SMOS OS Level 3

Algorithm Theoretical Basis Document (v400)

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Signatures

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1 Introduction

1.1 Scope of the document

The purpose of this Algorithm Theoretical Basis Document is to describe the procedure that is used in the SMOS CATDS Production Data Center (CPDC) to generate operational sea surface salinity (SSS) maps (also called L3OS/L4OS product, Level 3/4 Ocean Salinity product).

Moreover, this document gives an overview of the different steps of the global processing, from Level 1b to Level 3 and Level 4 products knowing that only L3OS/L4OS products are provided to users by the CATDS (intermediate products are not officially distributed).

1.2 Reference Documents

The following table presents the Reference Document (RD).

Table 1: Reference Document

ID	Title	Ref
[RD- 1]	SMOS L1 Full Polarisation Data Processing	SO-TN-DME-L1PP-0024, 16/07/07
[RD- 2]	SMOS L2 OS Algorithm Theoretical Baseline Document	SO-TN-ARG-GS-0007, 12/02/21 https://earth.esa.int/eogateway/documents/20142/3762 7/SMOS-L2OS-ATBD.pdf
[RD- 3]	Boutin, J., et al. (2016), Satellite and In Situ Salinity: Understanding Near-Surface Stratification and Subfootprint Variability, Bulletin of the American Meteorological Society, 97(8), 1391-1407.	doi:10.1175/bams-d-15-00032.1
[RD- 4]	Boutin, J., J. L. Vergely, S. Marchand, F. D'Amico, A. Hasson, N. Kolodziejczyk, N. Reul, G. Reverdin, and J. Vialard (2018), New SMOS Sea Surface Salinity with reduced systematic errors and improved variability, Remote Sensing of Environment, 214, 115-134.	doi:https://doi.org/10.1016/j.rse.2018.05.022.
[RD- 5]	Bretherton, F. P., R. E. Davis, and C. B. Fandry (1976), A technique for objective analysis and design of oceanographic experiments applied to MODE-73, Deep Sea Research and Oceanographic Abstracts, 23(7), 559-582.	doi:https://doi.org/10.1016/0011-7471(76)90001-2.
[RD- 6]	Brodzik, M. J., B. Billingsley, T. Haran, B. Raup, and M. H. Savoie (2012), EASE-Grid 2.0: Incremental but Significant Improvements for Earth-Gridded Data Sets, ISPRS International Journal of Geo-Information, 1(1), 32-45.	



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	T	
[RD- 7]	Kolodziejczyk, N., J. Boutin, JL. Vergely, S. Marchand, N. Martin, and G. Reverdin (2016), Mitigation of systematic errors in SMOS sea surface salinity, Remote Sensing of Environment, 180, 164-177.	doi:https://doi.org/10.1016/j.rse.2016.02.061
[RD- 8]	Kolodziejczyk, N., M. Hamon, J. Boutin, J L. Vergely, G. Reverdin, A. Supply, and N. Reul (2021), Objective Analysis of SMOS and SMAP Sea Surface Salinity to Reduce Large-Scale and Time-Dependent Biases from Low to High Latitudes, Journal of Atmospheric and Oceanic Technology, 38(3), 405-421.	doi:10.1175/jtech-d-20-0093.1.
[RD- 9]	Supply, A., J. Boutin, JL. Vergely, N. Martin, A. Hasson, G. Reverdin, C. Mallet, and N. Viltard (2018), Precipitation Estimates from SMOS Sea-Surface Salinity, Quarterly Journal of the Royal Meteorological Society, 144(S1), 103-119.	doi:https://doi.org/10.1002/qj.3110
[RD- 10]	Kolodziejczyk, N., M. Hamon, J. Boutin, JL. Vergely, G. Reverdin, A. Supply, and N. Reul (2021), Objective Analysis of SMOS and SMAP Sea Surface Salinity to Reduce Large-Scale and Time-Dependent Biases from Low to High Latitudes, <i>Journal of Atmospheric and Oceanic Technology</i> , 38(3), 405-421.	doi:10.1175/jtech-d-20-0093.1
[RD- 11]	Ide, K., P. Courtier, M. Ghil, and A. C. Lorenc, 1997: Unified notation for data assimilation: Operational, sequential and variational. J. Meteor. Soc. Japan, 75, 181–189.	https://doi.org/10.2151/jmsj1965.75.1B_181

1.3 Definitions, Acronyms and Abbreviations

1.3.1 Definition

- Brightness temperature measurement: brightness temperature (BT) measured in one MIRAS polarisation mode, along with relevant information (radiometric noise, observation conditions, contributions as computed by the model, flags, polarisation direction). A measurement is associated with one Grid point and one Snapshot at a spatial resolution of about 40 km.
- **Grid Point:** point on Earth surface where Measurements are available in SMOS L1c, L2 and L3 product. Note that only L3 products are delivered by CATDS.
- **Dwell line:** ensemble of Measurements at the same Grid Point available in SMOS L1c product.



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- **SSS:** Sea Surface Salinity. Salinity of the upper ocean that contributes to L-band emission (approx. 1 cm depth).
- SSS bulk: SSS corrected from rain effects
- **SST:** Sea Surface Temperature. What matters for SMOS it is the temperature of the upper fraction of the ocean that contributes to L-band emission (approx. 1 cm)
- EASE grid: set of Grid Points on Earth Surface where the BTs are reconstructed and the salinities are retrieved. This grid used by the CATDS is different from ISEA grid used by ESA DPGS (Data Processing Ground Segment). Pixels have a constant area, longitudes are equally spaced but not latitudes (see RD-6).
- **Snapshot:** Ensemble of measurements acquired at the same time. Distinction of snapshots per polarization is done.
- **Polarization direction**: axes of the polarization frames: **X** and **Y** for the MIRAS antenna polarization frame.
- MIRAS operating mode: MIRAS has two operating modes (see RD1):
 - **Dual polarization mode:** measurement sequence is XX YY XX YY –XX YY -...
- Retrieval Polarization mode: to derive SSS, one can use:
 - Stokes 1 parameter, i.e. the sum of BTs in X and Y polarization directions (Stokes 1 retrieval mode).
 - BTs in X and Y polarization directions (dual pol retrieval mode).
 - BTs in X and Y directions and real and imaginary part in XY (full pol retrieval mode).



