for event detection. This time series is a chronological data reorganization of daily products, ascending and descending, over a period of 7 days. This number of days is configurable with the parameter TEMP_SERIE in the L3 SM filtering processor configuration file, the default value being 7 days. It includes the products of the reference day and the complementary products from the 6 days before the reference day. The reference day is then the last day of the time series (Figure 17).

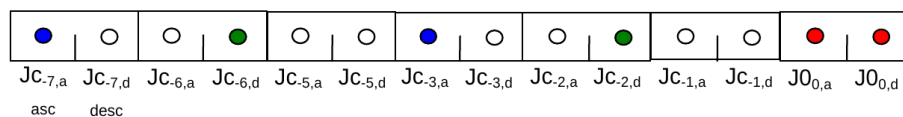


Figure 17: time series of daily products, J0 being the reference day. Jc is a complementary day. Red dots are the reference day, blue are previous ascending retrievals and green are previous descending retrievals used for the event detection

In the time series, ascending products are always placed before descending products in the same day, because the solar local time for ascending orbits is about 6 a.m. (in the morning) and for descending orbits the solar local time is about 6 p.m. (in the afternoon). Ascending and descending products are thus distinguished by even and odd subscripts. Daily products contain event detection flags updated at the end of the analysis of each reference day. The time series contain these updated daily products with the information of event detection of the previous days.

7.2.2.2 Time series analysis

The time series analysis aims at determining the value of the reference day events flags. The inputs of this step are the time series and the ECMWF files associated with the reference day. For a reference day, 2 measurements can be available in ascending and descending products. If both measurements are available, the analysis should be done on the afternoon orbit first (descending orbit type) and then on the morning orbit (ascending orbit type) because the frost risk is higher in the morning, so the knowledge of the state of the event flag in the afternoon will help to detect the frost in the morning.

The event detection is based on a 3 stages detection algorithm. For each event, the following processing is applied:

1. Verification of spatio-temporal constraints:
First, the probability of occurrence of the event on a DGG is assessed. This probability depends on spatio-temporal constraints, or climatic constraints from ancillary data. For example, freezing conditions occur only in some regions of the Earth.
2. "State tests":
Then, the values of geophysical retrieved parameters on the reference day are an indication on the state of the surface, and are also tested. If we keep the example above, freezing conditions need low temperature near 0°C or less. A list of thresholds is defined for each constraint taking into account their uncertainties. An event is declared as probable if all the tests are positive.

Bit Code	Value of the flag FL_EV_XXX	Meaning
00	-1	Missing value
01	0	The event is not verified
10	1	The event is plausible but not validated by the temporal analysis
11	2	The plausible event is verified by the time series analysis

Table 12: Meaning of the event flag

3. Temporal evolution:

The last stage consists in testing the temporal evolution of a list of selected geophysical parameters for each event over a 7 days period. This period ensures a minimum of 2 revisits per grid node. The evolution ($\Delta X = X_{J_c} - X_{J_0}$) is computed between complementary maps that are probable and the reference day map. X is the analyzed parameter in the temporal evolution step. The event is confirmed if the parameters evolutions coincide with the expected evolution for the tested event and that for all parameters. The changes of state or, on the contrary, the stagnation are indicators of the actual state of the surface. For example, during a freezing event the soil dielectric constant decreases drastically and can be detected. It is the combination of all the indicators that can bring to light some events.

It is the combination of all the indicators that can bring to light some events.

The stages of the event detection algorithm are presented on Figure 18. In this example, a chronicle of soil moisture is presented with a temporal sampling representative of this period. The values are given for information purposes only.

At the end of the analysis, event flags are updated in the daily product that corresponds to the reference day processed ($J_{0,a}$ or $J_{0,d}$). The different values of an event flag (named FL_EV_XXX, xxx depending on the name of the event) is presented in Table 18.

