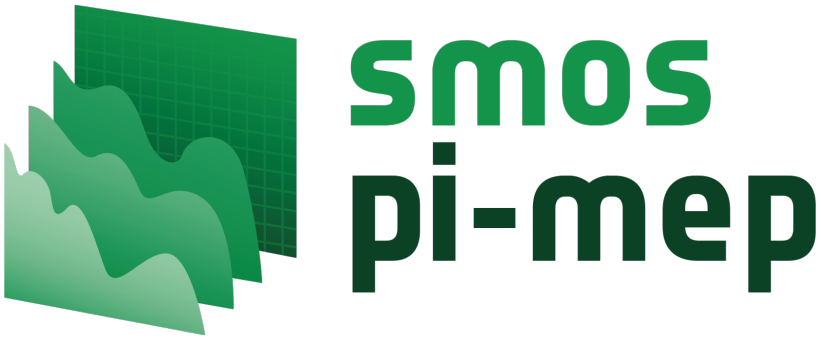

Match-up database Analyses Report

Aquarius SSS L4 OI v5 - Monthly (IPRC)

Sea mammals

Atlantic Ocean

prepared by the Pi-MEP Consortium

June 15, 2021

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Acronym

Aquarius	NASA/CONAE Salinity mission
ASCAT	Advanced Scatterometer
ATBD	Algorithm Theoretical Baseline Document
BLT	Barrier Layer Thickness
CMORPH	CPC MORPHing technique (precipitation analyses)
CPC	Climate Prediction Center
CTD	Instrument used to measure the conductivity, temperature, and pressure of seawater
DM	Delayed Mode
EO	Earth Observation
ESA	European Space Agency
FTP	File Transfer Protocol
GOSUD	Global Ocean Surface Underway Data
GTMBA	The Global Tropical Moored Buoy Array
Ifremer	Institut français de recherche pour l'exploitation de la mer
IPEV	Institut polaire français Paul-Émile Victor
IQR	Interquartile range
ISAS	*In Situ* Analysis System
Kurt	Kurtosis (fourth central moment divided by fourth power of the standard deviation)
L2	Level 2
LEGOS	Laboratoire d'Etudes en Géophysique et Océanographie Spatiales
LOCEAN	Laboratoire d'Océanographie et du Climat : Expérimentations et Approches Numériques
LOPS	Laboratoire d'Océanographie Physique et Spatiale
MDB	Match-up Data Base
MEOP	Marine Mammals Exploring the Oceans Pole to Pole
MLD	Mixed Layer Depth
NCEI	National Centers for Environmental Information
NRT	Near Real Time
NTAS	Northwest Tropical Atlantic Station
OI	Optimal interpolation
Pi-MEP	Pilot-Mission Exploitation Platform
PIRATA	Prediction and Researched Moored Array in the Atlantic
QC	Quality control
R_{sat}	Spatial resolution of the satellite SSS product
RAMA	Research Moored Array for African-Asian-Australian Monsoon Analysis and Prediction
r^2	Square of the Pearson correlation coefficient
RMS	Root mean square
RR	Rain rate
SAMOS	Shipboard Automated Meteorological and Oceanographic System
Skew	Skewness (third central moment divided by the cube of the standard deviation)
SMAP	Soil Moisture Active Passive (NASA mission)
SMOS	Soil Moisture and Ocean Salinity (ESA mission)
SPURS	Salinity Processes in the Upper Ocean Regional Study
SSS	Sea Surface Salinity
SSS_{insitu}	*In situ* SSS data considered for the match-up

SSS_{SAT}	Satellite SSS product considered for the match-up
ΔSSS	Difference between satellite and *in situ* SSS at colocalized point ($\Delta SSS = SSS_{SAT}$- SSS_{insitu})
SST	Sea Surface Temperature
Std	Standard deviation
Std*	Robust Standard deviation = median(abs(x-median (x)))/0.67 (less affected by outliers than Std)
Stratus	Surface buoy located in the eastern tropical Pacific
Survostral	SURVeillance de l'Océan AuSTRAL (Monitoring the Southern Ocean)
TAO	Tropical Atmosphere Ocean
TSG	ThermoSalinoGraph
WHOI	Woods Hole Oceanographic Institution
WHOTS	WHOI Hawaii Ocean Time-series Station
WOA	World Ocean Atlas