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1.3.2 Acronyms and abbreviations

Table 2: List of Acronyms

Acronym	ruble 2. List Of Acronyms			
/ torony m	Description			
ADF	Auxiliary Data File			
ATBD	Algorithm Theoretical Baseline Document			
ВТ	Brightness Temperature			
CATDS	Centre Aval de Traitement des Données SMOS			
CNES	Centre National d'Etudes Spatiales			
DDI	Dossier des Interfaces			
DPGS	Data Processing Ground Segment			
DPM	Data Processing Model			
ECMWF	European Centre for Medium-Range Weather Forecasts			
EASE-Grid	Equal-Area Scalable Earth Grid (used in the CATDS)			
ESA	European Space Agency			
ESRIN	ESA Centre for Earth Observation			
ESTEC	European Space Research and Technology Center			
IFREMER	Institut français de recherche pour l'exploitation de la mer			
ISEA-grid	Icosahedral Snyder Equal Area grid (used in the DPGS)			
L1OP	SMOS Level 1 Operational Processor			
L1PP	SMOS Level 1 Prototype Processor			
L2OS, L3OS	Level 2 or 3 Ocean Salinity			
LOCEAN	Laboratoire d'Océanographie et du Climat Expérimentation et Approches Numériques			
LUT	Look Up Table			
MIRAS	Microwave Imaging Radiometer using Aperture Synthesis			
OS	Ocean Salinity			
отт	Ocean Target Transformation			
sigSSS	SSS L2OS error			
SMOS	Soil Moisture and Ocean Salinity			
SSS	Sea Surface Salinity			
SST	Sea Surface Temperature			
SUM	Software User Manual			
UDP	User Data Product			



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1.3.3 Product name convention

The complete logical file name is to be of the following structure:

MM_CCCC_FFF_DDDDDD_<instance ID>

The meaning of the different subset of character string is given in the following table.

Table 3: File name convention

Naming element	Value	Description	Format
ММ	SM	SMOS mission ID	2 characters
сссс	OPER (operational product), REnn (reprocessing nn product)	File Class, i.e. the type of activity for which the file is used.	4 characters
FFF	MIR or NRT	MIR=MIRAS : Nominal product – ~5day delay NRT=Near Real Time - ~1 day delay	3 characters
DDDDDD=abcdef	a = C	From CATDS	1 character
	b = S	Sea product	1 character
	 c = D (dual pol acquisition) or F (full pol acquisition); other letters for more evoluted products : P=pre-qualified products (not distributed), Q=bias corrected products 	Dual or Full pol acquisition mode Pre-qualified or bias corrected products	1 character
d=2 or 3 Level pro		Level product	1 character
	e=A, B, P (not distributed), Q	Product resolution if d=2, e=P corresponds to prequalification products and e=Q to corrected products. if d=3, e=A or e= B correspond to 25 km or 50 km resolution respectively	1 character
	f = A, D or _	for ascending, descending or both	1 character
<instance id=""></instance>	yyyymmddThhmmss_	Validity start time	16 characters
	YYYYMMDDTHHMMSS_	Validity stop time	16 characters
	vvv_	Processor version number	4 characters
	ccc_	file counter	4 characters
	S	Code of the data center ('7' for CPDC)	1 character



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In this document, reduced names are used in order to name the different products (Erreur! Source du renvoi introuvable.).

Table 4: product reduced names

Reduced Name	Content	Frequency
UDP	L2OS user product. Contains estimated SSS from BTs and other flags and descriptors useful for L3 processing. Not distributed.	Daily, A and D separately. NRT products (~1day delay). Operational product (5days delay).
DAP	L2OS product. Contains UDP information + additional information like BT residuals and other retrieved parameters. Not distributed.	Daily, A and D separately. NRT products. Operational product.
L2P	L2OS prequalified products. Contains estimated SSS + SSS classification according to the retrieval conditions or geophysical conditions. Distributed under request.	Daily, A and D separately. NRT products. Operational product.
L2Q	L2OS corrected products. Contains estimated SSS corrected from latitudinal biases and land-sea contamination biases. Distributed.	Daily, A and D separately. NRT products. Operational product.
L3P	Level 3 SSS: average of SSS from uncorrected L2 SSS (from L2P products). Distributed under request.	daily products (average over 10 days, slipping window), A and D merge. MIR products. Operational product.
L3Q	Level 3 SSS : average of SSS from corrected L2 SSS (from L2Q products). Distributed.	daily products (average over 10 days, slipping squared window), A and D merge. MIR and NRT products. Operational product.

1.3.4 Global attributes

CATDS product files are always in netcdf format. Attributes for these files are common to all products and are as follows:

Table 5: Global attribute of CATDS files

Attribute name	Description	Value
title	File title	
netcdf_version_id	NetCDF library version	
creation_date	Creation date	
product_version	Product version	
institution	From what institution the file is built	
source	Name of the processor which built the file	
references	Document reference name	
conventions	Product norm: « CF-1.4 »	« CF-1.4 »
history	Not used	« none »



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ease_projection	Type of projection used to generate the CATDS DGG	
ease_resolution	Resolution used to generate the CATDS DGG (km)	
ease_global	Indicate if the CATDS DGG used for the product is global or not	
ease_origin_lat	Latitude of the origin point	
ease_origin_lon	Longitude of the origin point	



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2 Processing overview

2.1 L1 to L2 processing

This section gives an overview of the whole processing, including ESA DPGS processing which is done upstream of the CATDS processing.

The mission ground segment is organized around a Level 1 processor, which has for main task the reconstruction of SMOS BTs, and an Ocean Salinity Level 2 processor (L2OS) aimed at retrieving Sea Surface Salinity from SMOS data.

CATDS uses DPGS processed (under the ESA responsibility) products up to L1B. DPGS processing begins from Level 0 and ends at Level 2.

The CATDS processing is dedicated to L3 and L4 products, i.e. SMOS SSS gridded fields and derived products. Because the CATDS does not use the same grid and not exactly the same L2OS processor than the ones used by the DPGS, the CATDS processing begins from DPGS L1b products.

2.1.1 L1 processing

SMOS Level 1 processing (RD1) ingests raw SMOS data and produces inputs (Level 1c products) to the level 2 processors. Three out of the numerous aspects of level 1 processing are detailed here because either they contribute to the detailed definition of SMOS BT provided in the Level 1c products or they shape the Level 1c products.

The reconstruction

The L1b reconstruction process consists in obtaining BT Fourier components from visibilities in the antenna plan. At this level, apodization window and interpolation procedure are applied in order to obtain BTs on a regular grid.

The data are sorted in order to obtain for each grid point the set of BTs corresponding to different snapshots, i.e. different incidence angles (L1c data).