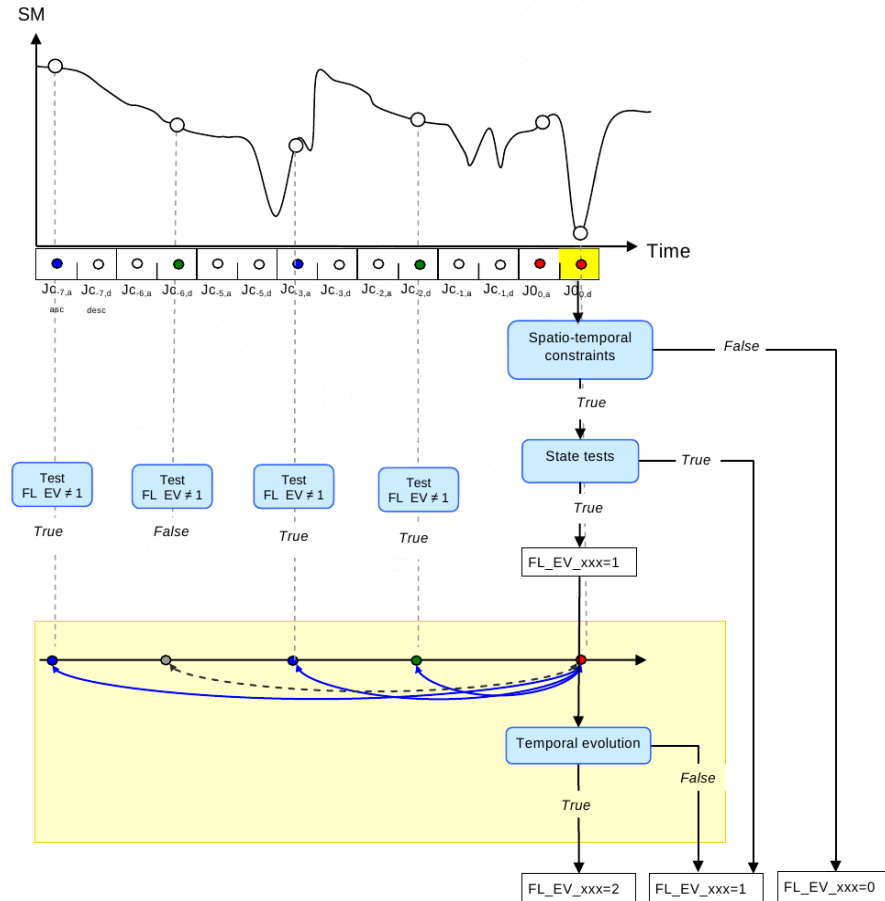


Figure 18: Time series analysis for the reference day J0

7.2.2.3 Event characterization

The event detection algorithm is parameterized according to the event to identify. Each event has its own temporal signature on the retrieved parameters. The parameterization of the algorithm is defined for freezing soil and freezing vegetation. The frost can affect soil and/or vegetation. Some experiences has shown that soil dielectric properties of frozen soil are very close to a dry soil, whereas water frost on the vegetation or vegetation freezing make the vegetation almost transparent in L-band [13]. The freezing/thawing is characterized by an important variation of the emitted L-band brightness temperature, which can be detected, if a non-negligible proportion of the surface contributing to the signal is affected by the frost. Freezing soil and freezing vegetation have not the same effect on the signal; the 2 events are thus processed separately. For the forests, branches and trunks contribute strongly to the signal because their dimensions are comparable to the wavelength in L-band ($\lambda = 21$ cm). However, during freezing period, the water contained in these elements does not often freeze. So, it will be difficult to observe a case of freezing forest. if the freezing of the soil is superficial (low penetration depth), the measured brightness temperatures are affected by contributions from deeper layers. It is thus possible not to be able to measure a significant effect of the frost on the signal, and so to not detect the event. The next tables present the characteristics and the parameters that are used in the CATDS algorithms to detect a case of freezing soil (Table 13) and freezing vegetation (Table 14).

The spatio-temporal constraints are undifferentiated between the two terrestrial hemispheres. Although the risk of freezing is generally not identical between the two hemispheres at a given date, this solution gives the possibility to detect punctual freezing events.

All the threshold values in Table 13 and Table 14 are given in the L3 SM filtering processor configuration file and can be modified if needed.

Other events can be detected by SMOS and may be considered in the future evolutions of the CATDS algorithm. It includes:

- The relative variations of the equivalent dielectric constant should allow us to detect rapid changes of the surface state
- Flood could be detected by a strong increase in SM and dielectric constant and a high value of ECMWF total precipitation
- Rain interception could be detected by a strong increase in Tau and a high value of ECMWF total precipitation
- Some diurnal effects like dew and frost show different values of Tau in the morning and in the afternoon

Nevertheless, the algorithms are not so simple and have to be tested before being implemented in the CATDS chain.

7.2.2.4 Verification of spatio-temporal constraints

This first analysis is to identify DGG nodes that can be a priori affected by the event being detected. The geographical location of the node DGG is tested. It can also be defined by an occurrence map of the tested event. Several maps of occurrence may exist for the same event depending on the season. This approach needs climatic information from ancillary data, and is not implemented. For the time being, the test for freezing is reduced to check the latitude and the day of the year. The Table 13 and Table 14 show the settings to use depending on the event. If the result of a test is "FALSE", the event detection on the DGG node stops and the flag is set $FL_EV_xxx = 0$. If it is "TRUE", it continues with the additional tests presented in the next paragraph.

7.2.2.5 Test of the state of the reference day map

This second step determines whether or not an event is plausible, depending on the values of some parameters. The analysis is conducted on the reference day products. The Table 13 and Table 14 show the settings to use depending on the event.

Table 15 shows the list of parameters to be tested for each event E_i .

Freezing soil	
Flag name	FL_EV_FRS
Description	
When the surface temperature is negative, the soil freezes: the water in the soil becomes solid to a certain depth and the resulting dielectric constant is greatly reduced. The soil emissivity increases. The L-band signal becomes closer to the signal of a dry soil.	
Spatio-temporal constraints	
Geographic constraints: Select the latitudes from where the event is probable	$TH_FRS_LATMIN < abs(LAT) < TH_FRS_LATMAX$ LAT: Latitude
Temporal constraints: Select the seasons where the event is probable	$TH_FRS_DMIN < DOY < TH_FRS_DMAX$ DOY: Day Of Year
State tests	
Nominal fraction of the retrieval: Work only on nominal soil FNO or frozen soil FRZ	$FMO = TH_FRS_FMO$ FMO: Nominal fraction of the retrieval Test on the decision tree branch (FNO or FRZ)
Surface temperature is low	$STL1 < TH_FRS_TS$ STL1: temperature of the first soil layer (K), from the ECMWF data
Retrieved soil moisture is low	$SM + \sigma_{SM} < TH_FRS_SM$ SM: soil moisture σ_{SM}: SM uncertainty = Soil_Moisture_Dqx
The module of the retrieved dielectric constant (MOD_EPS) is low	$MOD_EPS + \sigma_{MOD_EPS} < TH_FRS_MOD_EPS$ $MOD_EPS = \sqrt{\epsilon'^2 + \epsilon''^2}$ MOD_EPS: dielectric constant module ϵ' : real part of the dielectric constant ϵ'' : imaginary part of the dielectric constant σ_{MOD_EPS} : MOD_EPS uncertainty $\sigma_{MOD_EPS} = \frac{1}{2} \cdot \frac{\sqrt{\sigma_{\epsilon'}^2 + \sigma_{\epsilon''}^2}}{\sqrt{\epsilon'^2 + \epsilon''^2}}$ $\sigma_{\epsilon'}$: ϵ' uncertainty = $\Re(\text{Dielect_Const_Dqx})$ $\sigma_{\epsilon''}$: ϵ'' uncertainty = $\Im(\text{Dielect_Const_Dqx})$
Threshold values	
Decision tree branch number	$TH_FRS_FMO = [9, 10, 12]$
Threshold on soil moisture value	$TH_FRS_SM = 0.10 \text{ m}^3/\text{m}^3$
Threshold on surface temperature value	$TH_FRS_TS = 273.15 \text{ K}$
Variation of soil moisture	$TH_FRS_DSM = 0.15 \text{ m}^3/\text{m}^3$
Variation polarization ratio	$TH_FRS_DPR = 0.02$
Threshold on the dielectric constant module value	$TH_FRS_MOD_EPS = 15$
Latitudes of interest	$TH_FRS_LATMIN = 0.0^\circ$ $TH_FRS_LATMAX = 87.0^\circ$
Day Of Year start and stop	$TH_FRS_DMIN = 1$ $TH_FRS_DMAX = 365$

Table 13: Characteristics of the event "freezing soil"

