Copernicus Marine Service

QUALITY INFORMATION DOCUMENT

Multi Observation Global Ocean Daily SMOS Sea Surface Salinity Product

MULTIOBS_GLO_PHY_SSS_L3_MYNRT_015_014

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Contributors: Ana Parracho, Jacqueline Boutin, Stéphane Tarot

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I EXECUTIVE SUMMARY

I.1 Products covered by this document

This document covers the external product **MULTIOBS_GLO_PHY_SSS_L3_MYNRT_015_014**, which is the Sea Surface Salinity (SSS) from Soil Moisture Ocean Salinity (SMOS) Level-3 daily data (ascending and descending passes separately), corrected for the seasonal latitudinal bias and land-sea contamination, with and without rain freshening correction. The product is on a grid at 25 km spatial resolution and daily temporal resolution. Data in each pixel correspond to spatially integrated SSS over the native resolution of SMOS observations, which is around 50 km on average over all geometries of acquisitions. The product runs for a period from 2010-01-10 to present (for more detail see section on General Description and the PUM). It is obtained from the “Centre Aval de Traitement des Données SMOS” (CATDS), operated for the “Centre National d’Etudes Spatiales” (CNES, France) by IFREMER (Brest, France).

This is the base product used to build the weekly input fields that are used to create the MULTIOBS_GLO_PHY_SSS_L3_MYNRT_015_015 product.

I.2 Summary of the results

The quality of the SSS dataset MULTIOBS_GLO_PHY_SSS_L3_MYNRT_015_014 for the period between 2010 and 2021 has been assessed by comparison with independent Argo in situ measurements. The results are summarized below.

Sea surface salinity: The mean difference with respect to the Argo near surface salinity is slightly negative and equal to -0.17 globally and very close to zero (0.02) when considering only data > 800 km offshore (where the rain rate is zero, the mean daily wind ranges from 3 to 12 m/s and the SST is over 5°C). The STD of the difference is equal to 2.10 when considering the full data set, and 0.84 when considering only data far from the coast. When we remove the effect of outliers by considering the median and robust standard deviation results are improved. The median difference is very close to zero and the robust standard deviation is 0.81 for the global data and 0.72 at >800 km.

The monthly time series of the median difference is mostly between -0.2 and 0.2 and the time series of the robust standard deviation is around 1. Overall biases are relatively low in regions of moderate SST (between -0.2 and 0.2 within 45°N and 45°S) and are improved by the application of the quality flag and the rain correction. This is also observed for the standard deviation, which is mostly under 1, except at higher latitudes and close to the coast.

Sea surface salinity error: Uncertainties provided in the product are consistent with observed differences between SMOS SSS and in situ SSS. They can be used to filter out very noisy data and to weigh L2Q SSS when computing SSS means. Weighted averages of L2Q SSS are less noisy than instantaneous SSS. For instance, STD difference, RMS difference between L2Q SSS averaged over 10 days and Argo SSS are improved by a factor 3 to 4.

I.3 Estimated Accuracy Numbers

Table 1: Estimated accuracy numbers (with regards to Argo, retaining only good quality flags and rain corrected data)

SEA SURFACE SALINITY

	Global	>800 km offshore, moderate wind speed and not very cold conditions*
MEDIAN BIAS	0.00	0.02
ROBUST STANDARD DEVIATION **	0.81	0.72
MEAN BIAS	-0.17	0.02
STANDARD DEVIATION	2.10	0.84

* and rain rate equal to zero, mean daily wind range from 3 to 12 m/s and SST over 5°C

** Robust standard deviation, STD*, filters out outliers (STD*(x) is defined as the median(abs(x -median (x)))/0.67; STD*(x) is equal to STD(x) in case of a Gaussian distribution of x). Notice that representativity errors between punctual Argo measurements and spatially integrated SMOS measurements are not taken into account and can generate some outliers, especially in very variable near coast areas, which are filtered out in median and STD* estimates.

II PRODUCTION SYSTEM DESCRIPTION

II.1 General Description

Table 2: MULTIOBS_GLO_PHY_SSS_L3_MYNRT_015_014 product specification

Production system's name	MULTIOBS_GLO_PHY_SSS_L3_MYNRT_015_014
Production center's name	MULTIOBS-CATDS-BREST-FR (CATDS-CPDC at Ifremer, Brest, France)
Geographical coverage	Global: 83.517°S-83.517°N, 179.87°W-179.87°E
Variables	**Sea_Surface_Salinity**: Practical sea surface salinity **Sea_Surface_Salinity_Rain_Corrected**: Practical sea surface salinity corrected from rain instantaneous freshening effect (equivalent to a bulk salinity in rainy conditions) **Sea_Surface_Salinity_Error:** Random uncertainty on sea surface salinity **Sea_Surface_Salinity_Rain_Corrected_Error:** Random uncertainty on sea surface salinity corrected from rain effect **Sea_Surface_Salinity_QC:** quality flag on the sea surface salinity
Product Type	Satellite observation
Available time series	2010/01/12 – ongoing (D-1)
Temporal resolution	Daily
Target delivery time	**Detailed in the document: CMEMS-MOB-PUM-015-014** There are 3 steps of processing for each day of observation (D): • 1 – operational processing at D+1 (uncentered OTT calibration) • 2 – operational processing at D+5 (centered OTT calibration) • 3 – reprocessing
Delivery mechanism	CMEMS Information Service
Horizontal resolution	~25 km at 30° latitude on the EASE 2.0 cylindrical grid
Number of vertical levels	N/A (sea surface data)
Format	NetCDF 4.0 CF1.8

II.2 Processing Overview

SMOS Level 1 processing ingests raw SMOS data and produces Level 1c (L1c) products. The L2OS processor then takes the L1c brightness temperatures (BTs) as input. 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 measured BT.

Since after L1 reconstruction, BT systematic errors have been detected, an empirical correction (called OTT) is applied on the BT before SSS retrieval. This correction is derived using orbits accumulated over ~10 days in the south-east Pacific Ocean and is applied according to the position of the BT in the FOV (field of view). Due to RFI (radio frequency interference) contamination and reconstruction biases, a specific module allows to detect BT outliers which are removed before SSS retrieval. Finally, a retrieved SSS at a grid point is identified following an iterative process that allows minimization of the difference between modelled and measured values. 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 (order of 150 BTs).

A correction for seasonal latitudinal bias and land-sea contamination (Boutin et al., 2018; Kolodziejczyk et al., 2016) is then applied on the retrieved SSS. The corrected product is called L2Q and contains daily SSS on a 25 km EASE grid. A quality flag is provided that retains only salinities within +/-400 km from the center of the track, for wind speed less than 16 m/s and within a reasonable range. **We recommend to take this flag into account when using this product.**

II.2.1 Correction of latitudinal bias and land-sea contamination

The first step of this correction is to characterize as accurately as possible the biases as a function of the across swath location (distance to the center of the track). We first characterize the seasonal variation of the latitudinal biases using SSS in the Atlantic and part of the Pacific Ocean further than 800 km 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 slowly during a given period, then, the different satellite passes crossing the same pixel during the given period should give consistent salinities. 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 estimates do not use any external climatology, therefore, it allows checking that all the across swath locations and orbit types (ascending or descending) give consistent results.

In a last step, these relative salinity variations are converted to absolute salinities, by adding a single constant computed for each pixel, using quantiles (quantiles between 50 and 80%, depending on the variability) of SSS climatology over the whole period (ISAS data). Because it uses only one SSS climatology value per grid point as reference, the correction for latitudinal bias and land-sea contamination preserves the whole SMOS temporal dynamic independently of any information coming from in situ information, it is only the absolute value of the whole time series that is adjusted considering an external information.