1 Overview

In this report, we present systematic analyses of the Match-up DataBase (MDB) files generated by the Pi-MEP platform within the following Pi-MEP region and for the below pair of Satellite/*in situ* SSS data:

- Pi-MEP region: Atlantic Ocean (download the corresponding mask in NetCDF here)
- SSS satellite product (SSS_{SAT}): Aquarius SSS L4 OI v5 - Monthly (IPRC)
- *In situ* dataset (SSS_{Insitu}): Sea mammals (download the corresponding *in situ* report here)

In the following, $\Delta SSS = SSS_{SAT} - SSS_{Insitu}$ denotes the difference between the satellite and *in situ* SSS at the colocalized points that form the MDB.

This report presents successively:

The MDB file DataSets (Section 2)

- A short description of the satellite SSS product considered in the match-up (2.1)
- A short description of the *in situ* SSS dataset considered in the match-up (2.2)
- A short description of the auxiliary geophysical datasets co-localized with SSS pairs (2.3)
- An overview of how the Match-ups were evaluated (2.4)
- An overview of the MDB characteristics for the particular *in situ*/satellite pairs (2.5)

The major results of the MDB file Analyses (Section 3)

- Spatial Maps of the Time-mean and temporal Std of *in situ* and satellite SSS and of the ΔSSS (3.1)
- Time series of the monthly median and Std of *in situ* and satellite SSS and of the ΔSSS (3.2)
- Zonal mean and Std of *in situ* and satellite SSS and of the ΔSSS (3.3)
- Scatterplots of satellite vs *in situ* SSS by latitudinal bands (3.4)
- Time series of the monthly median and Std of the ΔSSS sorted by latitudinal bands (3.5)
- ΔSSS sorted as function of geophysical parameters (3.6)
- ΔSSS maps and statistics for different geophysical conditions (3.7)

All analyses are conducted over the Pi-MEP Region specified above and over the full satellite SSS product period. Original figures appearing in this report can be downloaded as PNG files here or by clicking directly on the figure.

2 The MDB file datasets

2.1 Satellite SSS product

2.1.1 Aquarius SSS L4 OI v5 - Monthly (IPRC)

This product is a monthly SSS analysis on a near-global 0.5° grid for the period for the period September 2011 - June 2015, spanning the complete 3 year, 9 month period of Aquarius science data availability. The input data for the analysis are the Level-2 (swath) SSS data provided by Aquarius/SAC-D satellite, a collaborative space mission between NASA and Argentina's space agency. The analysis method is optimal interpolation (OI) that takes into account analyzed errors on the observations, specific to the Aquarius instrument. The method also includes a large-scale correction for satellite biases, filtering of along-track SSS data prior for OI, and the use of realistic correlation scales of mesoscale SSS anomalies (Melnichenko et al. (2014a)). The description of the mapping methodology can be found in Melnichenko et al. (2014b), which also includes results of statistical validation of the product against concurrent in situ data.

Table 1: Satellite SSS product characteristics

Aquarius SSS L4 OI v5 - Monthly (IPRC)	
Spatial resolution	0.5°x0.5°
Temporal repeat	Monthly
Temporal coverage	From 2011-08-27 to 2015-05-28
Spatial coverage	Global [-180 180 -90 90]
Data Provider	Oleg Melnichenko at IPRC
Release Date	2014-10-17 (updated 2018-07)
Version	5
Documentation	Technical_Notes.pdf and Addendum_1.pdf
Data access	OISSS_V5.0_monthly

2.2 *In situ* SSS dataset

Instrumentation of southern elephant seals with satellite-linked CTD tags proposes unique temporal and spatial coverage. This includes extensive data from the Antarctic continental slope and shelf regions during the winter months, which is outside the conventional areas of Argo autonomous floats and ship-based studies. The use of elephant seals has been particularly effective to sample the Southern Ocean and the North Pacific. Other seal species have been successfully used in the North Atlantic, such as hooded seals. The marine mammal dataset (MEOP-CTD database) is quality controlled and calibrated using delayed-mode techniques involving comparisons with other existing profiles as well as cross-comparisons similar to established protocols within the Argo community, with a resulting accuracy of ±0.03 °C in temperature and ±0.05 in salinity or better (Treasure et al. (2017)). The marine mammal data were collected and made freely available by the International MEOP Consortium and the national programs that contribute to it (`http://www.meop.net`). This dataset is updated once a year and can be downloaded here (Roquet et al. (2018)). A preprocessing stage is applied to the database before being used by the Pi-MEP which consist to keep only profile with salinity, temperature and pressure quality flags set to 1 or 2 and if at least one measurement is in the top 10 m depth. Marine mammal SSS correspond to the top (shallowest) profile salinity data provided that profile depth is 10 m or less.