Freezing vegetation	
Flag name	FL_EV_FRV
Description	
When the air temperature is negative, the vegetation can freeze. A frozen vegetation becomes transparent at L-band, so only the soil contributes significantly to the signal. The result is a strong decrease in the vegetation optical thickness.	
Spatio-temporal constraints	
Geographic constraints: Select the latitudes from where the event is probable	$TH_FRS_LATMIN < abs(LAT) < TH_FRS_LATMAX$ LAT: Latitude
Temporal constraints: Select the seasons where the event is probable	$TH_FRS_DMIN < DOY < TH_FRS_DMAX$ DOY: Day Of Year
State tests	
Nominal fraction of the retrieval: Work only on nominal soil FNO or frozen soil FRZ	$FMO = TH_FRS_FMO$ FMO: Nominal fraction of the retrieval Test of the decision tree branch (FNO or FRZ)
Low vegetation temperature is low	$SKT < TH_FRV_TC$ SKT: Soil skin temperature (K) from ECMWF data
Retrieved vegetation optical thickness is low	$TAU + \sigma_TAU < TH_FRV_TAU$ Tau: vegetation optical thickness σ_TAU : TAU uncertainty = Optical_Thickness_NadDqx
Temporal evolution	
Strong decrease in the vegetation optical thickness compared to unfrozen vegetation	$DTAU - \sigma_DTAU > TH_FRV_DTAU$ DTAU: Tau variation between a complementary day J_{Ci} and the reference day J_0 $DTAU = TAU_{J_{Ci}} - TAU_{J_0}$ σ_DTAU : DTAU uncertainty $\sigma_DTAU = \sqrt{\sigma_Tau_{J_C}^2 + \sigma_Tau_{J_0}^2}$
Threshold values	
Decision tree branch number	$TH_FRS_FMO = [9, 10, 12]$
Threshold on canopy temperature	$TH_FRV_TC = 273.15 \text{ K}$
Threshold on vegetation optical thickness	$TH_FRV_TAU = 0.1$
Variation of vegetation optical thickness	$TH_FRV_DTAU = 0.2$
Latitudes of interest	$TH_FRS_LATMIN = 0.0^\circ$ $TH_FRS_LATMAX = 87.0^\circ$
Day Of Year start and stop	$TH_FRS_DMIN=1$ $TH_FRS_DMAX=365$

Table 14: Characteristics of the event "freezing vegetation"

	FM0	SM	Tau	MOD_EPS	PR	STL1	SKT
E ₁ : Freezing soil	X	X		X		X	
E ₂ : Freezing vegetation	X		X				X

Table 15: "State tests" to apply for event detection

For an event E_i, a set of parameters {X_i} is tested, the test status of each parameter is noted RX_i, it is given by the following rules:

- If a parameter X_i is not available (missing value), it is not included in the tests: RX_i = -1
- If the test result is "True": RX_i = 1
- If the test result is "False": RX_i = 0

The final result of "state tests" on a DGG node and for an event E_i is given by the following rules:

- If one test is "FALSE" (RX_i = 0) or if no test is performed: FL_EV_xxx = 0
- If at least one test is performed and all results are "TRUE" (RX_i = 1): FL_EV_xxx = 1

It can be summarized by this formula

$$FL_EV_xxx = \prod_{X_i} (RX_i / RX_i \neq -1) \quad (36)$$

An event is declared as **probable** if all the tests are positive (FL_EV_xxx = 1).

7.2.2.6 Temporal evolution

The last step tests the temporal dynamics and identifies unexpected evolutions linked with an event. The idea is that for a DGG node some changes can be observed between the reference day and the complementary days. The temporal evolution of a list of selected geophysical parameters is tested for each event over a 7 days period.

The state of the complementary days is known throughout the event flags (updated when the previous reference days were analyzed), except for initialization (see §7.2.2.7). If two days have a different state, it must be sufficiently strong to be attributed to an event (this variation is small for similar states).

As shown in Figure 17, only probable events are tested, i.e. FL_EV_xxx = 1 for the reference day J₀.

For the event E_i, the evolution of several parameters {DX_i} is computed between complementary maps that are probable and the reference day map. It is tested with DX_i = DX_{J_i} - DX_{J₀}. X is the analyzed parameter in the temporal evolution step. Table 16 shows the list of parameters tested for each event E_i.

	DSM	DPR	DTAU
E_1: Freezing soil	X	X	
E_2: Freezing vegetation			X

Table 16: Evolution tests to apply for event detection

For a given parameter, the set of pair of days (J_c, J₀) are tested. The example in Figure 18 has the following pairs: {DX_{J-7a,J₀}, DX_{J-6d,J₀}, DX_{J-3a,J₀}, DX_{J-2d,J₀}. The test result of each DX_i is RDX_{J_{ci},J₀}, which is given by the following rules:

- If a parameter X_i is not available (missing value), it is not included in the tests: RX_i = -1
- If the test result is "True": RX_i = 1
- If the test result is "False": RX_i = 0
- If a parameter X_j is not available (missing value), the test is not applied on this parameter: RDX = -1
- The additional day J_c with a flag FL_EV_xxx = 1 are not included in the tests, because the event is not confirmed, so we are not sure of its state: RDX = -1
- If the additional day J_c has no event detected, i.e. with a flag FL_EV_xxx = 0: If DX - σ_{DX} > TH_FRX_DX, the result is "True": RDX = 1, there was no event before the reference day, the parameters have evolved significantly at the reference day, so it is confirmed that a change of state happened between the 2 days J_c and J₀.
else the result is "False": RDX = 0, there was no event before the reference day, the parameters have not evolved significantly at the reference day, so it is confirmed that there is no change of state between the 2 days J_c and J₀.

- If the additional day J_c has a detected event, i.e. with a flag $FL_EV_xxx = 2$:

If $abs(DX - \sigma_DX) < TH_FRX_DX$, the test is "True": $RDX = 1$, an event was detected before the reference day, the parameters have not evolved at the reference day. It is confirmed that no change of state happened between the 2 days J_c and J_0 . The event is still present.

Else the test is "False": $RDX = 0$, an event was detected before the reference day, the parameters have evolved significantly at the reference day. A change of state happened between the 2 days J_c and J_0 and so the event is confirmed.

Every complementary day is tested, and finally a result of the evolution test is available for each day: $RDX = 0$ or $RDX = 1$. Then, every day in the time series is weighted by its distance from the reference day. The idea is to give more importance to the days closest to the reference day, in order to enhance the sudden appearance of the event (like freezing).