II.2.2 Rain correction

In rainy conditions, the SSS retrieved from L-Band radiometers are much lower than the ones measured at a few meters' depth 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 at 10 mm hr^{-1} (Boutin et al., 2016, Supply et al., 2018). Even when it is averaged in time and space, the signature of this effect remains larger than -0.1 in rainy regions like ITCZ (Supply, PhD thesis, 2020). Removing this effect from level 2 SMOS SSS, leads to much decreased systematic differences when compared to Argo derived salinities.

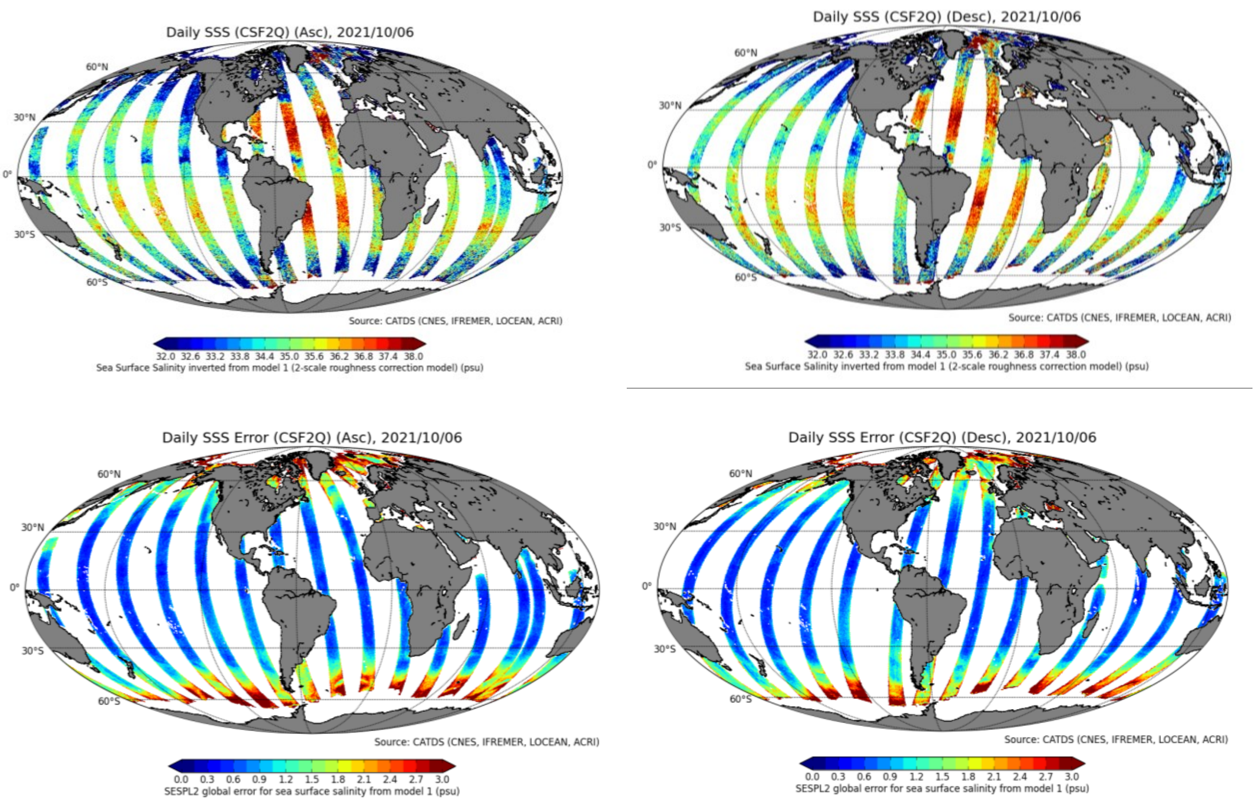

Figure 1: Example of top) Sea Surface Salinity for ascending orbits (left) and descending orbits (right) and (bottom) of their errors, as derived from the retrieval algorithm, for ascending orbits (left) and descending orbits (right) (no quality flag has been applied here).

II.2.3 Quality check

A quality flag (QC) is provided with the data set. Good QC are for the salinities between a (minSSS-2*ErrorSSS) and (maxSSS+2*ErrorSSS) value, with minimum and maximum values (Figure 2) derived from statistics of SMOS retrieved SSS for each grid point and with wind speed between 0 and 16 m/s.

We advise the users to apply this flag by default except if they are interested in strongly variable areas (e.g. river plumes regions) where this flag can eliminate correct values appearing as outliers.

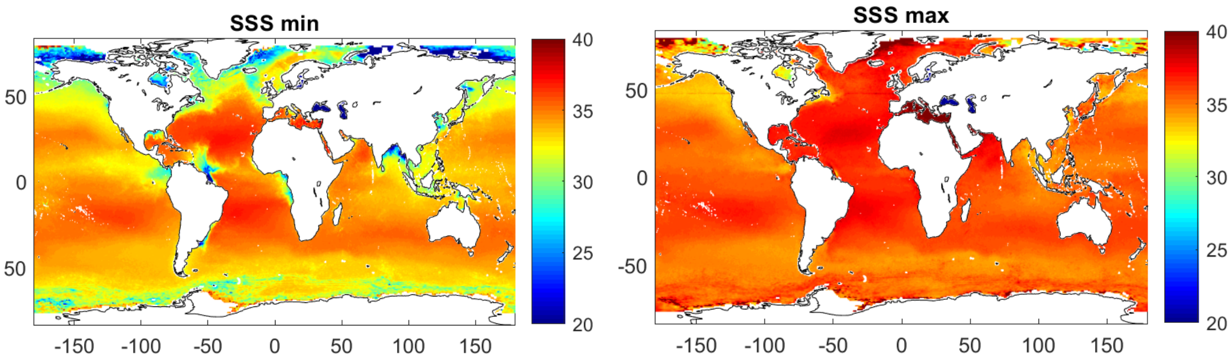

Figure 2: Maps of minimum and maximum value of SSS used to compute the quality flags.

III VALIDATION FRAMEWORK

MULTIOBS_GLO_PHY_SSS_L3_MYNRT_015_014 L2Q SSS and its estimated error is compared with the fully independent in situ Argo SSS data, where matchups are found between the two datasets.

Different metrics of comparison are computed, including mean, median, standard deviation and robust standard deviation, and root mean square of the difference between the satellite and in situ data. Both SSS and its estimated error are validated using metrics of comparisons applied to SSS and to centered reduced variable ((SSS_{SMOS} – SSS_{insitu})/Error).

The results are shown in global maps, time series, histograms and a summary table.

Metric name	*Description*
SSS_CLASS4_INS_N_MEAN_STD	L2Q SSS and SSS error comparison with Argo in situ observations Mean, median, Robust Std and Std differences and number (N) of matchups paired between satellite L2Q data and Argo.

IV VALIDATION RESULTS

IV.1 Sea surface salinity

IV.1.1 Description of the data match up

The data matchups are created by the PiMEP platform (see https://www.salinity-pimep.org/). We summarize below the procedure followed by the PiMEP, more information can be found in PiMEP reports.

The first step consists in filtering Argo in situ data using quality flags, so that only valid salinity data remain in the final match-up files. For each Argo data collected in the Pi-MEP database during 1 day, the platform searches for all satellite SSS data of the composite product found at grid nodes located within a radius of 12.5 km from the in-situ data location. If several satellite SSS product samples are found to meet these criteria, the final satellite SSS match-up point is chosen to be the satellite SSS with central time to which is the closest in time from the in-situ data measurement date.