From the v700 L1 processing, the so called "gibbs 2" algorithm has been implemented. This algorithm allows decreasing Gibbs effect close to coast (created by the shrp BT gradient between land and sea surfaces) by subtracting approximate land-sea scene in Fourier space before image reconstruction.

One feature of the reconstruction process is the reconstruction grid, which is the ensemble of geographic locations where SMOS BTs are derived. It is worth noting that in SMOS processing, the centre of picture elements (grid points) are not driven by the instrument but are in the hands of the SMOS project team. At CATDS, the reconstruction grid has been chosen to be an EASE2 grid [RD-6].



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The apodization window

The apodization function is applied in the image reconstruction and participates to the definition of the synthetic antenna beam. This way, it shapes the measurement footprints. In the Level 2 SSS processor, the footprint information is provided by the level 1c, i.e. the semi-minor and semi-major axis of the equivalent 3dB ellipse (footprint can be approximated by pseudo ellipsoidal function), to which definition of the apodization function shall be added.

Sorting SMOS data

The CATDS C-PDC generates its own L1c products, starting from L1b, on the EASE grid (which is different from the ISEA grid used in ESA processing made at DPGS). These L1 products are internal to the CATDS and are not distributed to the users.

In the Level 1c product, SMOS data are sorted out in such a way that all BTs reconstructed at the same grid point and auxiliary information are packed together. A single Level 1c product includes SMOS acquisitions during one day (from pole to pole), with a separation between ascending and descending orbits. The ability of SMOS to capture signal variations as a function of viewing conditions is a constraint contributing to a better retrieval of sea surface salinity.

2.1.2 L2OS processing

The L2OS processor takes as input the L1c BTs provided by the L1 processor at antenna level. The main output of the L2OS processor is the retrieved salinity which is computed at grid point level using multi incidence angle observations (see a detailed description in RD2 and the main steps below).

The CATDS L2OS products are provided on the EASE specific grid with a 24 km resolution (at the latitude 30°). These L2OS products are internal to the CATDS and are not distributed to the users.

Forward models

In this processor, a forward model is implemented in order to retrieve the salinity and other geophysical parameters. This is done using a series of physical models (dielectric constant model, roughness model, sun glint contribution, galactic glint, atmospheric effect) which are applied to auxiliary parameters (SST, wind, etc.) and a first guess SSS, in order to compute the BT that should be measured at a specific polarization and geometric configuration. These values are transported to SMOS antenna level and then compared to actually measured BT. These models are the same as in the ESA L2OS processor (RD2).

OTT correction

Because after L1 reconstruction, BT systematic errors depending on the location of BT in the FOV have been detected, an empirical correction, called OTT, is applied on the BT before SSS retrieval. The correction is applied according to the position of the BT in the FOV and differs from one polarization to the other. This correction is derived using orbits accumulated over



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~10 days. The nominal (MIR) product derived at CATDS uses OTT centered in time, hence being delayed by 5 days. In order to fulfil user needs for near-real-time data, a NRT product is also derived using non centered OTTs (similar to ESA L2OS products). Difference between NRT and MIR products is generally small except during periods with rapid OTT changes.

BT filtering

Because of RFI contamination and reconstruction biases, a specific module allows to detect BT outliers which are removed before SSS retrieval.

Iterative scheme

An iterative process (considering all measurements/views of a single grid point obtained in consecutive snapshots) allows minimization of the difference between modelled and measured values, until identifying a retrieved SSS for this grid point. This minimization is done using a Bayesian (Levenberg-Marquardt) algorithm which allows the estimation of one salinity and its error based on multi-incidence BTs (on the order of 150 BTs).

Post processing

A post processing step allows building quality indicators of the retrieved SSS. These indicators are used in input of the prequalification L3OS processor, in order to qualify the SSS as "valid" or "not valid".

2.2 CATDS algorithm steps

The **Erreur! Source du renvoi introuvable.** presents the main different steps of the processing and the associated products:

- SSS classification stored in L2P products (internal product)
- L2 SSS corrected from systematic uncertainties stored in L2Q products (CATDS public dissemination)
- L3 corrected SSS stored in L3Q products (CATDS public dissemination)
- L3 uncorrected SSS stored in L3P products (internal product).

The classification step allows identifying the salinities to be kept or discarded before the averaging step.

The salinity average is done at different resolutions: 25 and/or 50 km and 10 days or month. The 10 day maps (L3Q) are given every day of the year. All the products are in NetCDF format.



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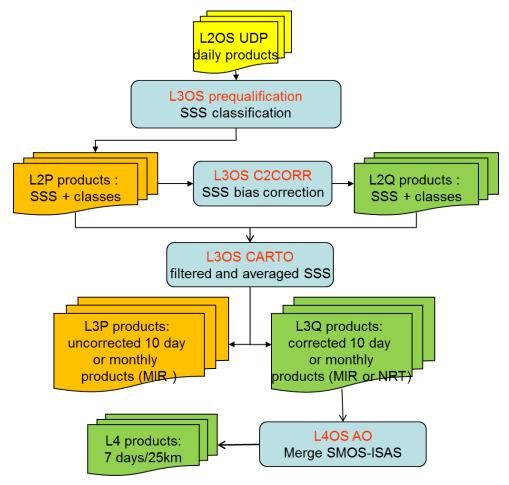


Figure 1: Scheme of the processing from L2OS products to L3OS products. See Table 3 for product name definition. In yellow, products not distributed; in orange, products distributed on request; in green, distributed products.

2.3 CATDS L2 post processing (L2Q)

2.3.1 Algorithms

A prequalification processing allows classifying salinities in about 30 different classes using retrieved SSS and L2OS Flags and descriptors associated to the salinities and external data files (SSS climatology, land-sea mask).

The prequalification products (L2P) are daily products given on a 24 km EASE grid. A correction for seasonal latitudinal bias and coastal bias is applied (see below). The corrected product is called L2Q and contains, as L2P, daily SSS.

The SMOS SSS are affected by biases coming from various unphysical contaminations such as the so-called land contamination and latitudinal biases likely due to the thermal drift of the



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instrument. For retrieved salinity, the impact is non-negligible and can reach more than 1 salinity unit in some regions close to the coasts.

These biases are not easy to characterize because they exhibit very strong spatial gradients and they depend on the coast orientation in the FOV. Moreover, these biases are dependent on the position on the swath.