The result of each day is thus weighted, to compute a weighted mean of the results, $MRDX$:

$$MRDX = \frac{C_1 \cdot RDX_{J_{c1}} + C_2 \cdot RDX_{J_{c2}} + C_3 \cdot RDX_{J_{c3}} + C_4 \cdot RDX_{J_{c4}} + C_5 \cdot RDX_{J_{c5}} + C_6 \cdot RDX_{J_{c6}} + C_0 \cdot RDX_{J_{c0}}}{\sum_i C_i} \quad (37)$$

The values $RDX_{J_{ci}} = -1$ are not taken into account in the sum. The coefficients c_i , that are the weight of each day in the temporal evolution analysis, are given by an exponential law:

$$C_i = WMAX \cdot \exp\left(-\frac{|T_i - T_{ref}|}{TCW}\right) \quad (38)$$

With:

$WMAX$ is the maximum weight at T_{ref} , by default $WMAX = 1$

T_i is the time of the day i , expressed in seconds

T_{ref} is the time of the reference day, expressed in seconds

$$TCW = \frac{(TEMP_SERIE - 1) * 86400}{\ln\left(\frac{WMAX}{WMIN}\right)} \quad (39)$$

$WMIN$ is the minimum weight at the beginning of the time series, by default $WMIN = 0.5$.

For a given test on the parameter X , the weighted mean of the results ($MRDX$) is compared to a threshold (TH_FL_EVENT , default value = 0.5):

If $MRDX > TH_FL_EVENT$, then the result is "True", else it is "False". If all the tests on the several parameters X give a result "True" with at least one test applied, then the evolution test is positive, **the event is confirmed: $FL_EV_xxx = 2$** . The parameters evolutions coincide with the expected evolution for the tested event and that for all parameters. Else, if at least one test is negative (false), **$FL_EV_xxx = 1$, the event is not confirmed by the temporal analysis, it is just "probable"**. The event flags FL_EV_xxx are updated in the daily product.

The parameters $WMIN$ (Minimal temporal weighting), $WMAX$ (Maximal temporal weighting), and TH_FL_EVENT (Threshold of evolution test flags consistency) are defined in the L3 SM filtering processor configuration file. If we want to give the same weight to every days in the time series, the default values of $WMIN$ can be changed by a number very close to 1. Note that a value of 1 will lead to an indecision in the computing of TCW (see equation above).

7.2.2.7 Initialization

Initialization is required **only the first time a time series is analyzed during the processing**. The complementary days do not have yet a valid flag for FL_EV_xxx ($FL_EV_xxx = -1$). It consists in applying the "state tests" to the complementary days, and then all the events considered probable will be confirmed. Then, all flag $FL_EV_xxx = 1$ will be replaced by $FL_EV_xxx = 2$.

7.3 DAILY PRODUCTS

This subsection provides the list of data present in the **L3 SM daily products**, at the end of the L3 SM filtering processing. The format of the product is NetCDF. Only retrieved parameters are in the product, i.e. no default value is reported. Table 17 L3 SM daily product contains the following fields:

Table 17: L3 SM daily products description

	Parameters	Description	Units
1	lat	Latitude of each point in the product	degree
2	lon	Longitude of each point in the product	degree
3	Mean_Acq_Time_Days	Day of mean time of acquisition associated with the selected soil moisture value of DGG point	day
4	Mean_Acq_Time_Seconds	Seconds of mean time of acquisition associated with the selected soil moisture value of DGG point	s
5	Mean_Acq_Time_Days2	Day of mean time of acquisition associated with the selected dielectric constant value of DGG point	day
6	Mean_Acq_Time_Seconds2	Seconds of mean time of acquisition associated with the selected dielectric constant value of DGG point	s
7	Soil_Moisture	Retrieved soil moisture value	$m^3.m^{-3}$
8	Soil_Moisture_Dqx	DQX for Soil_Moisture	$m^3.m^{-3}$
9	Optical_Thickness_Nad	Nadir optical thickness estimate for vegetation layer associated to the Soil_Moisture, DGG per DGG	neper
10	Optical_Thickness_NadDqx	DQX for Optical_Thickness_Nad	neper
11	Optical_Thickness_Nad2	Nadir optical thickness estimate associated to the Dielectric Constant, DGG per DGG	neper
12	Optical_Thickness_NadDqx2	DQX of Optical_Thickness_Nad2	neper
13	Dielect_Const	Dielectric constant (complex value)	$F.m^{-1}$
14	Dielect_Const_Dqx	DQX of Dielectric constant (complex value)	$F.m^{-1}$
15	Hr	Maximal roughness	
16	Hr_Dqx	DQX of Maximal roughness	
17	Scattering_Albedo_H	Albedo on H polarization	
18	Scattering_Albedo_H_Dqx	DQX of Albedo on H polarization	
19	Diff_Albedos	Albedo difference on H and V polarization	
20	Diff_Albedos_Dqx	DQX of Albedo difference on H and V polarization	
21	Surface_Temperature	Surface temperature associated to the Soil_Moisture, DGG per DGG	K
22	Surface_Temperature_Dqx	DQX of surface temperature	K
23	Temp_STL1	ECMWF temperature of the first soil layer associated with the selected SM	K
24	Temp_SKT	ECMWF soil skin temperature associated with the selected SM	K
25	S_Tree_1	Decision tree branch associated with the selected SM	
26	Tb_Toa_Theta_B_X	Top of the atmosphere TB computed from forward model at specific incidence angle theta_B (42.5°), for X polarization, at the antenna frame	K
27	Tb_Toa_Theta_B_X_Dqx	DQX of Tb_Toa_Theta_B_X	K
28	Tb_Toa_Theta_B_Y	Top of the atmosphere TB computed from forward model at specific incidence angle theta_B (42.5°), for Y polarization, at the antenna frame	K
29	Tb_Toa_Theta_B_Y_Dqx	DQX of Tb_Toa_Theta_B_Y	K
30	Tb_Asl_Theta_B_H	Surface level TB (corrected from sky/atmosphere contribution) computed from forward model with a specific incidence angle theta_B (42.5°) for H polarization, at the Earth frame	K
31	Tb_Asl_Theta_B_H_Dqx	DQX of Tb_Asl_Theta_B_H	K