2.3 Auxiliary geophysical datasets

Additional EO datasets are used to characterize the geophysical conditions at the *in situ*/satellite SSS pair measurement locations and time, and 10 days prior the measurements to get an estimate of the geophysical condition and history. As discussed in Boutin et al. (2016), the presence of vertical gradients in, and horizontal variability of, sea surface salinity indeed complicates comparison of satellite and *in situ* measurements. The additional EO data are used here to get a first estimates of conditions for which L-band satellite SSS measured in the first centimeters of the upper ocean within a 50-150 km diameter footprint might differ from pointwise *in situ* measurements performed in general between 10 and 5 m depth below the surface. The spatio-temporal variability of SSS within a satellite footprint (50–150 km) is a major issue for satellite SSS validation in the vicinity of river plumes, frontal zones, and significant precipitation. Rainfall can in some cases produce vertical salinity gradients exceeding 1 pss m^{-1}; consequently, it is recommended that satellite and *in situ* SSS measurements less than 3–6 h after rain events should be considered with care when used in satellite calibration/validation analyses. To identify such situation, the Pi-MEP platform is first using CMORPH products to characterize the local value and history of rain rate and ASCAT gridded data are used to characterize the local surface wind speed and history. For validation purpose, the ISAS monthly SSS *in situ* analysed fields at 5 m depth are collocated and compared with the satellite SSS products. The use of ISAS is motivated by the fact that it is used in the SMOS L2 official validation protocol in which systematic comparisons of SMOS L2 retrieved SSS with ISAS are done. In complement to ISAS, monthly std climatological fields from the World Ocean Atlas (WOA13) at the match-up pairs location and date are also used to have an a priori information of the local SSS variability.

2.3.1 CMORPH

Precipitation are estimated using the CMORPH 3-hourly products at 1/4° resolution (Joyce et al. (2004)). CMORPH (CPC MORPHing technique) produces global precipitation analyses at very high spatial and temporal resolution. This technique uses precipitation estimates that have been derived from low orbiter satellite microwave observations exclusively, and whose features are transported via spatial propagation information that is obtained entirely from geostationary satellite IR data. At present NOAA incorporate precipitation estimates derived from the passive microwaves aboard the DMSP 13, 14 and 15 (SSM/I), the NOAA-15, 16, 17 and 18 (AMSU-B), and AMSR-E and TMI aboard NASA's Aqua, TRMM and GPM spacecraft, respectively. These estimates are generated by algorithms of Ferraro (1997) for SSM/I, Ferraro et al. (2000) for AMSU-B and Kummerow et al. (2001) for TMI. Note that this technique is not a precipitation estimation algorithm but a means by which estimates from existing microwave rainfall algorithms can be combined. Therefore, this method is extremely flexible such that any precipitation estimates from any microwave satellite source can be incorporated.

With regard to spatial resolution, although the precipitation estimates are available on a grid with a spacing of 8 km (at the equator), the resolution of the individual satellite-derived estimates is coarser than that - more on the order of 12 x 15 km or so. The finer "resolution" is obtained via interpolation.

In effect, IR data are used as a means to transport the microwave-derived precipitation features during periods when microwave data are not available at a location. Propagation vector matrices are produced by computing spatial lag correlations on successive images of geostationary satellite IR which are then used to propagate the microwave derived precipitation estimates. This process governs the movement of the precipitation features only. At a given location, the shape and intensity of the precipitation features in the intervening half hour periods between microwave scans are determined by performing a time-weighting interpolation between microwave-derived

features that have been propagated forward in time from the previous microwave observation and those that have been propagated backward in time from the following microwave scan. NOAA refer to this latter step as "morphing" of the features.