The zero order bias is the so-called Ocean Target Transformation (OTT) which is a correction applied at BT level. Here, we consider remaining biases on the SSS retrieved from BTs corrected with an OTT. CATDS SSS maps are obtained from an additive correction applied at salinity level. This correction is determined using simultaneously the July 2010-September 2019 period of SMOS observations. Indeed, it is possible to build salinity time series for each grid point depending on the observation conditions (for instance depending on the orbit direction) and check, from a statistical point of view, the consistency of the salinities.

The first step of this empirical approach is to characterize as accurately as possible these biases as a function of the dwell line position. We first characterize the seasonal variation of the latitudinal biases using SSS in the Atlantic and part of the Pacific Ocean further than 800km from the coast. The second step is to correct for biases in the vicinity of land. We have found that these biases vary little in time, and can be characterized according to the grid point geographical location (latitude, longitude) and to its location across track. If we assume that the salinity at a given grid point varies very slowly during a given period, then, the different satellite passes crossing the same pixel during the given period should give consistent salinities. Additionally, assuming that the bias does not vary temporally for a given grid point implies that the relative salinity variation over the whole period should be the same whatever the distance to the center of the track. It is then possible to estimate the relative biases between the various distances across track and to obtain, with a least squares approach, a time series of relative salinity variations obtained from all the passes. Note that these steps estimation do not use any external climatology. It allows checking that all the dwell-lines and orbit types (ascending or descending) give consistent results.

These relative salinity variations are then converted, in a last step, to absolute salinities by adding a single constant determined, in each pixel, using quantiles (quantiles between 50 and 80%, depending on the variability) of SSS climatology over the whole period (ISAS data). This last step, because it uses only one SSS climatology value per grid point as reference totally preserves the SMOS temporal dynamic. The corrected SSS are stored in the so-called L2Q products.

In rainy areas, the SSS retrieved from L-Band radiometers are much lower than the ones measured at a few meters' depths or in the non-rainy surrounding regions. Since most applications are using bulk salinities, it is important to evaluate this effect. At first order, it is possible to relate the satellite SSS decrease, ΔS , observed just after a rain event to the instantaneous rain rate, RR provided by IMERG—like products. The instantaneous effect is typically ~-1.5 pss at 10 mm hr-1 (RD-3, RD-9). Even when it is averaged in time and space, the signature of this effect remains larger than -0.1 psu in rainy regions like ITCZ (Supply, PhD



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thesis, 2020). Removing this effect from level 2 SMOS SSS, leads to much decreased systematic differences when compared to Argo derived salinities.

2.3.2 L2Q product name

See section 1.3.3 for general information.

Table 6: List of products built by the bias correction L3-OS processor

Name	Description	Туре
MIR_CSD2QA	This product contains corrected salinity (ascending orbits, dual pol)	NETCDF
MIR_CSD2QD	This product contains corrected salinity (descending orbits, dual pol)	
MIR_CSF2QA	This product contains corrected salinity (ascending orbits, full pol)	
MIR_CSF2QD	This product contains corrected salinity (descending orbits, full pol)	

2.3.3 L2Q product content

The MIR_CSD2QA, MIR_CSD2QD, MIR_CSF2QA MIR_CSF2QD products have the same data format. They contain information about the L2 salinity corrected from coastal and latitudinal biases.

The grid points on which are given the results of corrected SSS are the same as those of the L2OS UDP product. Part of the L2 and L2P product is copied in the corrected SSS product: salinities and salinity errors, X_Swath, Mean_Acq_Time and L2P Classes. For the classes, we have added one bit (bit number 30) which gives an out-of-range SSS qualification after correction. Another class (bit number 31) contains the SSS mask to remove high WS regions.

The format of these products is the NetCDF format.

The data are given on an EASE grid which is defined in the product ((nlat,nlon) dimensions).

Table 7: MIR_CSD2Q and MIR_CSF2Q content

	Parameter	Description	Туре	Unit
1	Grid_point_ID(nlat,nlon)	Grid number ID	int	
2	lat(nlat)	Grid point latitude	float	degree
3	lon(nlon)	Grid point longitude	float	degree
4	Sea_Surface_Salinity_Model1_Value(nlat,nlon)	SSS estimator (corrected from latitudinal bias, SST bias and land-sea contamination bias)	short	psu



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5	Sea_Surface_Salinity_Model2_Value(nlat,nlon)	Bulk SSS estimator (corrected from latitudinal bias, SST bias, land-sea contamination bias and rain effect)	short	psu
6	Sea_Surface_Salinity_Model3_Value(nlat,nlon)	Acard	short	psu
7	Sea_Surface_Salinity_Model1_Error(nlat,nlon)	SSS error from model 1	short	psu
8	Sea_Surface_Salinity_Model1_Bias(nlat,nlon)	SSS bias applied on L2OS SSS estimator from model 1	short	psu
9	Sea_Surface_Salinity_Model2_Error(nlat,nlon)	Not used	short	psu
10	Sea_Surface_Salinity_Model2_Bias(nlat,nlon)	Not used	short	psu
11	Sea_Surface_Salinity_Model3_Error(nlat,nlon)	Not used	short	psu
12	Sea_Surface_Salinity_Model3_Bias(nlat,nlon)	dAcard (Acardsmos- Acardmodel)	short	psu
13	X_Swath(nlat,nlon)	Distance from grid node to the satellite ground track	short	km
14	Mean_Acq_Time(nlat,nlon)	Mean acquisition time	float	dd
15	Sea_Surface_Salinity_Model1_Classes(nlat,nlon)	Classification of SSS model 1 (see A1.1)	Int (31 bits used)	
16	Sea_Surface_Salinity_Model2_Classes(nlat,nlon)	Not used	Int (31 bits used)	
17	Sea_Surface_Salinity_Model3_Classes(nlat,nlon)	Not used	Int (31 bits used)	

2.3.4 Algorithm evolutions of systematic SSS corrections

The algorithms for correcting land-sea contamination and seasonal-latitudinal systematic errors (described in previous section) have evolved following research work performed in the frame of the CATDS expertise center (RD3 and RD7). Evolutions of the corrections are summarized in Table 8. With respect to RD3, the CPDC v700 employs a more elaborated bias correction method, aligned with CATDS CEC V5.