32	Tb_Asl_Theta_B_V	Surface level TB (corrected from sky/atmosphere contribution) computed from forward model with a specific incidence angle theta_B (42.5°) for V polarization, at the Earth frame	K
33	Tb_Asl_Theta_B_V_Dqx	DQX of Tb_Asl_Theta_B_V	K
34	Scientific_Flags	They are the Science_Flags associated with the selected SM See Table XXX	
35	Fno	Mean fraction in FM0 class for FNO	
36	Ffo	Mean fraction in FM0 class for FFO	
37	M_Ava0	number of TB measurements available in L1C	
38	M_Ava	Pre-processing number of TB measurements available in L1C	
39	N_Rfi_X	Count of deleted TBs due to suspected RFI	
40	N_Rfi_Y	Count of deleted TBs due to suspected RFI	
41	Min_Soil_Moisture	Minimum value of available SM	m ³ .m ⁻³
42	Max_Soil_Moisture	Maximum value of available SM	m ³ .m ⁻³
43	Min_Soil_Moisture_Dqx	Dqx associated with the minimum value of SM	m ³ .m ⁻³
44	Max_Soil_Moisture_Dqx	Dqx associated with the maximum value of SM	m ³ .m ⁻³
45	Soil_Moisture_Init_Val	Initial value for free parameter SM	m ³ .m ⁻³
46	Soil_Moisture_Init_Std	Initial standard deviation for free parameter SM	
47	Gqx	Global Quality Index associated to the Soil_Moisture, DGG per DGG	
48	Gqx2	Global Quality Index associated to the Dielectric Constant, DGG per DGG	
49	Event_Flags	See Table 18	
50	Rfi_Prob	RFI Probability	

The parameter Event_Flags contains flags from temporal series analysis. Each flag is composed of 2 bits with the following meaning:

00 | 0 ⇒ Not verified
01 | 1 ⇒ Possible
10 | 2 ⇒ Sure
11 | 3 ⇒ Not processed, stands for -1 (missing value)

Table 18: Event flags

At the moment, only the freezing of the soil can be detected by the processor. The freezing of the vegetation, even though implemented, is not activated and is under validation: the event flags are organised like that:

[00 00 00 00 00 00 XX XX] where X = 0 or 1
VEG SOIL

With this convention, the fill value of this parameter is [00 00 00 00 00 00 11 11], which corresponds to a numerical value of 15.

The Table 19 presents the event flags organization:

Parameter	Description	Size (bits)
FL_EV_Frost_soil	Event flag on the detection of soil freezing, result of the time series analysis	2
FL_EV_Frost_veg	Event flag on the detection of vegetation freezing, result of the time series analysis	2
Spare	Padded with 0	12

Table 19: Event flags description

8 L3 SM AGGREGATION

8.1 OBJECTIVE

The objective of this last processing is to generate the CATDS L3 SM temporal syntheses over different time steps with global coverage. Daily maps are aggregated over several time periods. The need for temporal syntheses is not the same depending on the application, so 3 aggregation types have been defined:

- Over a 3-day period
- Over a 10-day period
- Over one month

The inputs and outputs of L3 SM aggregation processor are schematized in Figure 19.

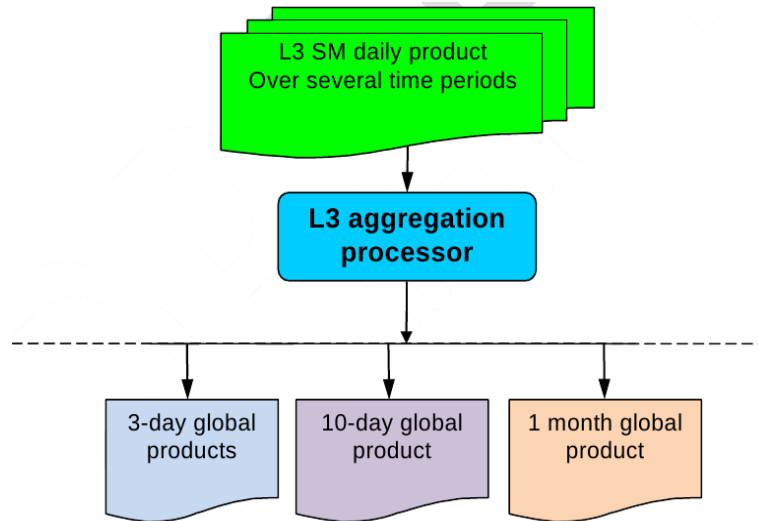


Figure 19: CATDS L3 SM aggregation processor inputs and outputs

8.2 DETAILED DESCRIPTION OF THE ALGORITHMS

The algorithm deals with time aggregation only, i.e. no space averaging is considered. The aggregation of ascending orbits and descending orbits are processed separately. The 3 aggregation types lead to 3 separate processing. The L3 SM aggregation processor has 3 modules that work separately but with common daily products as input, as schematized in Figure 20.

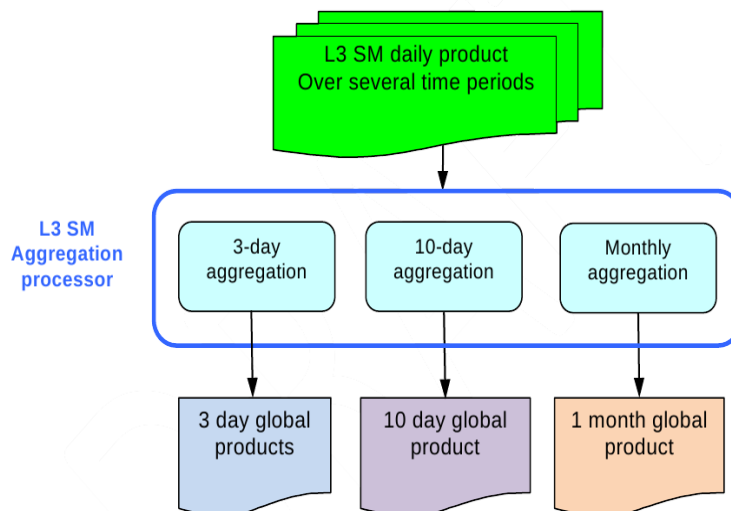


Figure 20: L3 SM Aggregation modules

The next paragraphs present the algorithms used on these 3 kinds of aggregation methods.

8.2.1 THREE DAY AGGREGATION

The 3-day aggregation generates, on a daily basis, global L3 SM and products on a 3-day sliding window. The main advantage is that **the whole Earth's surface is covered in this 3-day product**.

The first step to compute the 3-day product for a given day "n" is to select the daily products at days "n-2", "n-1" and "n". Ascending and descending orbits are processed separately. The **aggregation consists in selecting the best retrieval available on the period of 3 days if there are several values available**.