For the present Pi-MEP products, we only considered the 3-hourly products at 1/4 degree resolution. The entire CMORPH record (December 2002-present) for 3-hourly, 1/4 degree lat/lon resolution can be found at: ftp://ftp.cpc.ncep.noaa.gov/precip/CMORPH_V1.0/CRT/. CMORPH estimates cover a global belt (-180°W to 180°E) extending from 60°S to 60°N latitude and are available for the complete period of the Pi-MEP core datasets (Jan 2010-now).

2.3.2 ASCAT

Advanced SCATterometer (ASCAT) daily data produced and made available at Ifremer/CERSAT on a 0.25°x0.25° resolution grid (Bentamy and Fillon (2012)) since March 2007 are used to characterize the mean daily wind at the match-up pair location as well as the wind history during the 10-days period preceding the in situ measurement date. These wind fields are calculated based on a geostatistical method with external drift. Remotely sensed data from ASCAT are considered as observations while those from numerical model analysis (ECMWF) are associated with the external drift. The spatial and temporal structure functions for wind speed, zonal and meridional wind components are estimated from ASCAT retrievals. Furthermore, the new procedure includes a temporal interpolation of the retrievals based on the complex empirical orthogonal function (CEOF) approach, in order to enhance the sampling length of the scatterometer observations. The resulting daily wind fields involves the main known surface wind patterns as well as some variation modes associated with temporal and spatial moving features. The accuracy of the gridded winds was investigated through comparisons with moored buoy data in Bentamy et al. (2012) and resulted in rms differences for wind speed and direction are about 1.50 $m.s^{-1}$ and 20°.

2.3.3 ISAS

The In Situ Analysis System (ISAS), as described in Gaillard et al. (2016) is a data based reanalysis of temperature and salinity fields over the global ocean 70°N–70°S on a 1/2° grid. It was initially designed to synthesize the temperature and salinity profiles collected by the Argo program. It has been later extended to accommodate all type of vertical profile as well as time series. ISAS gridded fields are entirely based on *in situ* measurements. The methodology and configuration have been conceived to preserve as much as possible the data information content and resolution. ISAS is developed and run in a research laboratory (LOPS) in close collaboration with Coriolis, one of Argo Global Data Assembly Center and unique data provider for the Mercator operational oceanography system. In Pi-MEP, the products in used are the INSITU_GLO_TS_OA_REP_OBSERVATIONS_013_002_b for the period 2010 to 2019 and INSITU_GLO_TS_OA_NRT_OBSERVATIONS_013_002_a for the Near-Real Time (2020-2021) derived at the Coriolis data center and provided by the Copernicus Marine Environment Monitoring Service (CMEMS). The major contribution to the data set is from Argo array of profiling floats, reaching an approximate resolution of one profile every 10-days and every 3-degrees over the satellite SSS period (http://www.umr-lops.fr/SNO-Argo/Products/ISAS-T-S-fields/); in this version SSS from ship of opportunity thermosalinographs are not used, so that we can consider SMOS SSS validation using these measurements independent of ISAS. The ISAS optimal interpolation involves a structure function modeled as the sum of two Gaussian functions, each associated with specific time and space scales, resulting in a smoothing over typically 3 degrees. The smallest scale which can be retrieved with ISAS analysis is not smaller than 300–500 km (Kolodziejczyk et al. (2015)). For validation purpose, the ISAS monthly SSS fields at 5 m

depth are collocated and compared with the satellite SSS products and included in the Pi-MEP Match-up files. In addition, the "percentage of variance" fields (PCTVAR) contained in the ISAS analyses provide information on the local variability of *in situ* SSS measurements within 1/2°x1/2° boxes.

2.3.4 World Ocean Atlas Climatology

The World Ocean Atlas 2013 version 2 (WOA13 V2) is a set of objectively analyzed (1° grid) climatological fields of *in situ* temperature, salinity and other variables provided at standard depth levels for annual, seasonal, and monthly compositing periods for the World Ocean. It also includes associated statistical fields of observed oceanographic profile data interpolated to standard depth levels on 5°, 1°, and 0.25° grids. We use these fields in complement to ISAS to characterize the climatological fields (annual mean and std) at the match-up pairs location and date.

2.4 Overview of the Match-ups generation method

The match-up production is basically a three steps process:

1. preparation of the input *in situ* and satellite data, and,
2. co-localization of satellite products with *in situ* SSS measurements.
3. co-localization of the *in situ*/satellite pair with auxiliary information.