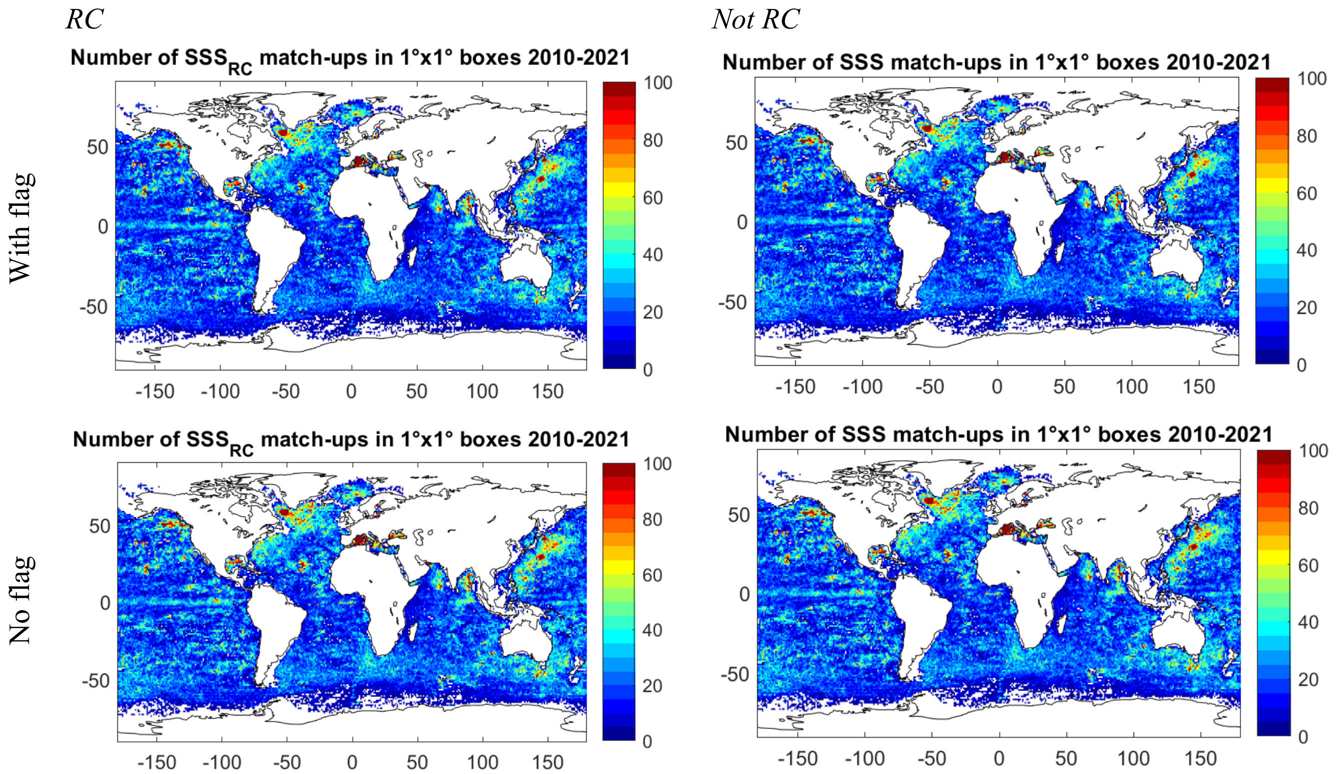

Figure 3: Number of SSS match-ups between Argo SSS and the SMOS SSS L2Q v330 - 0.25 Deg (CATDS-CPDC) SSS product for the Global Ocean Pi-MEP region over 1°×1° boxes and for the full satellite product period. Top left with QC flag and rain correction, top right with QC flag, without rain correction, bottom left without QC and rain correction, and bottom right without flag and without rain correction.

IV.1.2 SSS-CLASS4-INS-MEAN-STD

The mean and standard deviation between SMOS and Argo were computed for:

- Global data, which includes all data with and without quality flag, with (Figure 4a) or without rain correction (Figure 4b);
- C1, where global, rain rate (from IMERG) is zero, mean daily wind is in the range [3, 12] m/s, the SST is > 5 ◦C and distance to coast is > 800 km (Figure 4c).

The results are shown in the maps in Figure 4, for 2010-2021 data, gridded in 1°x1° boxes. Mean difference between SMOS and Argo is mostly between -0.2-0.2 within 45N-45S, where SST is moderate, and increases in absolute value up to 1 at high latitudes in cold waters and the standard deviation is mostly under 1, except at higher latitudes and close to the coast. Most regions with largest bias and STD are removed when considering C1, although there are still regions where the standard deviation is over 1, outside mid-latitudes and in the western North Pacific where numerous radio frequency interferences contaminate the radiometric signal. The application of the quality flag improves these results.

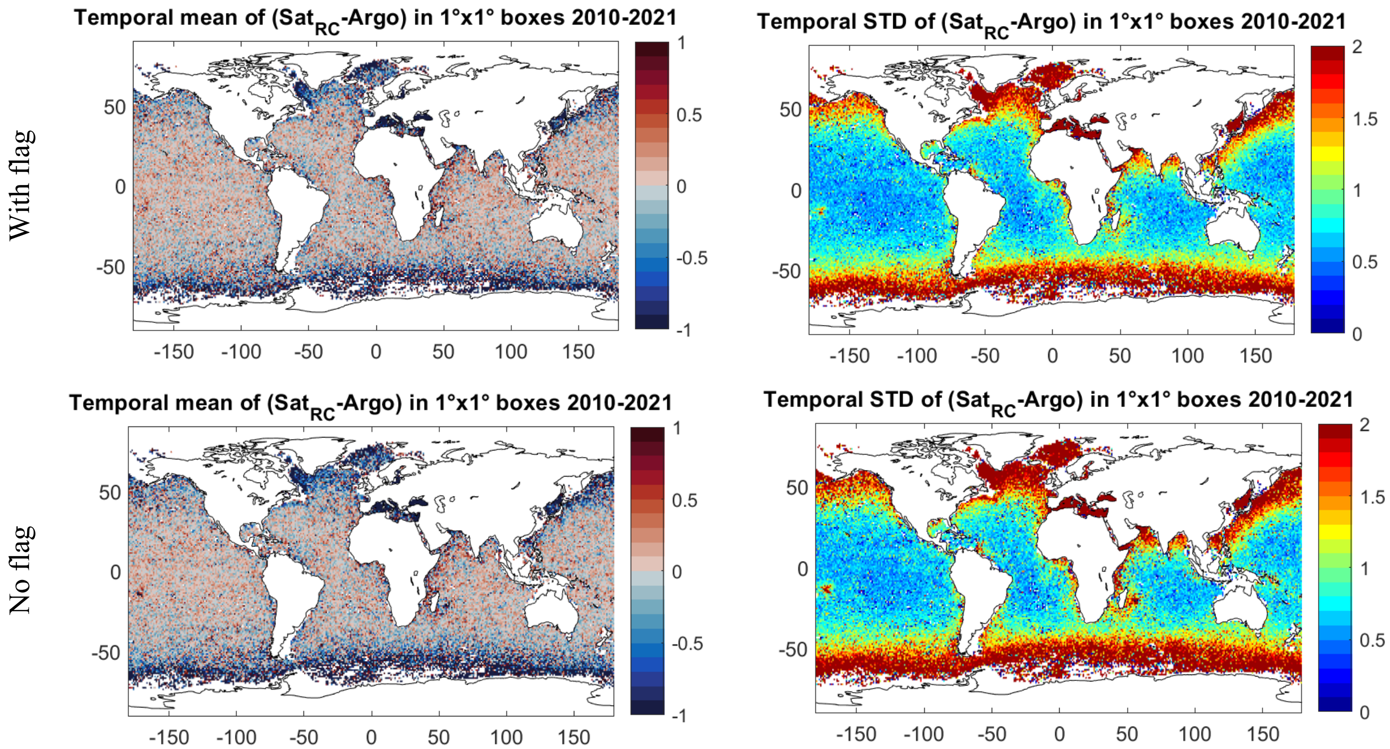

Figure 4 a: Temporal mean (left) and Std (right) of ΔSSS (Satellite - Argo), rain corrected. Only match-up pairs are used to generate these maps, with the quality flag applied to L2Q data (top) and without the quality flag applied to the data (bottom).