For the soil moisture product, the best estimation is chosen from the set of retrievals of soil moisture available on the period of 3 days by selecting the **lowest soil moisture CHI2 TO BO CHECKED**. The other parameters are those retrieved at the same time as the selected SM, in order to be consistent in the same product daily L3 product. All the geophysical parameter estimations are relative to the same date.

For the dielectric constant product, the best estimation is chosen from the set of retrievals of dielectric constant available on the period of 3 days by selecting the lowest dielectric constant DQX **TO BO CHECKED**. As for the daily product, the other parameters retrieved at the same time as the selected dielectric constant are selected, in order to have a consistent product, i.e. having all the geophysical parameter estimations relative to the same date.

These 2 products, 3days soil moisture and dielectric constant are generated on a daily basis, with a 3-day sliding window (Figure 21).

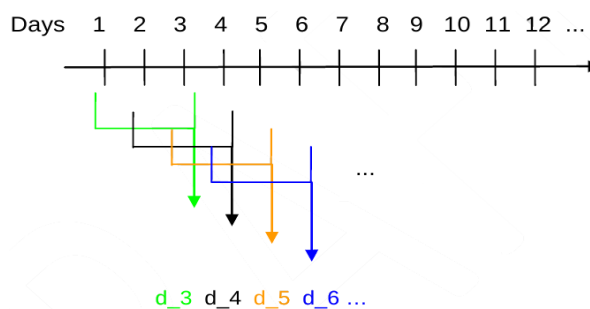


Figure 21: 3-day products

The 3 day aggregation is activated by the parameter FlagAgreger3j that must be "true" in the L3 SM Aggregation processor configuration file. In addition, a minimal number of days from which computations can be performed is defined: NbJoursMinAgr3j. This parameter is in the L3 SM Aggregation processor configuration file, its default value is 1.

8.2.2 10-DAY AGGREGATION

The 10-day aggregation generates global L3 SM products on a 10-day period (no sliding window), from 10 intermediate daily products, see Figure 22. Ascending and descending orbits are processed separately.

This product is composed of three soil moisture values per grid node: **the median, minimum and maximum values of soil moisture** that are extracted out of 10 daily products. The corresponding other parameters, retrieved at the same time as the selected SM, (nominal retrieval fraction, tau, DQX, etc.) are also extracted and included in this product. Three products per month are delivered, meaning that the last one of each month can cover from 8 to 11 days according to the month.

Figure 22 shows aggregation strategy for 10-day period.

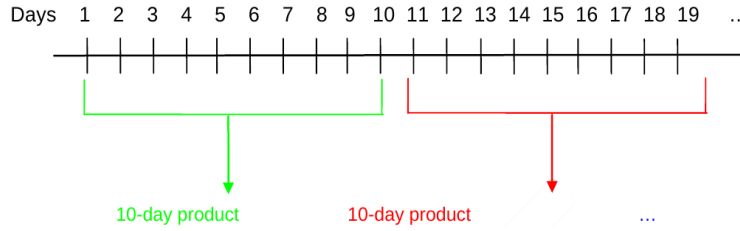


Figure 22: 10 day product obtained at the dates d_5, d_15

The mean GQX (quality indicator) on the 10-day product is computed as follow:

$$GQX_{decade} = \frac{\sum_i^n GQX_i}{n} \quad (40)$$

Where i corresponds to the day i

The sum is computed considering n days of the 10 days when data are available and not contaminated by an event. The 10-day aggregation is activated by the parameter FlagAgreger10j that must be "true" in the L3 SM Aggregation processor configuration file. In addition, a minimal number of days from which computations can be performed is defined: NbJoursMinAgr10j. This parameter is in the L3 SM Aggregation processor configuration file and its default value is 3. It means that the processor needs at least 3 days in the 10-day period to process this product, otherwise there will not be a median, a minimum and a maximum value. In order to have a full coverage of the world, the missing soil moisture is replaced by the mean value of the initial soil moisture values over the period of 10 days, computed from the ECMWF data. In that case, their GQX are set to missing value.

8.2.3 MONTHLY AGGREGATION

The monthly aggregation generates global L3 SM products per month, from daily products. Ascending and descending orbits are still processed separately. This kind of product is useful for climate monitoring.

For each DGG node, it provides a weighted mean of soil moisture, vegetation optical thickness, and RFI statistics over a month, without taking into account the detected events reported in the daily product. There is no sliding window, an estimation is done month by month, as presented on Figure 23. The number of days to be considered depends on the number of days in the month (28 to 31 days).

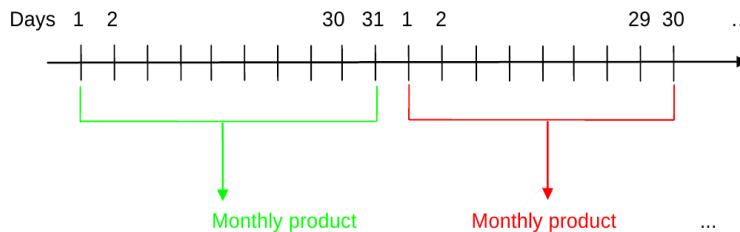


Figure 23: monthly products

The values taken into account in the computation of the weighted mean of a parameter must not be affected by an event. So, only values from daily products with all the event flags FL_EV_XXX set to 0 are taken into account. The decision tree branch in the majority over the month is considered. Only soil moisture values associated with this decision tree branch are taken into account in the computation of the weighted mean. For the computation of the weighted mean of low vegetation optical thickness, only retrievals over a nominal fraction are taken into account (decision tree branch = 12). For the computation of the weighted mean of forest optical thickness, only retrievals over a forest fraction are taken into account (decision tree branch = 11).

- The average parameter over a month, P_month, to be estimated (soil moisture SM, tau, etc) is obtained with a weighted error (DQX). This temporal mean (no spatial average) is computed for each grid node. The weighted

average for a parameter P, is computed as:

$$P_{month} = \frac{\sum_{i=1}^n \frac{P_i}{(DQX_{P_i})^2}}{\sum_{i=1}^n \frac{1}{(DQX_{P_i})^2}} \quad (41)$$

Where i corresponds to the day i

The sum is computed considering n days of the month when data are available and not contaminated by an event. DQX_P_i corresponds to the theoretical uncertainty for parameter P, at the day i.