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Table 8: Summary of SMOS CATDS CEC LOCEAN-ACRI-st evolutions

CEC Versions	CPDC Versions	Main evolutions	Main improvements	Reference
	RE07/v335	=V5 (but applied to L1 and L2OS v7) + rain rate correction	SSSbulk closer to bulk in situ SSS. Improved temporal stability. Decreased RFI contamination	
V5 (2020)		=V4+ refined absolute correction	Decrease of biases in very variable and noisy regions (high latitudes, RFI contaminated areas)	Boutin et al., IGARSS 2021
V4 (2019)		=V3 + wind speed limited to 16m/s, Acard filtering, update of SST correction in cold waters, refined absolute correction	Decrease of mean bias over the open ocean, improved ice filtering, improved SSS at high latitudes (especially in the Southern Ocean)	(Thouvenin- Masson,2020 10.5194/egusphere- egu2020-7545)
V3 (2018)	RE06/V317	= V2 + SSS natural variability varying seasonally; latitudinal bias correction applied everywhere; SSS correction at low SST; improved absolute correction	=V2 + improved adjustment of land-sea biases close to coast; adjustment of high latitudinal biases	
V2 (2017)		= V1 + SSS natural variability varying spatially; no latitudinal bias correction outside 47S-47N	= V1 + improved land- sea contamination in very dynamic areas	(Boutin et al., 2018)
V1 (2016)		= V0 + seasonal latitudinal correction (same SSS natural variability everywhere)	= V0+ Reduced latitudinal biases	
V0 (2015)			Reduced land-sea contamination	(Kolodziejczyk et al., 2016)

In CPDC RE07/v335, the absolute adjustment of the long term mean biases has been estimated from the 2012-2018 median (or from an upper quantile in very variable regions) of SMOS SSS relative to the one obtained with ISAS delayed time SSS (https://doi.org/10.17882/52367 up to 2015 and http://marine.copernicus.eu/services-portfolio/access-to-products/?option=com_csw&view=details&product_id=INSITU_GLO_TS_OA_REP_OBSERVA TIONS_013_002_b later on).



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2.4 Salinity averages (L3P and L3Q 'simple average' products)

2.4.1 Algorithms

This averaging is done by using uncorrected SSS (L2P) for L3P generation and corrected SSS (L2Q) for L3Q generation.

Before salinity averaging, a filtering is performed as follows:

For L3P (uncorrected SSS), a selection of the salinities with the following criteria (so far, only five classes are used by the L3OS processor) is done:

- Class 1: valid salinities: only these salinities are kept for the averaging. The conditions of belonging to this class are described below.
- class 29: salinities which belong to the edge of the swath (further than 400 km from the ground track). These salinities are discarded before the averaging because they are very noisy.
- class 5a: salinities associated to large wind speed (WS > 12 m/s). These salinities are removed before the averaging because roughness model is inaccurate for high wind speed.
- class 5b: salinities associated to low wind speed (WS < 3 m/s). These salinities are removed before the averaging because errors on ECMWF WS are large at low WS, relationship between roughness and WS at low WS is badly known and the sensitivity of BT to wind speed increases at low WS (increasing the errors on retrieved SSS).
- class of salinities associated to high sea state. These salinities are removed before the averaging because roughness model is inaccurate for swell.

For L3Q (corrected SSS), a selection of the salinities with the following criteria is done:

- class 29: salinities which belong to the edge of the swath (further than 400 km from the ground track). These salinities are discarded before the averaging because they are very noisy.
- class 30: only salinities pertaining to a min/max interval according to the GP is kept.
- class 31: salinities associated to WS between 0m/s and 16m/s are kept.
- In this case (corrected SSS), the class 1 (SSS validity class) is not used because we consider that the applied correction is able to make valid a data that was not valid before correction.
- SSS is corrected from rain effects in order to provide a bulk SSS.

The L2OS SSS values which are used for averaging belongs to the interval [5 40 psu]. Salinities outside this interval are excluded (same SSS interval applied whatever the latitude is).

The averaging algorithm is the same for L3P and L3Q SSS:



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- 1. For each considered grid point, a selection of the spatio-temporal neighbour salinities is done: this selection is done using a distance criteria expressed in km (25 or 50) and an interval time (month or decade). The time interval is given in the product name (validity start time and validity stop time, see section 1.3.3). The spatial resolution is given in the product header and/or directly in the product name (see section 1.3.3).
- 2. From the neighbour salinities and for each pixel, the SSS mean, \bar{S} , is computed using weighted average algorithm:

$$\bar{S} = \frac{\frac{S_1}{\text{sigSSS}_1^2} + \dots + \frac{S_n}{\text{sigSSS}_n^2}}{\frac{1}{\text{sigSSS}_1^2} + \dots + \frac{1}{\text{sigSSS}_n^2}}$$

where S_1 , S_2 , ... S_n are the selected salinities (see 1. and 2.) and ${\rm sigSSS}_1$, ${\rm sigSSS}_2$, ... ${\rm sigSSS}_n$, the associated errors. These errors are obtained from L2OS least square iterative processing. They come from the propagation of the BT errors and the auxiliary data errors (like errors on wind speed or sea surface temperature which are used in the L2OS inversion scheme).

Note that the previous equation gives the better estimator of the mean salinity in the least square sense.

3. For each grid point, the error on the mean salinity, SSS_Standard_Deviation, is computed as follows:

$$SSS_error_mean = \sqrt{\frac{1}{\frac{1}{sigSSS_1^2} + ... + \frac{1}{sigSSS_n^2}}}$$

4. For each grid point the empirical standard deviation, Sss_Rms_Mean, is computed as follows:

SSS_standard_deviation =
$$\sqrt{\frac{\sum_{i=1}^{n} (\bar{S} - S_i)^2}{n-1}}$$

with \bar{S} computed in 3/ and S_i the selected salinities.

2.4.2 L3Q product names.

See section 1.3.3 for general information.



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Name	Description	Туре
(MIR,NRT)_CSQ3(A,B)_	Average corrected SSS map derived from L2Q products, ascending + descending orbits, dual or full polarization for (A=25km or B=50km) resolution	

Note that "full polarization" products are in majority. Dual polarization products are only available for few weeks at the beginning of the mission.