In the following, we successively detail the approaches taken for these different steps.

2.4.1 *In situ*/Satellite data filtering

The first step consists in filtering Sea mammals *in situ* data using the quality flags as described in 2.2 so that only valid salinity data remain in the final match-up files.

For high-spatial resolution *in situ* SSS measurements such as the Thermo-SalinoGraph (TSG) SSS data, as well as SSS data from surface drifters, an additional spatial filtering step is performed on the *in situ* data that will be in fine compared to the satellite SSS products. If R_{sat} is the spatial resolution of the satellite SSS product (L2 to L3-L4), the *in situ* data are spatially low pass filtered using a running median filter with a window width=R_{sat} to try to minimize the spatial representativeness uncertainty when comparing to the lower spatial resolution of the satellite SSS product. Both original and filtered *in situ* data are finally stored in the MDB files.

Only for satellite L2 SSS data, a third step consist in filtering spurious data using the flags and associated recommendation as provided by the official data centers and described in 2.1.

2.4.2 *In situ*/Satellite Co-localization

In this step, each SSS satellite acquisition is co-localized with the filtered *in situ* measurements. The method used for co-localization differ if the satellite SSS is a swath product (so-called Level 2-types) or a time-space composite product (so-called Level 3/level 4-types).

- For L2 SSS swath data :

  If R_{sat} is the spatial resolution of the satellite swath SSS product, for each *in situ* data sample collected in the Pi-MEP database, the platform searches for all satellite SSS data found at grid nodes located within a radius of $R_{sat}/2$ from the *in situ* data location and acquired with a time-lag from the *in situ* measurement date that is less or equal than ± 12

hours. If several satellite SSS samples are found to meet these criteria, the final satellite SSS match-up point is selected to be the closest in time from the *in situ* data measurement date. The final spatial and temporal lags between the *in situ* and satellite data are stored in the MDB files.

- For L3 and L4 composite SSS products :

  If R_{sat} is the spatial resolution of the composite satellite SSS product and D the period over which the composite product was built (e.g., periods of 1, 7, 8, 9, 10, 18 days, 1 month, etc..) with central time t_o, for each *in situ* data sample collected in the Pi-MEP database during period D, the platform searches for all satellite SSS data of the composite product found at grid nodes located within a radius of $R_{sat}/2$ 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 composite SSS with central time t_o which is the closest in time from the *in situ* data measurement date. The final spatial and temporal lags between the *in situ* and satellite data are stored in the MDB files.

2.4.3 MDB pair Co-localization with auxiliary data and complementary information

MDB data consist of satellite and *in situ* SSS pairs but also of auxiliary geophysical parameters such as local and history of wind speed and rain rates, as well as various information (climatology, distance to coast, mixed layer depth, barrier layer thickness, etc) that can be derived from *in situ* data and which are included in the final match-up files. The collocation of auxiliary parameters and additional information is done for each *in situ* SSS measurement contained in the match-up files as follows :

If t_{insitu} is the time/date at which the *in situ* measurement is performed, we collect:

- The ASCAT wind speed product of the same day than t_{insitu} found at the ASCAT 1/4° grid node with closest distance from the *in situ* data location and the time series of the ASCAT wind speed at the same node for the 10 days prior the *in situ* measurement day.
- If the *in situ* data is located within the 60°N-60°S band, we select the CMORPH 3-hourly product the closest in time from t_{insitu} and found at the CMORPH 1/4° grid node with closest distance from the *in situ* data location. We then store the time series of the CMORPH rain rate at the same node for the 10 days prior the *in situ* measurement time.

For the given month/year of the *in situ* data, we select the ISAS and WOA fields for the same month (and same year for ISAS fields) and take the SSS analysis (monthly mean, std) found at the closest grid node from the *in situ* measurement.

The distance from the *in situ* SSS data location to the nearest coast is evaluated and provided in km. We use a distance-to-coast map at 1/4° resolution where small islands have been removed.