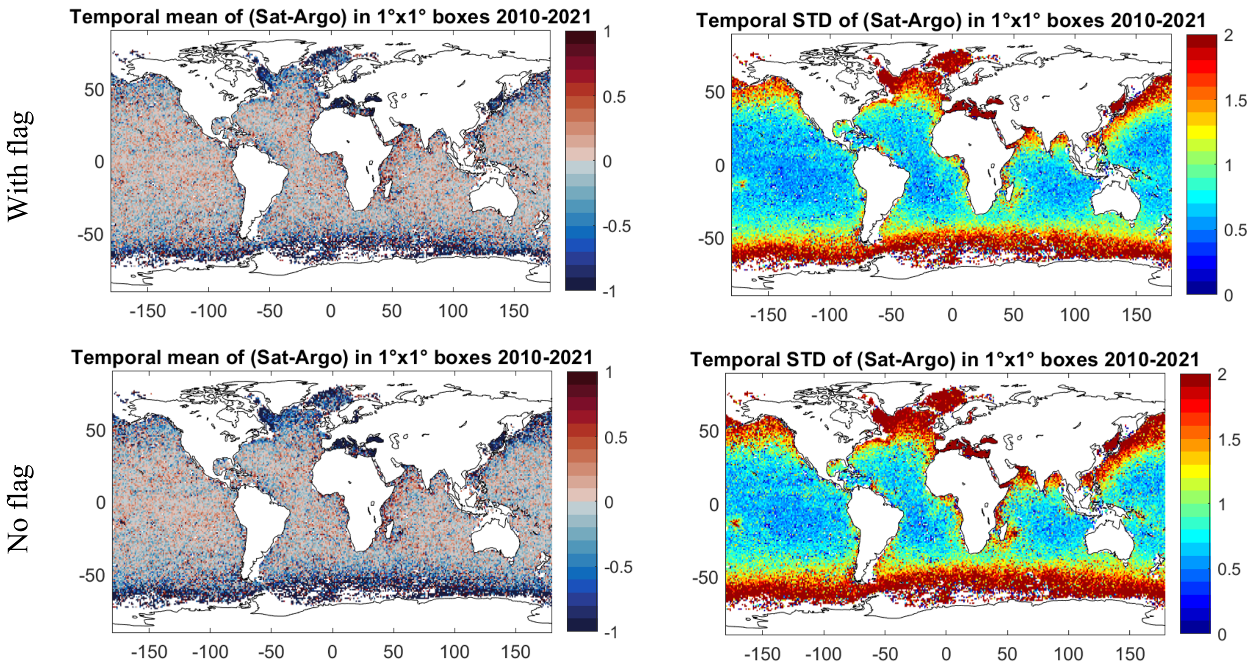

Figure 4 b: Temporal mean (left) and Std (right) of ∆SSS (Satellite - Argo), not rain corrected. Only match-up pairs are used to generate these maps, with the quality flag applied to L2Q data (top) and without the quality flag applied to the data (bottom).

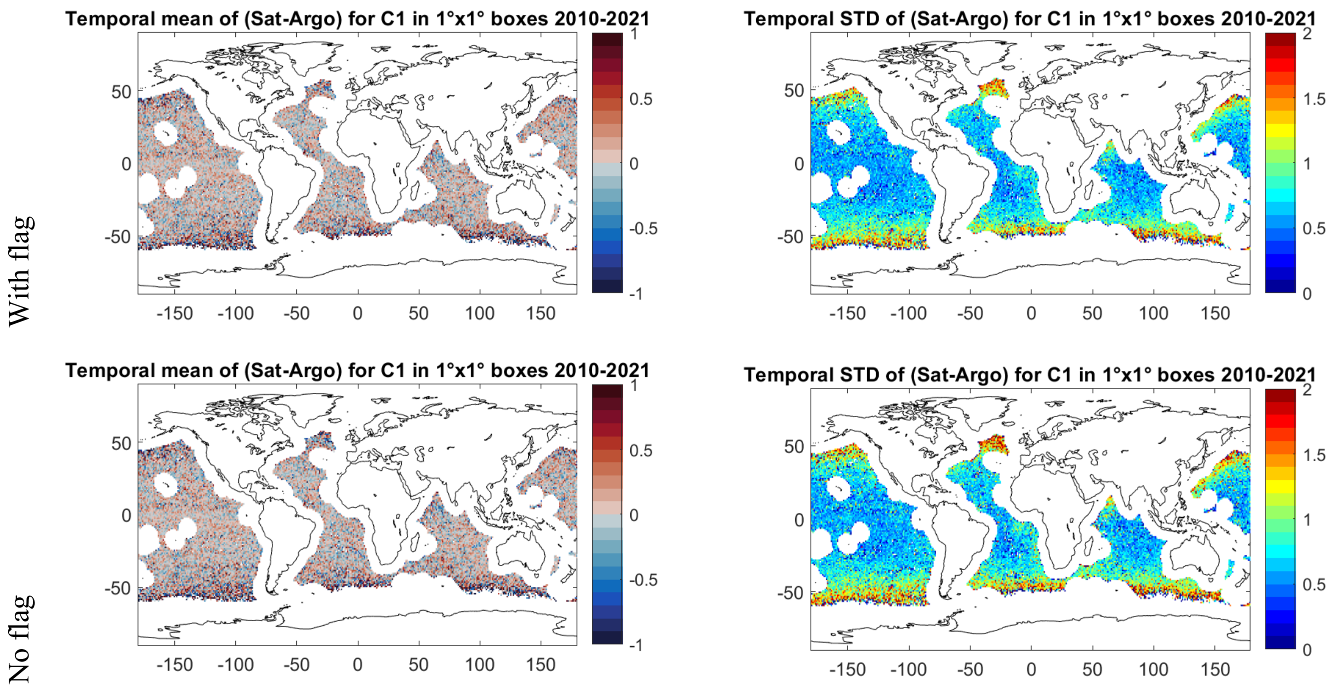

Figure 4 c: Temporal mean (left) and Std (right) of ∆SSS (Satellite - Argo), for C1. Only match-up pairs are used to generate these maps, with the quality flag applied to L2Q data (top) and without the quality flag applied to the data (bottom).

Figure 5 shows the difference between rain corrected SSS and not rain corrected SSS, both without and with the flag applied. As expected, the differences are negative everywhere, most often less than 0.1 in absolute value when averaged over the whole time period, and maximum in the Intertropical Convergence Zone and in the South Pacific Convergence Zone.