- The variance in the monthly product, VAR_P is computed as follow:

The total variance (VAR_total) observed on the parameter P over one month is due to the combined effect of the real geophysical variance coming from climatic events (VAR_P) and the variance of the retrieval coming from the uncertainty of instrument and the errors of the retrieval algorithm. The latest one can be assimilated to a "noise" it may not be stationary if the instrument is presenting a drift or if special events occurs like RFI burst ... So if the user is interested in the geophysical variance we have, VAR_P = VAR_total - VAR_P_month and

$$VAR_P = \frac{\sum_{i=1}^n (P_i - P_{month})^2}{n} - \frac{\sum_{i=1}^n (DQX_{P_i})^2}{n} \quad (42)$$

The associated standard deviation is then

$$STD_P = \sqrt{VAR_P} = \sqrt{\frac{\sum_{i=1}^n (P_i - P_{month})^2}{n} - \frac{\sum_{i=1}^n (DQX_{P_i})^2}{n}} \quad (43)$$

The idea of taking into account the DQX in the formula allows us to check if the variation is due to a geophysical phenomenon and not due to significant noise measurements. When the number of retrieved values n increases, the monthly DQX decreases and the impact of instrument noise is less important.

- The mean DQX_P_month is the mean error of P_i over one month (and not the error associated to P_month). It has to be taken at the quadratic point of view:

$$DQX_{P_{month}} = \sqrt{\frac{\sum_{i=1}^n (DQX_{P_i})^2}{n}} \quad (44)$$

- The mean GQX (quality indicator) is computed as follows (without DQX weighting):

$$GQX_{month} = \frac{\sum_{i=1}^n (GQX_i)^2}{n} \quad (45)$$

- Concerning the RFI field, the percentage of the contaminated views will be aggregated for each EASE grid node. RFI_month is the number of RFI-contaminated SMOS TB for a given grid node in the considered month:

$$RFI_{month} = \sum_{i=1}^n RFI_i \quad (46)$$

TOTview_month is the number of SMOS TB for a given grid node in the considered month:

$$TOTview_{month} = \sum_{i=1}^n VIEW_i = \sum_{i=1}^n MAVA_i \quad (47)$$

fracRFI_month presents the fraction of contaminated SMOS TB in the considered month:

$$fracRFI_{month} = \frac{RFI_{month}}{TOTview_{month}} \quad (48)$$

the fraction of RFI in the month is polarization dependent:

$$RFI_X_Frac = \frac{\sum_{i=1}^n NRFI_X_i}{\sum_{i=1}^n MAV_A_i} \quad (49)$$

$$RFI_Y_Frac = \frac{\sum_{i=1}^n NRFI_Y_i}{\sum_{i=1}^n MAV_A_i} \quad (50)$$

So we have

$$fracRFI_{month} = RFI_X_Frac + RFI_Y_Frac \quad (51)$$

The monthly aggregation is activated by the parameter FlagAgreger1m that must be "true" in the L3 SM Aggregation processor configuration file. In addition, a minimal number of days from which computations can be performed is defined: NbJoursMinAgr1m. This parameter is in the L3 SM Aggregation processor configuration file, its default value is 3. It means that the processor needs at least 3 days in the month to process the monthly product. In the monthly products, to cover the entire the world, missing soil moisture values are replaced by the mean value of initial soil moisture over the month, computed from the ECMWF data. In that case, their associated GQX are set to missing value.

8.3 PRODUCTS

This subsection provides the list of data present in the **L3 SM temporal syntheses (3-day, 10- day, monthly)** at the end of the L3 SM aggregation processing. All the products are in the NetCDF format.

8.3.1 L3 SM 3-DAY PRODUCT

The L3 SM 3-day product, dedicated to soil moisture, contains the following fields:

	Parameter	Description	Units
1	Lat	Latitude of each point in the product	degree
2	Lon	Longitude of each point in the product	degree
3	Nb_Sm	Number of soil moisture estimates available on the period	
4	Soil_Moisture	Retrieved soil moisture value	$\text{m}^3.\text{m}^{-3}$
5	Soil_Moisture_Dqx	DQX of retrieved soil moisture value	$\text{m}^3.\text{m}^{-3}$
6	Nominal_Fraction	Nominal fraction associated to soil moisture value (Mean fraction in FM0 class for FNO)	
7	Optical_Thickness_Nad	Nadir optical thickness value associated to soil moisture value	neper
8	Optical_Thickness_Nad_Dqx	DQX of Nadir optical thickness value	neper
9	Scientific_Flags	They are the Science_Flags associated with the selected SM, See Table XXX	
10	Event_Flags	See Table 18	
11	Gqx	Global Quality index	
12	Mean_Acq_Time_Days	Day of mean time of acquisition associated with the selected soil moisture value of DGG point	d
13	Mean_Acq_Time_Seconds	Seconds of mean time of acquisition associated with the selected soil moisture value of DGG point	s
14	Dielect_Const	Dielectric constant from MD retrieval (complex value), associated to soil moisture value	F.m^{-1}
15	Dielect_Const_Dqx	DQX of Dielectric constant from MD retrieval (complex value), associated to soil moisture value	F.m^{-1}
16	list_of_data_set	Extract of the product header. It is an XML structure containing the number of Data_Set structures, compacted as array of string	

Table 20: L3 SM 3 day product description

8.3.2 L3 SM 10-DAY PRODUCT

The **L3 SM 10-day product** contains the following fields:

	Parameter	Description	Units
1	Lat	Latitude of each point in the product	degree
2	Lon	Longitude of each point in the product	degree
3	Mean_Acq_Time_Days	Day of mean time of acquisition associated with the soil moisture values (median, minimum, maximum) of DGG point	day
4	Mean_Acq_Time_Seconds	Seconds of mean time of acquisition associated with the soil moisture values (median, minimum, maximum) of DGG point	s
5	Nb_Sm	Number of soil moisture estimates available on the period	
6	Soil_Moisture	Retrieved soil moisture values median, minimum, maximum	$\text{m}^3.\text{m}^{-3}$
7	Soil_Moisture_Dqx	DQX of retrieved soil moisture value median, minimum, maximum	$\text{m}^3.\text{m}^{-3}$
8	Optical_Thickness_Nad	Nadir optical thickness value associated with the soil moisture values median, minimum, maximum	neper
9	Optical_Thickness_Nad_Dqx	DQX of Nadir optical thickness value associated with the soil moisture values, median, minimum, maximum	neper
10	Hr	Maximal roughness associated with the soil moisture values median, minimum, maximum	
11	Hr_Dqx	DQX of Maximal roughness associated with the soil moisture values (with the order: median, minimum, maximum)	
12	Scattering_Albedo_H	Scattering albedo for horizontal polarization associated with the soil moisture values median, minimum, maximum	
13	Scattering_Albedo_H_Dqx	DQX of scattering albedo for horizontal polarization associated with the soil moisture values median, minimum, maximum	
14	Diff_Albedos	Difference of albedos wh-wv associated with the soil moisture values (with the order: median, minimum, maximum)	
15	Diff_Albedos_DQX	DQX of difference of albedos wh-wv associated with the soil moisture values median, minimum, maximum	
16	Nominal_Fraction	Nominal fraction (Mean fraction in FM0 class for FNO) associated with the soil moisture values median, minimum, maximum	
17	Science_Flags	They are the Science_Flags associated with the soil moisture values median, minimum, maximum. See Table 8	
18	Gqx	Global Quality index on the 10-day period	
19	list_of_data_set	Extract of the product header. It is an XML structure containing the number of Data_Set structures, compacted as array of string	