2.4.3 L3Q product content

These products have a matrix structure with two dimensions (nlat, nlon) which depend on the spatial resolution. The definition of these products is as follows:

Table 10: MIR_CSD3 and MIR_CSF3 content

	Parameter	Description	Туре	Unit
1	Mean_Sea_Surface_Salinity_1(nlat,nlon)	Bulk mean sea salinity (corrected from rain)	short	psu
2	N_Used_Meas_1(nlat,nlon)	Number of measures used to compute the mean of bulk salinity	short	
3	N_Rejected_Meas_1(nlat,nlon)	Number of rejected measures before bulk salinity computation	short	
4	Class_Majority_1(nlat,nlon)	Majority class among used input salinity classes	short	
5	SSS_standard_deviation_1(nlat,nlon)	Sea salinity std of bulk salinity	short	psu
6	SSS_error_mean_1(nlat,nlon)	Sea salinity mean error of bulk salinity	ushort	psu
7	lat(nlat)	Grid point latitude	Float	degree
8	Lon(nlon)	Grid point longitude	Float	degree
9	Mean_Sea_Surface_Salinity_2(nlat,nlon)	Mean sea surface salinity (not corrected from rain)	short	psu
10	N_Used_Meas_2(nlat,nlon)	Number of measures used to compute the mean SSS	short	
11	N_Rejected_Meas_2(nlat,nlon)	Number of rejected measures before mean SSS computation	short	
12	Class_Majority_2(nlat,nlon)	Majority class among used input salinity classes	short	
13	SSS_standard_deviation_2(nlat,nlon)	Sea surface salinity std	short	psu
14	SSS_error_mean_2(nlat,nlon)	Sea surface salinity mean error	ushort	psu



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2.5 L4 products

2.5.1 Algorithms

Full details on the method are described in (RD-10).

Optimal interpolation (OI) of satellite L3 SSS data is performed following (RD-5), presented here in the formalism of (RD-11). The interpolated SSS fields consist of the sum of a reference field (or first guess) and an anomaly field obtained by linear combination of satellite SSS data as follows:

$$x^a = x^f + K^{OI}(y^o - y^f)$$
 (1)

where:

$$K^{\text{OI}} = C_{\text{ao}} (C_{\text{oo}} + R)^{-1}$$
 (2)

where x^a are the vectors of the estimates at the grid point and y^o is the vector of observation, respectively; and x^f and y^f are the vectors of the reference field values at the grid and observation points, respectively. K^{OI} is the weight's matrix constructed from co-variance and error matrix. C_{ao} is the covariance matrix between the analyzed fields at the grid and observation points; C_{oo} is the covariance matrix between the observations, and R is the observation error matrix.

The SMOS L3Q debias are mapped on an EASE horizontal grid with a resolution of 25km. The optimal analysis is calculated on anomalies relative to the reference field used as a first guess i.e. ISAS. The analysis modifies the first guess according to observations a priori statistics and chosen scales and covariance model. Thus, in poorly sampled areas or if the observational errors are relatively large, the solution may remain close to the reference field.

The covariance matrices C_{oo} and C_{ao} are constructed using the same covariance model C(dr,dt), using a Gaussian function of time and space :

$$C_{i,j}(dr,dt) = \sigma_{i,j}e^{-\left(\frac{dr_{i,j}^2}{2L^2} + \frac{dr_{i,j}^2}{2T^2}\right)}$$
 (3)

where dr and dt are the spatial and temporal distances, and L and T are the associated decorrelation scales. The weight given at each scale of variability corresponds to the variance. The variance field, $\sigma_{i,j}$, has been computed from filtered historical SMOS data (Fig. 3a; Boutin et al., 2018). The error matrix for SMOS L3 data is derived from the model error provided by the L2 SMOS inversion and provided along with the L3 fields. Two Optimal Interpolations are used: a first to estimate the bias, a second to re-project and filter out the corrected data onto the EASE grid.



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The first step consists in a first OI using Equation 1. SMOS L3 SSS data are mapped over a period of 7 days separately for each satellite using a 'large' correlation scale comparable to that used in ISAS. This large scale has been estimated to be on average 500 km in the Tropic and Subtropics. This correlation scale has been chosen empirically since the sampling strategy and the scale chosen for ISAS resolves on average a 500 km horizontal feature. This scale is introduced into the Gaussian correlation model (Equation 3) and the first OI is perfomed using the ISAS monthly fields as first guess. Smoothed seasonal and large-scale corrections are then deduced from the comparison of the SMOS smoothed fields with ISAS SSS monthly fields interpolated for the corresponding analyzed weeks. Note that, by construction the ISAS SSS fields are relaxed to climatology in regions where no in situ data are available (especially at high latitude). It is likely that in these regions the large-scale bias correction is less accurate.

In the tropical regions, SMOS L3 large scale and seasonal systematic errors are reduced to values lower than 0.3 pss locally. This is on the order of the expected uncertainty on SMOS weekly gridded data. Thus, seasonal and large-scale corrections are relaxed within the tropics using a Gaussian function centered at the equator:

$$\alpha(y) = 1 - e^{\frac{-y^2}{l^2}}$$
 (4)

where the length scale I= 30°. This relaxation allows to keep the information content in the data of the low salinity plume of large tropical river runoff as well as the Tropical Instability Wave signature in SSS found in SMOS products. The large-scale correction is also relaxed in the Gulf of Mexico and off Rio de la Plata river mouth regions.

Finally, the corrected SMOS L3 SSS are mapped using an interpolation scheme by introducing into the Gaussian function (Equation 3) spatial and temporal correlation scales corresponding to the synoptic scales resolved by SMOS, i.e. 7 days and 25 km.

2.5.2 L4 product names

See section 1.3.3 for general information.

Table 11: List of products built by the L4 OI processor (optimal interpolation)

Name	Description	Туре
SMOS OI	Optimal Interpolated SSS map derived from L3Q SMOS SSS 9 days debias products and using a large scale correction from ISAS NRT near surface salinity SSS product.	



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2.5.3 L4 product content

These products have a matrix structure with three dimensions (ntime=1,nlat=584, nlon=1388) corresponding to the EASE grid. The definition of these products is as follows:

Table 12: L4 OI content

	Parameter	Description	Туре	Unit
1	SSS	Corrected Sea Surface Salinity	Float	pss-78
2	sss_isas	Reference SSS from ISAS in situ gridded product	Float	pss-78
3	sss_corr_smos	Sea Surface Salinity Correction for SMOS	Float	pss-78
8	sst	Sea Surface Temperature	Float	Degree C
9	spiciness0	Spiciness at p = 0 dbar (75-term equation) computed from TEOS-10 MATLAB Toolbox	Float	Kg m ⁻³
10	SA	Absolute Salinity from Practical Salinity computed from TEOS-10 MATLAB Toolbox	Float	g kg ⁻³
11	СТ	Conservative Temperature from in-situ temperature computed from TEOS-10 MATLAB Toolbox	Float	Degree C
12	rho	In-situ density computed from TEOS-10 MATLAB Toolbox	Float	Kg m ⁻³
13	Alpha	Thermal expansion coefficient with respect to Conservative Temperature computed from TEOS-10 MATLAB Toolbox	Float	K ⁻¹
14	beta	Haline contraction coefficient at constant Conservative Temperature computed from TEOS-10 MATLAB Toolbox	Float	none
15	ice_mask	Ice Mask. Sea Ice Fraction (>=15 %) from multi-sensor L4 foundation SST product from Remote Sensing Systems	Float	none
16	lat	Latitude grid points. EASE grid	Float	degree
17	lon	Longitude grid points.EASE grid.	Float	degree
18	time	Time in days .gregorian (MATLAB format)	Float	day



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Annex A

The Annex describes intermediate products not officially distributed.