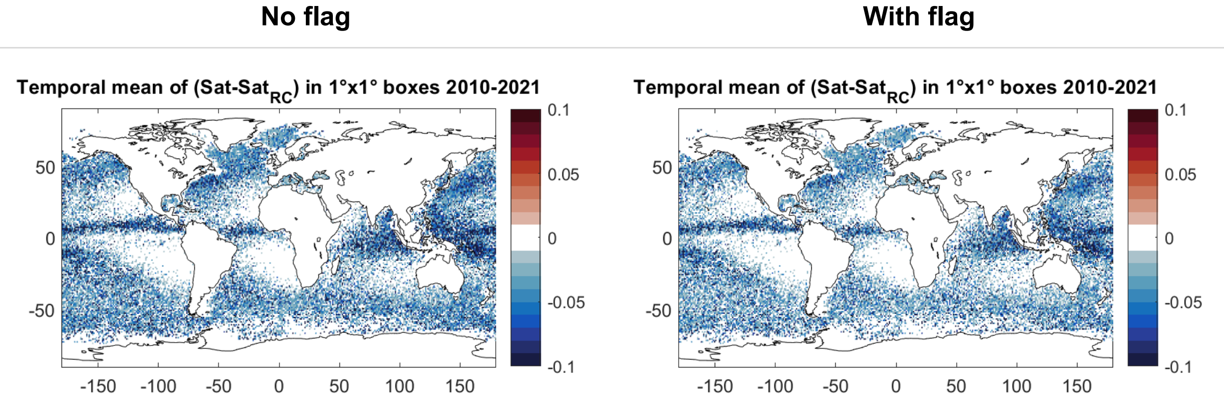

Figure 5: Temporal mean (left) and Std (right) of the difference between SSS and SSS rain corrected, without (left) and with quality flag applied to the data (right).

Figure 6 shows the monthly mean time series of the median SSS (a), mean and median of the difference between satellite and Argo (b), and STD and robust STD of the difference between satellite and Argo (c), after applying the quality flag. Figure 7 shows the same results as Figure 6, but for the case where no quality flag is applied. A comparison between Figure 6 and Figure 7 shows an overall improvement of the statistics when the flag is applied.

Considering the case with the QC flag applied (the figures in Figure 6), the highest negative mean and median differences (about -0.4 and -0.2 respectively) are observed at the beginning of the data period, in 2010, due to numerous radio frequency interferences and a less stable calibration, and are smaller after the QC flag has been applied (down from around -0.6 mean difference). The mean difference is negative most of the time, due to the presence of outliers and numerous negative biases at high latitudes which are only partly filtered out by QC flag; these outliers are filtered out by the median which is close to 0.

The standard deviation of the differences is stable and around 2, whereas the robust standard deviation is much lower, at less than 1 (when the QC flag is applied). This large difference between STD and STD* also points out the presence of outliers.

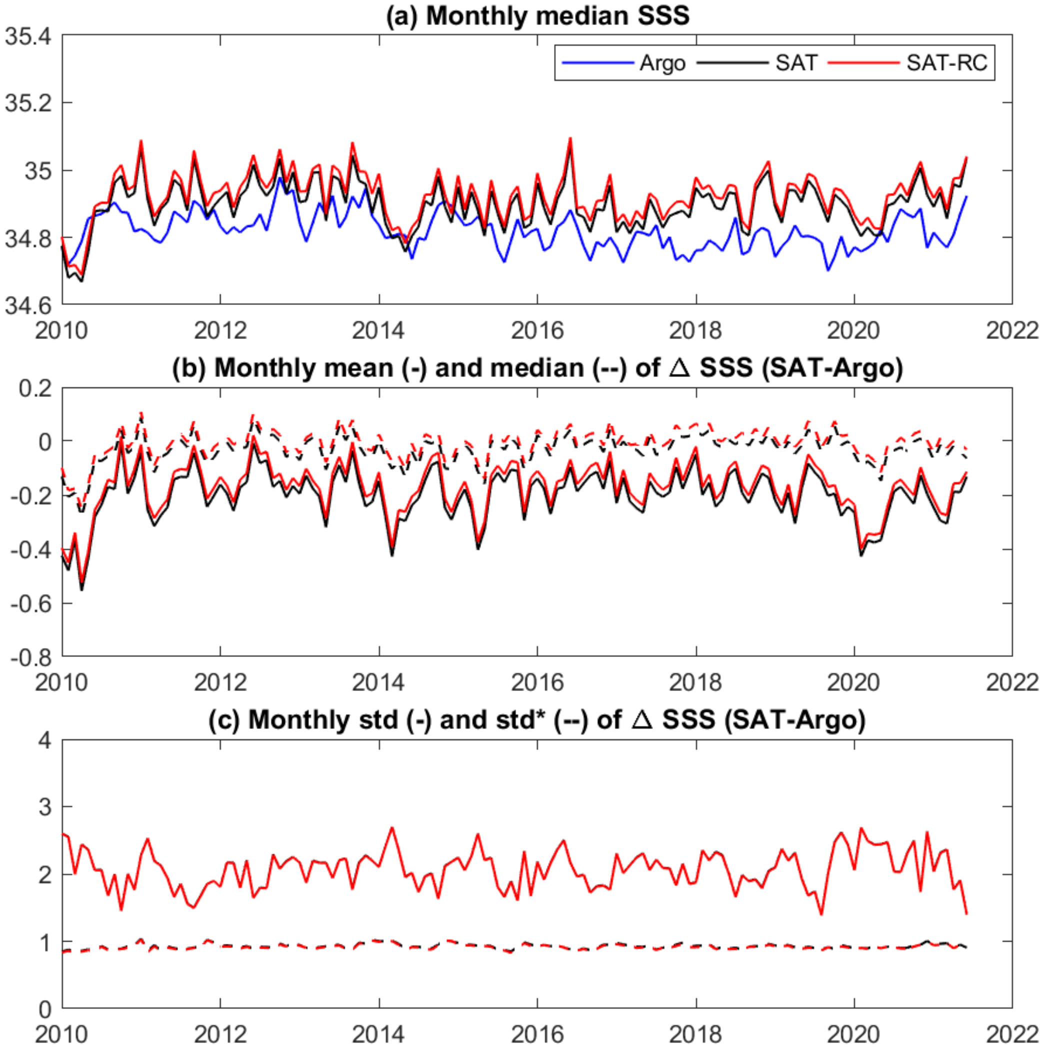

Figure 6: Time series of the monthly median SSS (top), median of ∆SSS (Satellite - Argo) and Std and robust STD of ∆SSS (Satellite - Argo) over the Global Ocean Pi-MEP region considering all match-ups collected by the Pi-MEP. (the quality flag has been applied to L2Q data and rain corrected data is in red, while not rain corrected is in black)