When vertical profiles of salinity (S) and temperature (T) are made available from the *in situ* measurements used to build the match-up (Argo or sea mammals), the following variables are included into each satellite/*in situ* match-up file:

1. The vertical distribution of pressure at which the profile were measured,
2. The vertical S(z) and T(z) profiles,
3. The vertical potential density anomaly profile $\sigma_0(z)$,

4. The Mixed Layer Depth (MLD). The MLD is defined here as the depth where the potential density has increased from the reference depth (10 meter) by a threshold equivalent to 0.2°C decrease in temperature at constant salinity: $\sigma_0 = \sigma_{010m} + \Delta\sigma_0$ with $\Delta\sigma_0 = \sigma_0(\theta_{10m} - 0.2, S_{10m}) - \sigma_0(\theta_{10m}, S_{10m})$ where θ_{10m} and S_{10m} are the temperature and salinity at the reference depth (i.e. 10 m) (de Boyer Montégut et al. (2004), de Boyer Montégut et al. (2007)).

5. The Top of the Thermocline Depth (TTD) is defined as the depth at which temperature decreases from its 10 m value by 0.2°C.

6. The Barrier Layer if present, is defined as the intermediate layer between the top of the thermocline and the bottom of the density mixed-layer and its thickness (BLT) is defined as the difference between the MLD and the TTD.

7. The vertical profile of the buoyancy frequency $N^2(z)$

The resulting match-ups files are serialized as NetCDF-4 files whose structure depends on the origin of the *in situ* data and is described in section 2.4.4.

2.4.4 Content of the Match-Up NetCDF files

netcdf pimep-mdb_aquarius-l4-iprc-v5-1m_mammal_20100116_v01 {
dimensions:
N_prof = 1 ;
N_LEVELS = 27 ;
N_DAYS_WIND = 10 ;
N_3H_RAIN = 80 ;
STRING = 8 ;
TIME_Sat = UNLIMITED ; // (1 currently)
variables:
float DATE_MAMMAL(N_prof) ;
DATE_MAMMAL:long_name = ”Date of marine mammal profile” ;
DATE_MAMMAL:units = ”days since 1990-01-01 00:00:00” ;
DATE_MAMMAL:standard_name = ”time” ;
DATE_MAMMAL:_FillValue = -999.f ;
float LATITUDE_MAMMAL(N_prof) ;
LATITUDE_MAMMAL:long_name = ”Latitude of marine mammal profile” ;
LATITUDE_MAMMAL:units = ”degrees_north” ;
LATITUDE_MAMMAL:valid_min = -90. ;
LATITUDE_MAMMAL:valid_max = 90. ;
LATITUDE_MAMMAL:standard_name = ”latitude” ;
LATITUDE_MAMMAL:_FillValue = -999.f ;
float LONGITUDE_MAMMAL(N_prof) ;
LONGITUDE_MAMMAL:long_name = ”Longitude of mammal profile” ;
LONGITUDE_MAMMAL:units = ”degrees_east” ;
LONGITUDE_MAMMAL:valid_min = -180. ;
LONGITUDE_MAMMAL:valid_max = 180. ;
LONGITUDE_MAMMALS:standard_name = ”longitude” ;
LONGITUDE_MAMMAL:_FillValue = -999.f ;
float SSS_DEPTH_MAMMAL(N_prof) ;
SSS_DEPTH_MAMMAL:long_name = ”Sea water pressure at marine mammal location