A.1 SMOS SSS L2P products

A.1.1 Class definition

As mentioned in section 2.2, salinities are classified before averaging. At this stage, the SSS is not modified and directly copied in the prequalification product.

The prequalification step allows classifying the salinities into 31 different classes using L2OS flags, external information and self-consistency tests.

Each SSS, associated to a ground grid point, is qualified by L2OS flags which are:

- Fg_ctrl_many_outliers: raised if a lot of BTs used for SSS retrieval have been identified as outliers
- Fg ctrl sunglint : raised if the grid point is affected by sun glint.
- Fg_ctrl_moonglint: raised if the grid point is affected by moon glint.
- Fg ctrl gal noise: raised if the grid point is affected by large galactic noise reflection.
- Fg sc TEC gradient: raised if BTs are affected by large TEC variations along the dwell line.
- Fg sc in clim ice: raised if grid point is contaminated by ice (from climatology)
- Fg sc ice: raised if grid point is contaminated by ice (from SST and BT values)
- Fg sc suspect ice: raised if grid point is contaminated by ice
- Fg_sc_rain: raised if grid point is contaminated by rain
- Fg sc Land Sea coast1/2 : raised if grid point is contaminated by coast
- Fg ctrl num meas low: raised if number of BT available for retrieval are too low
- Fg_ctrl sigma: raised if SSS a posteriori theoretical error is larger to 5 psu
- Fg ctrl chi2: raised if chi2 after convergence is larger than 1.35
- Fg_ctrl_chi2_P: raised if poor fit quality (chi2_P > 0.95 or chi2_P < 0.05
- Fg_ctrl_reach_maxiter: raised if iterative algorithm has reached the max number of iteration
- Fg ctrl marq: raised if Marquardt amplifier reaches a threshold
- Fg_ctrl_range : raised if SSS > 50 or < 10 psu
- Fg_oor_LUT_XXX_YYY: raised if forward model used for SSS retrieval is out of range of one LUT.



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If one or more of the previous flags is raised, the associated salinity is considered as invalid (it does not belong to the class of valid salinities) and is not used for averaging.

The following table presents the 31 classes available in the L2Q products (for advanced users). In L2P products, only classes 1 to 29 are available. The "green" classes are available. The "white" classes are specified and implemented but not computed.

Class	Flags used	Description	Thresholds	Bi
1	Fg_ctrl_X, Fg_sc_X, Fg_oor_X (UDP L2OS)	Valid salinities	No L3 thresholds (only flags from L2).	1
2a	Fg_grad_space_SST Fg_grad_space_SSS	SSS and SST not well mixed horizontally	(Tg_grad_space_SSS, Tg_grad_space_SST) Apply a threshold on the modulus of the spatial gradient of the SSS and SST.	2
2b	Fg_grad_space_SST Fg_grad_space_SSS	SSS not well mixed horizontally and SST well mixed horizontally	(Tg_grad_space_SSS, Tg_grad_space_SST) Apply a threshold on the modulus of the spatial gradient of the SSS and SST.	3
3	Fg_SSS_distrib_boiteX_seuilY	SSS far from climatology.	(Tg_SSS_distrib_boiteX_statY) Depends on the averaging box. Flag is raised if significant difference observed at least in one box.	4
4a	Fg_SSS_nsig_scale1	SSS not self-consistent with its neighbours (in space and in time)	(Tg_SSS_nsig2) Self-consistency indexes from box n°1.	5
4b	Fg_SSS_nsig_scale2	SSS not self-consistent with its neighbours (in space and in time)	(Tg_SSS_nsig2) Self-consistency indexes from box n°2.	6
4c	Fg_SSS_nsig_scale3	SSS not self-consistent with its neighbours (in space and in time)	(Tg_SSS_nsig2) Self-consistency indexes from box n°3.	7
5a	Fg_sc_high_wind (UDP L2OS)	SSS associated with high wind speed (instantaneous WS)	No L3 threshold WS > 12 m/s	8



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5b	Fg_low_wind (UDP L2OS)	SSS associated with high low speed (instantaneous WS)	No L3 threshold WS < 3 m/s.	9
5c	Fg_high_wind_48	SSS associated with high wind speed (average WS over 48h00)	(Tg_mean_WShigh_48)	10
5d	Fg_low_wind_48	SSS associated with high low speed (average WS over 48h00)	(Tg_mean_WSlow_48)	11
5e	Fg_sc_high_SST (UDP L2OS)	SSS measured with high SST	No L3 threshold SST > 28°C	12
5f	Fg_sc_low_SST (UDP L2OS)	SSS measured with low SST	No L3 threshold SST < 10°C	13
5g	Fg_high_SST_48	SSS measured with high SST (average over 48 H)	Tg_mean_SSThigh_48 Average SST over 48h > 28°C	14
5h	Fg_low_SST_48	SSS measured with low SST (average over 48 H)	Tg_mean_SSTlow_48 Average SST over 48h < 10°C	15
5i	Fg_SSS_distrib_boite1_seuil3	SSS climato with high variability	Tg_SSS_distrib_boite1_stat3 SSS variability > threshold for the box 1	16
5j	Fg_grad_time_WS_48[SSS from extreme geophysical conditions	(Tg_grad_time_WS_48) High WS time gradient	17
5k	Fg_grad_time_SSTC_48	SSS from extreme geophysical conditions	(Tg_grad_time_SSTC) High SST time gradient	18
51	Fg_grad_time_partot	SSS from extreme geophysical conditions	(Tg_Param1_prior_M1_gradti me) High geophysical parameter time gradient (other than SSS and SST)	19
5m	Fg_sc_low_wave_height1 (UDP L2OS)	« swell-dominated » SSS	No L3 threshold	20
5n	Fg_sc_low_wave_height2 (UDP L2OS)	« mixed sea » SSS	No L3 threshold	21
50	Fg_sc_low_wave_height3 (UDP L2OS)	« young sea » SSS	No L3 threshold	22