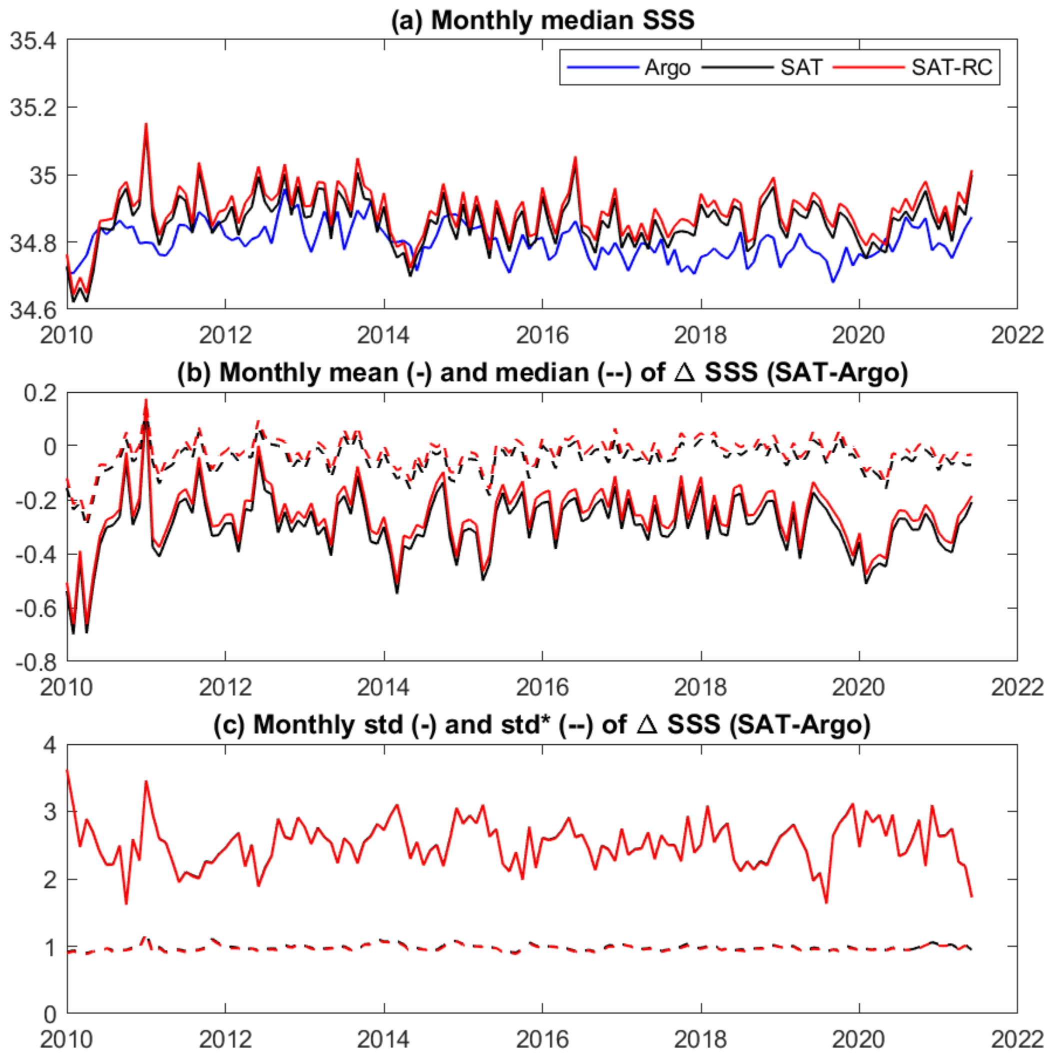

Figure 7: Time series of the monthly median SSS (top), median of ΔSSS (Satellite - Argo) and Std and robust STD of ΔSSS (Satellite - Argo) over the Global Ocean Pi-MEP region considering all match-ups collected by the Pi-MEP. (no quality flag has been applied to L2Q data and rain corrected data is in red, while not rain corrected is in black)

Finally, Table 3 reports global statistics about L2Q. We also report the statistics obtained for L2Q (good quality flags) averaged over 10 days (L3Q products, the L3Q fields are available at CATDS), in order to illustrate how the noise on daily fields is reduced by the temporal average.

Table 3: Statistics of ΔSSS (Satellite - Argo) for the L2Q data and the L3Q data averaged over 10 days. Statistics are shown for all available data, rain-corrected (RC) and not rain-corrected (NRC) and C1 data only.

Statistics of ΔSSS (Satellite - Argo) - MULTIOBS_GLO_PHY_SSS_L3_MYNRT_015_014

Condition	#	Median	Mean	STD	RMS	IQR	R^2	STD*
NRC (with quality flag)	667332	-0.03	-0.20	2.10	2.11	1.24	0.59	0.93
RC (with quality flag)	**667332**	**-0.00**	**-0.17**	**2.10**	**2.10**	**1.23**	**0.59**	**0.92**
C1 (with quality flag)	227144	0.02	0.02	0.84	0.84	0.96	0.55	0.72
NRC (no quality flag)	711901	-0.05	-0.29	2.55	2.57	1.32	0.55	0.98
RC (no quality flag)	711901	-0.02	-0.25	2.55	2.56	1.30	0.55	0.97
C1 (no quality flag)	233502	0.02	0.02	0.92	0.92	0.98	0.50	0.73
Statistics of ΔSSS (Satellite - Argo) averaged over 10 days (product available at catds: smos-l3-catds-cpdc-v335-10d-25km)								
all	1064253	-0.01	-0.04	0.55	0.55	0.45	0.92	0.34
C1	363831	0.00	0.00	0.30	0.30	0.36	0.95	0.27

For reference, other reports are available from Pi-MEP (https://www.salinity-pimep.org/), considering other in situ data as reference, and focused on various sub-regions.

IV.2 Sea surface salinity error

In this section we present a validation of the random uncertainty of the SSS (also called SSS error in the products) which is estimated together with the L2Q SSS by the retrieval algorithm, completely independently of any in situ measurement comparison. Maps of the error variables for both rain corrected and not rain corrected data are presented, both with and without the quality flag applied (Figure 8a). Since the signal to noise ratio of radiometric L-Band measurements to salinity decreases with the SST, we observe a large increase of the error towards high latitudes (cold waters). Figure 8b shows the temporal quadratic mean SSS error, which mirrors the temporal standard deviation of the difference between satellite and ARGO, providing a first qualitative validation of the SSS errors. The histogram of the error, shown in Figure 9, shows the error is between 0.5 and 5, with a predominant peak around 0.7.

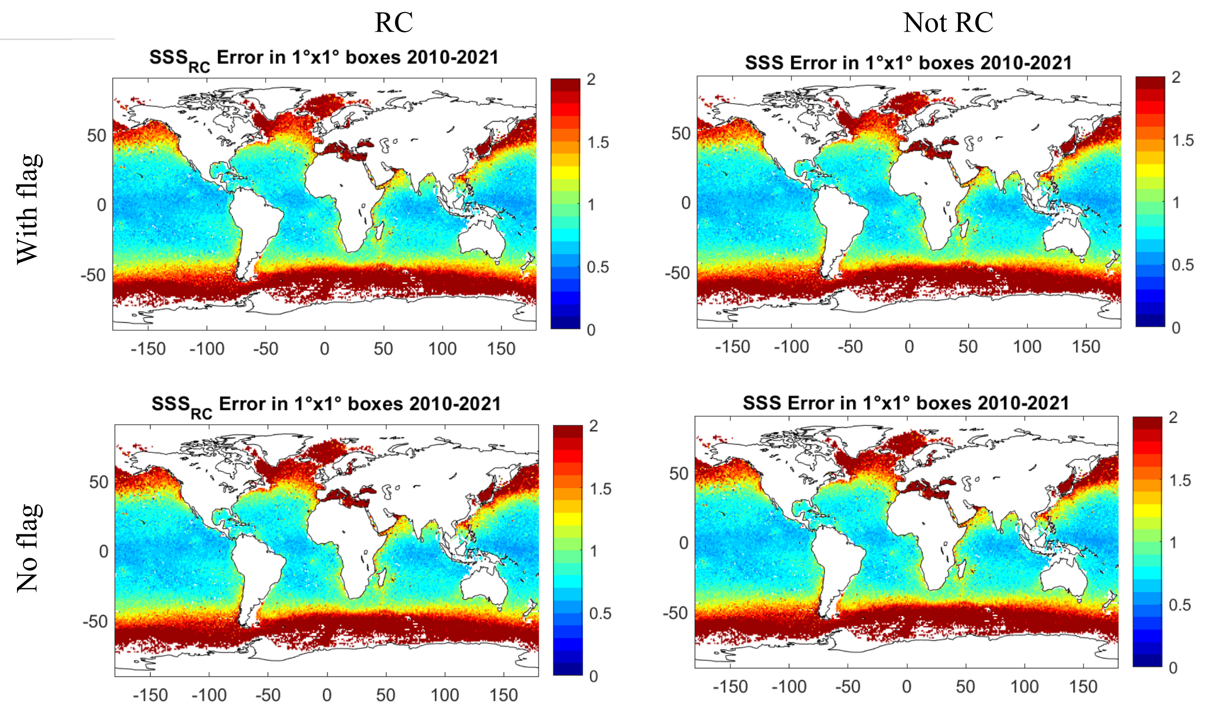

Figure 8 a: Maps of temporal quadratic mean SSS Error for match-ups between Argo SSS and the SMOS SSS L2Q v330 - 0.25 Deg (CATDS-CPDC) SSS product for the Global Ocean Pi-MEP region over 1°×1° boxes and for the full satellite product period (left, with rain correction; right without), with (top) and without quality flag applied to the data (bottom).