Table 21: L3 SM 10-day product description

8.3.3 L3 SM MONTHLY PRODUCT

The **L3 SM monthly** product contains the following fields:

	Parameter	Description	Units
1	Lat	Latitude of each point in the product	degree
2	Lon	Longitude of each point in the product	degree
3	Nb_Sm	Number of soil moisture estimates available on the period	
4	Soil_Moisture	Retrieved soil moisture mean value	$\text{m}^3.\text{m}^{-3}$
5	Soil_Moisture_Dqx	DQX of Retrieved soil moisture value over the month (mean error)	$\text{m}^3.\text{m}^{-3}$
6	Var_Soil_Moisture	Variance of Retrieved soil moisture value	
7	Optical_Thickness_Lv	Nadir optical thickness mean value for lower vegetation	neper
8	Optical_Thickness_Lv_Dqx	DQX of Nadir optical thickness value for lower vegetation over the month (mean error)	neper
9	Var_Optical_Thickness_Lv	Variance of Nadir optical thickness value for lower vegetation	
10	Optical_Thickness_Fo	Nadir optical thickness mean value for forest	neper
11	Optical_Thickness_Fo_Dqx	DQX of Nadir optical thickness value for forest over the month (mean error)	neper
12	Var_Optical_Thickness_Fo	Variance of Nadir optical thickness value for forest	neper
13	Nominal_Fraction	Nominal fraction (Mean fraction in FM0 class for FNO) mean value, associated to soil moisture	
14	Forest_Fraction	Forest fraction (Mean fraction in FM0 class for FFO) mean value, associated to soil moisture	
15	Gqx	Global Quality index on the month	
16	Rfi_X_Frac	Fraction of contaminated SMOS TB by RFI in the considered month, on the X polarization	
17	Rfi_Y_Frac	Fraction of contaminated SMOS TB by RFI in the considered month, on the Y polarization	
18	list_of_data_set	Extract of the product header. It is an XML structure containing the number of Data_Set structures, compacted as array of string	

Table 22: L3 SM monthly product description

8.3.4 L3 Dielectric constant 3-DAY PRODUCT

The L3 SM 3-day product dedicated to the dielectric constant contains the following fields:

	Parameter	Description	Units
1	Lat	Latitude of each point in the product	degree
2	Lon	Longitude of each point in the product	degree
3	Dielect_Const	Dielectric constant (complex value)	F.m^{-1}
4	Dielect_Const_Dqx	DQX of dielectric constant (complex value)	F.m^{-1}
5	Dielect_Const_Module	Module of Dielectric constant	F.m^{-1}
6	Dielect_Const_Module_Dqx	Module of DQX of Dielectric constant	F.m^{-1}
7	Optical_Thickness_Nad	Nadir optical thickness value associated to dielectric constant value	neper
8	Optical_Thickness_Nad_Dqx	DQX of Nadir optical thickness value	neper
9	Mean_Acq_Time_Days	Day of mean time of acquisition associated with the selected dielectric constant value of DGG point	day
10	Mean_Acq_Time_Seconds	Seconds of mean time of acquisition associated with the selected dielectric constant value of DGG point	s
11	Event_Flags	See Table 18	
12	Gqx	Global Quality index	
13	list_of_data_set	Extract of the product header. It is an XML structure containing the number of Data_Set structures, compacted as array of string	

Table 23: L3 SM 3-day product description

9 CONCLUSION AND FURTHER DEVELOPMENTS

The CATDS L3 soil moisture and brightness temperature chains have been described in this ATBD. The CATDS operational products are delivered at the CATDS production centre (C-PDC) (www.catds.fr). The main enhancements of this chain are: the use of a new map based gridding system (EASE 25 km), a user-friendly format for the products (NetCDF) and most important the use of multi-orbit information for the retrieval of soil moisture. Time synthesis products are delivered by the chain: daily, 3 day, 10-days, monthly products. The chain uses as input the L1B brightness temperature Fourier components and not the level 2 soil moisture products in order to deliver optimal brightness temperature products on the new grid that are then used in a multi-orbit retrieval schemes.

Many algorithmic improvements will be undertaken in the coming years, the retrieval algorithms for soil moisture remain at an early stage, because SMOS is the first satellite dedicated to the observation of soil moisture in L-Band. Improvements at the ESA Level 2 processor will continue to be implemented in the CATDS L3 SM optimal processor.

Currently, extensive validation, evaluation and sensitivity analysis studies of the L3 multi-orbit retrieval products are underway. These studies will enable to understand the specificities of the L3 multi-orbit retrievals compared to the ESA Level 2 processor and to find optimal parameter configuration for the retrieval.

The event detection has to be fine tuned and improved, by adjusting the configuration parameters, and the thresholds. Many improvements can be undertaken, by the use of occurrence maps for example. The algorithms for the event detection may then be extended to other events.

A coast processing, that uses simultaneously land and sea CATDS processor, on a dedicated EASE grid, may be studied.

Level 3 products are used to produce Level 4 products. As defined by EOS committee level 4 are products obtained from the combined use of different sensors or models to produce a higher level product. The opportunities for Level 4 are quite large but this is out of the scope of this ATBD. Here is a list of the main applications and products from CATDS L4:

- Assimilation of soil moisture or TBs in hydrological modelling for flood monitoring.
- Soil moisture in the root zone, drought index and Fire risk.
- Disaggregation of soil moisture at 1 km resolution using visible infrared remote sensing data
- Merging with other satellite datasets for a soil moisture historical dataset
- Enhanced rainfall products
- Advanced freezing and thawing products complementary to the event detection in the L3 daily product

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