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5p	Fg_sc_moderate_wave_heig ht4 (UDP L2OS)	« older seas/mix » SSS	No L3 threshold	23
5q	Fg_sc_moderate_wave_heig ht5 (UDP L2OS)	« young sea (steep) » SSS	No L3 threshold	24
5r	Fg_sc_extreme_wave_height 6 (UDP L2OS)	« high sea » SSS	No L3 threshold	25
6	Fg_param_retr	Problem with retrieved parameter other than the SSS (SST, WS, TEC)	(Tg_ParamX_prior_MY_retr) Estimated parameter too far from the prior	26
7	Fg_low_wind_48 (L3) Fg_low_wind (UDP L2OS)	SSS not well mixed vertically	(Tg_mean_WSlow_48) instantenous WS < 4 m/s and WS average over 48h < 4 m/s	27
8	Fg_ctrl_X, Fg_sc_X, Fg_oor_X	outlier SSS	Complementary of Class 1	28
9	Fg_sc_X,	outlier SSS SSS from the edge of the swath	Complementary of Class 1 (Tg_border_swath) Threshold to be applied on x_swath	28
	Fg_sc_X, Fg_oor_X		(Tg_border_swath) Threshold to be applied on	

A.1.2 L2P product names.

See section 1.3.3 for general information.

Table 13: List of products built by the prequalification L3-OS processor

Name	Description	Туре
MIR_CSD2PA	This product contains prequalified salinity (ascending orbits, dual pol)	NETCDF
MIR_CSD2PD	This product contains prequalified salinity (descending orbits, dual pol)	
MIR_CSF2PA	This product contains prequalified salinity (ascending orbits, full pol)	
MIR_CSF2PD	This product contains prequalified salinity (descending orbits, full pol)	



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A.1.3 L2P product content

The MIR_CSD2PA, MIR_CSD2PD, MIR_CSF2PA MIR_CSF2PD products have the same data format. They contain information about the prequalification of the L2 salinity. The grid points on which are given the results of pre-qualification are the same of those of the L2OS UDP product. Part of the L2 product is copied in the prequalification product: salinities and salinity errors, X_Swath and Mean_Acq_Time.

The format of these products is the NetCDF format. The data are given on an EASE grid which is defined in the product ((nlat,nlon) dimensions).

Table 14: MIR_CSD2P and MIR_CSF2P content

	Parameter	Description	Type	Unit	
1	Grid_point_ID(nlat,nlon)	Grid number ID	int		
2	lat(nlat)	Grid point latitude	float	degree	
3	lon(nlon)	Grid point longitude	float	degree	
4	Sea_Surface_Salinity_Model1_Value(nlat,nlon)	SSS estimator from model 1	short	psu	
5	Sea_Surface_Salinity_Model2_Value(nlat,nlon)	SSS estimator from model 2 (not relevant)	short	psu	
6	Sea_Surface_Salinity_Model3_Value(nlat,nlon)	SSS estimator from model 3 (not relevant)	short	psu	
7	Sea_Surface_Salinity_Model1_Error(nlat,nlon)	SSS error from model 1	short	psu	
8	Sea_Surface_Salinity_Model1_Bias(nlat,nlon)	SSS bias (external information) (not relevant)	short	psu	
9	Sea_Surface_Salinity_Model2_Error(nlat,nlon)	SSS error from model 2 (not relevant)	short	psu	
10	Sea_Surface_Salinity_Model2_Bias(nlat,nlon)	SSS bias (external information) (not relevant	short	psu	
11	Sea_Surface_Salinity_Model3_Error(nlat,nlon)	SSS error from model 3 (not relevant)	short	psu	
12	Sea_Surface_Salinity_Model3_Bias(nlat,nlon)	SSS bias (external information) (not relevant	short	psu	
13	X_Swath(nlat,nlon)	Distance from grid node to the satellite ground track	short	km	
14	Mean_Acq_Time(nlat,nlon)	Mean acquisition time	float	dd	
15	Sea_Surface_Salinity_Model1_Classes(nlat,nlon)	Classification of SSS model 1. 29 classes (only 5 used for averaging)	Int (29 bits used)		



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16	Sea_Surface_Salinity_Model2_Classes(nlat,nlon)	Classification of SSS model 2. 29 classes (only 5 used for averaging) (not relevant)	Int (29 bits used)	
17	Sea_Surface_Salinity_Model3_Classes(nlat,nlon)	Classification of SSS model 3. 29 classes (only 5 used for averaging) (not relevant)	Int (29 bits used)	

A.2 SMOS SSS L3P products

A.1.1 L3P product names.

L3P contains average SSS from L2 SSS not corrected from biases (see section 2.4.1).

See section 1.3.3 for general information.

Table 15: List of products built by the L3-OS CARTO processor (averaging salinities)

Name	Description	Туре
(MIR,NRT)_CSD3(A,B)_	Average SSS map derived from L2P products, ascending + descending orbits, dual polarization for (A=25km or B=50km) resolution	
(MIR,NRT)_CSF3(A,B)_	Average SSS map derived from L2P products, ascending + descending orbits, full polarization for (A=25km or B=50km) resolution	

Note that "full polarization" products are in majority. Dual polarization products are only available for few weeks at the beginning of the mission.

A.1.4 L3P product content

These products have a matrix structure with two dimensions (nlat, nlon) which depend on the spatial resolution. The definition of these products is as follows:

Table 16: MIR_CSD3 and MIR_CSF3 content

	Parameter	Description	Туре	Unit
1	Mean_Sea_Surface_Salinity(nlat,nlon)	Mean sea surface salinity	short	psu
2	N_Used_Meas(nlat,nlon)	Number of measures used to compute the mean	short	
3	N_Rejected_Meas(nlat,nlon)	Number of rejected measures	short	
4	Class_Majority(nlat,nlon)	Majority class among used input salinity classes	short	
5	SSS_standard_deviation(nlat,nlon)	Sea surface salinity std	short	psu
6	SSS_error_mean(nlat,nlon)	Sea surface salinity mean error	ushort	
7	lat(nlat)	Grid point latitude	Float	degree



Ref.: Erreur ! Nom de propriété de document inconnu.

Version: 4.Erreur! Nom de propriété de document

8 Lon(nlon) Grid point longitude Float degree