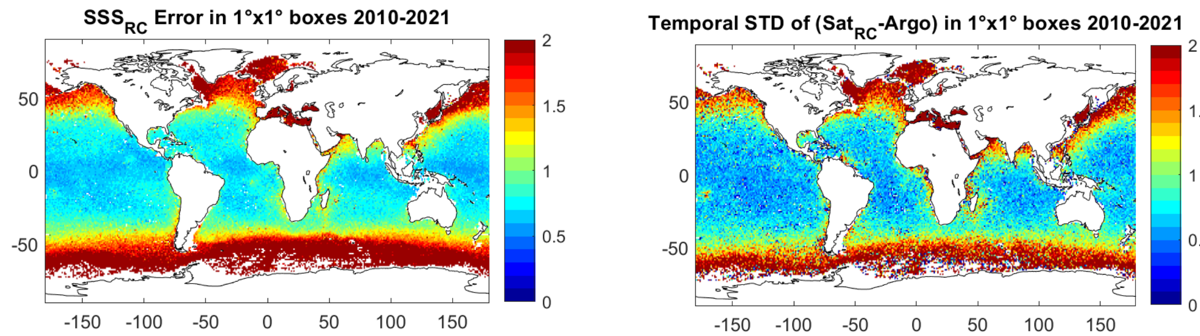

Figure 8 b: Map of SSS Error for match-ups between Argo SSS and the SMOS SSS L2Q v330 - 0.25 Deg (CATDS-CPDC) SSS product for the Global Ocean Pi-MEP region over 1°×1° boxes and for the full satellite product period (left) compared with the map of temporal standard deviation of the difference between satellite SSS and Argo SSS (right).

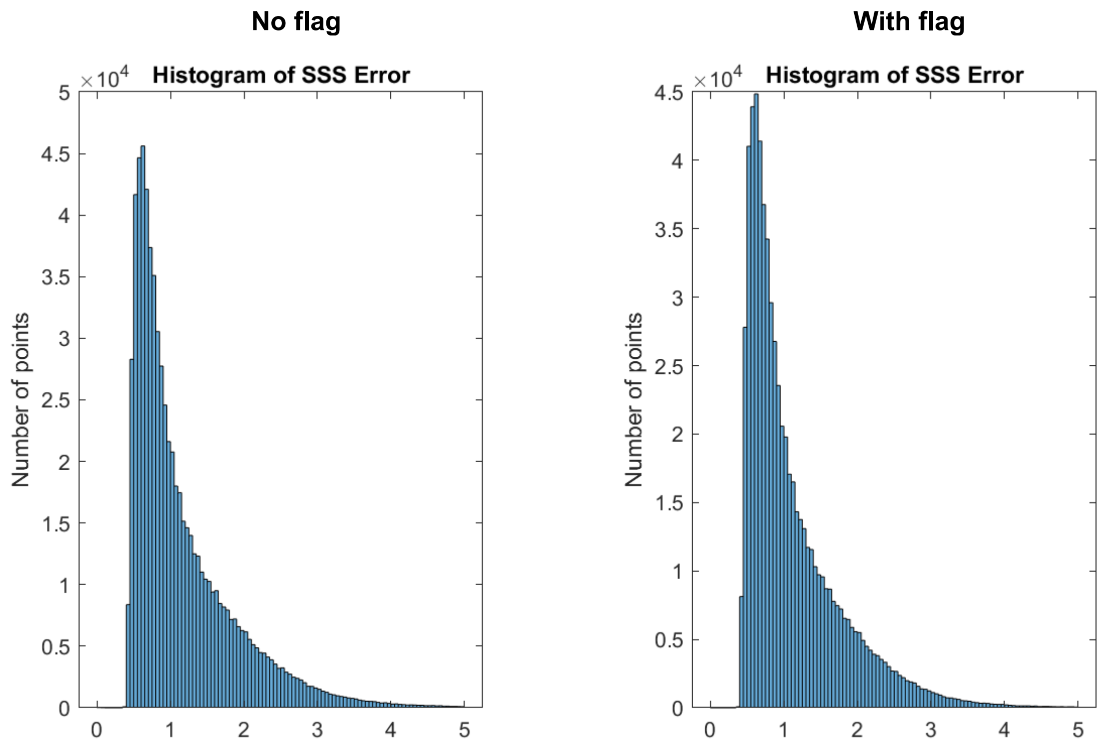

Figure 9: Histogram of SSS Error over the Global Ocean Pi-MEP region considering all match-ups collected by the Pi-MEP for the case where no quality flag has been applied to L2Q data (left) and the quality flag has been applied to L2Q data (right).

In order to validate more quantitatively the errors corresponding to each L2Q SSS, we look at the mean and STD of the reduced variable (ΔSSS/SSS_error), where ΔSSS is the difference between L2Q SSS and Argo. If the random uncertainties are correctly estimated the mean and STD should be very close to 0 and 1 respectively (STD might be slightly higher than 1 given that here we neglect the representativity error between Argo and SMOS SSS, but in most regions (except in river plumes), the SSS variability within a SMOS pixel is expected to be much less than the SMOS L2Q SSS error he) (see method details in Thouvenin-Masson et al. 2022).

Figures 10 and 11 shows the monthly time series of mean, median, STD* and STD of the reduced variable, for the data with and without the quality flag applied, respectively. The median and mean are very close to each other contrary to the mean and median of ΔSSS (Figures 6 and 7) indicating that ΔSSS and SSS error are consistent so that the normalization of ΔSSS by the SSS error reduces the impact of large ΔSSS on the mean. We still observe relatively high negative mean and median at the beginning of the observation period. They are around zero for the rest of the period, with a noticeable peak in January 2011, when the SSS bias is higher globally. This is improved after the application of the QC flag (Figure 9). The robust STD are close to 1 both with and without the quality flag applied. With the quality flag enabled, the STD is also around 1, which is what we expect when random uncertainties are correctly estimated, and the peaks found without the quality flag are removed (except for January 2011). In general, we see that with the quality flag and rain correction, the results are noticeably improved.

This is further evidenced in Figure 12, where we see the distribution of ΔSSS (Satellite - Argo)/SSS Error. Without the quality flag, the distribution follows a gaussian distribution with mean 0 and STD 1, but with outliers on both sides of the distribution (mostly on the negative side). When the quality flag is applied, these outliers are removed (Figure 12, on the right).

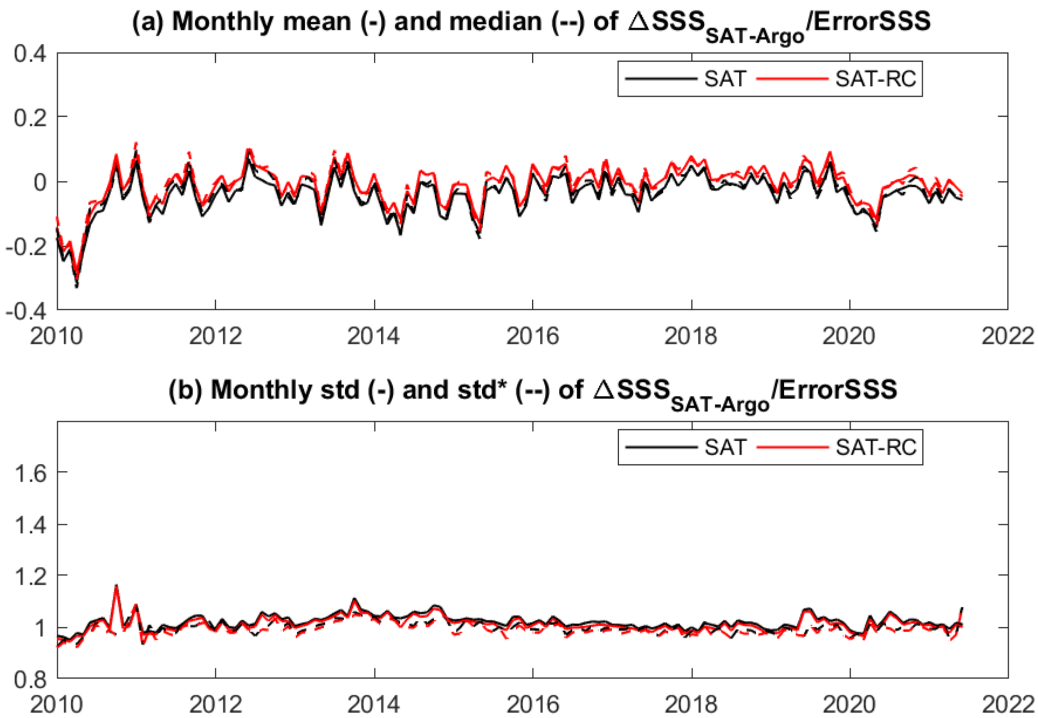

Figure 10: Time series of the monthly mean and median ΔSSS (Satellite - Argo)/SSS Error (top), and Std and robust STD of ΔSSS (Satellite - Argo)/SSS Error over the Global Ocean Pi-MEP region considering all match-ups collected by the Pi-MEP. (the quality flag has been applied to L2Q data)

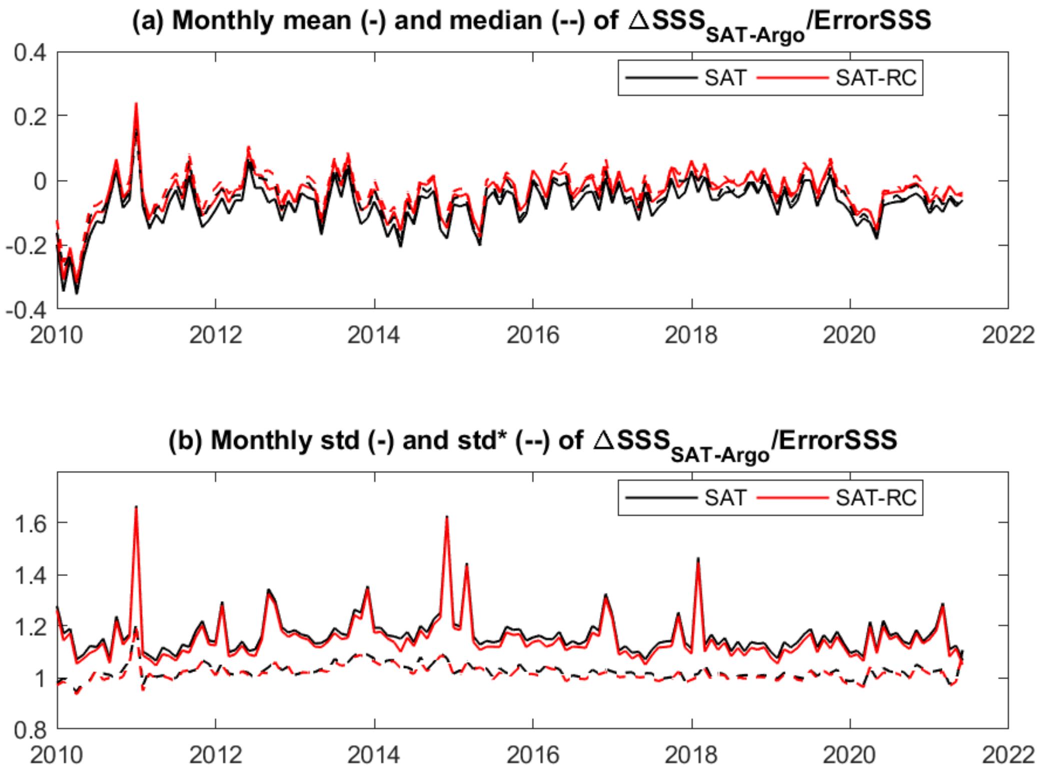

Figure 11: Time series of the monthly mean and median ΔSSS (Satellite - Argo)/SSS Error (top), and Std and robust STD of ΔSSS (Satellite - Argo)/SSS Error over the Global Ocean Pi-MEP region considering all match-ups collected by the Pi-MEP. (no quality flag has been applied to L2Q data)

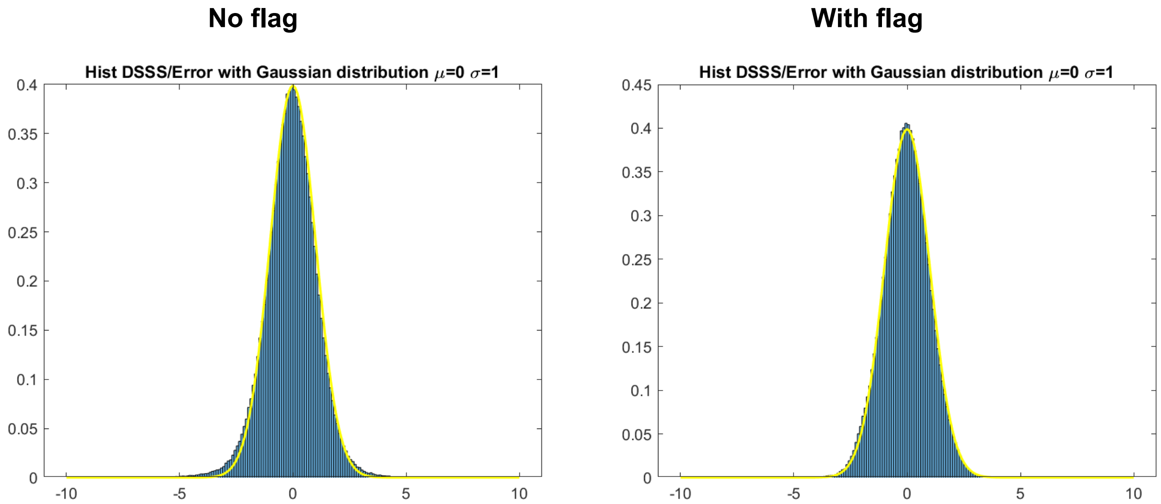

Figure 12: Histogram of ΔSSS (Satellite - Argo)/SSS Error (top), and Std and robust STD of ΔSSS (Satellite - Argo)/SSS Error over the Global Ocean Pi-MEP region considering all match-ups collected by the Pi-MEP.

V SYSTEM’S NOTICEABLE EVENTS, OUTAGES OR CHANGES

This is the first version of this document, therefore there are no changes to note.

VI QUALITY CHANGES SINCE PREVIOUS VERSION

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