(equals 0 at sea level)" ;
SSS_DEPTH_MAMMAL:units = "decibar" ;
SSS_DEPTH_MAMMAL:standard_name = "sea_water_pressure" ;
SSS_DEPTH_MAMMAL:_FillValue = -999.f ;
float SSS_MAMMAL(N_prof) ;
SSS_MAMMAL:long_name = "Mammals SSS" ;
SSS_MAMMAL:units = "1" ;
SSS_MAMMAL:salinity_scale = "Practical Salinity Scale(PSS-78)" ;
SSS_MAMMAL:standard_name = "sea_water_salinity" ;
SSS_MAMMAL:_FillValue = -999.f ;
float SST_MAMMAL(N_prof) ;
SST_MAMMAL:long_name = "Mammals SST" ;
SST_MAMMAL:units = "degree Celsius" ;
SST_MAMMAL:standard_name = "sea_water_temperature" ;
SST_MAMMAL:_FillValue = -999.f ;
float DISTANCE_TO_COAST_MAMMAL(N_prof) ;
DISTANCE_TO_COAST_MAMMAL:long_name = "Distance to coasts at marine mammal location" ;
DISTANCE_TO_COAST_MAMMAL:units = "km" ;
DISTANCE_TO_COAST_MAMMAL:_FillValue = -999.f ;
float PLATFORM_NUMBER_MAMMAL(N_prof) ;
PLATFORM_NUMBER_MAMMAL:long_name = "Mammals unique identifier" ;
PLATFORM_NUMBER_MAMMAL:conventions = "WMO float identifier : A9IIIII" ;
PLATFORM_NUMBER_MAMMAL:units = "1" ;
PLATFORM_NUMBER_MAMMAL:_FillValue = -999.f ;
float PSAL_MAMMAL(N_prof, N_LEVELS) ;
PSAL_MAMMAL:long_name = "Mammals salinity profile" ;
PSAL_MAMMAL:units = "1" ;
PSAL_MAMMAL:salinity_scale = "Practical Salinity Scale (PSS-78)" ;
PSAL_MAMMAL:standard_name = "sea_water_salinity" ;
PSAL_MAMMAL:_FillValue = -999.f ;
float TEMP_MAMMAL(N_prof, N_LEVELS) ;
TEMP_MAMMAL:long_name = "Mammals temperature profile" ;
TEMP_MAMMAL:units = "degree Celsius" ;
TEMP_MAMMAL:standard_name = "sea_water_temperature" ;
TEMP_MAMMAL:_FillValue = -999.f ;
float PRES_MAMMAL(N_prof, N_LEVELS) ;
PRES_MAMMAL:long_name = "Mammals pressure profile" ;
PRES_MAMMAL:units = "decibar" ;
PRES_MAMMAL:standard_name = "sea_water_pressure" ;
PRES_MAMMAL:_FillValue = -999.f ;
float RHO_MAMMAL(N_prof, N_LEVELS) ;
RHO_MAMMAL:long_name = "Mammals in-situ density profile" ;
RHO_MAMMAL:units = "kg/m" ;
RHO_MAMMAL:_FillValue = -999.f ;
float SIGMA0_MAMMAL(N_prof, N_LEVELS) ;
SIGMA0_MAMMAL:long_name = "Mammals potential density anomaly profile" ;
SIGMA0_MAMMAL:units = "kg/m^3" ;
SIGMA0_MAMMAL:_FillValue = -999.f ;

float N2_MAMMAL(N_prof, N_LEVELS) ;
N2_MAMMAL:long_name = ”Mammals buoyancy frequency profile” ;
N2_MAMMAL:units = ”$1/s^2$” ;
N2_MAMMAL:_FillValue = -999.f ;
float MLD_MAMMAL(N_prof) ;
MLD_MAMMAL:long_name = ”Mixed Layer Depth (MLD) calculated from marine mammal profile (depth where $\sigma_0 = \sigma_{010m} + \Delta\sigma_0$ with $\Delta\sigma_0 = \sigma_0(\theta_{10m} - 0.2, S_{10m}) - \sigma_0(\theta_{10m}, S_{10m})$)” ;
MLD_MAMMAL:units = ”m” ;
MLD_MAMMAL:_FillValue = -999.f ;
float TTD_MAMMAL(N_prof) ;
TTD_MAMMAL:long_name = ”Top of Thermocline Depth (TTD) calculated from marine mammal profile (depth where $\theta = \theta_{10m} - 0.2$)” ;
TTD_MAMMAL:units = ”m” ;
TTD_MAMMAL:_FillValue = -999.f ;
float BLT_MAMMAL(N_prof) ;
BLT_MAMMAL:long_name = ”Barrier Layer Thickness (TTD-MLD)” ;
BLT_MAMMAL:units = ”m” ;
BLT_MAMMAL:_FillValue = -999.f ;
float DATE_Satellite_product(TIME_Sat) ;
DATE_Satellite_product:long_name = ”Central time of satellite SSS file” ;
DATE_Satellite_product:units = ”days since 1990-01-01 00:00:00” ;
DATE_Satellite_product:standard_name = ”time” ;
float LATITUDE_Satellite_product(N_prof) ;
LATITUDE_Satellite_product:long_name = ”Satellite product latitude at marine mammal location” ;
LATITUDE_Satellite_product:units = ”degrees_north” ;
LATITUDE_Satellite_product:valid_min = -90. ;
LATITUDE_Satellite_product:valid_max = 90. ;
LATITUDE_Satellite_product:standard_name = ”latitude” ;
LATITUDE_Satellite_product:_FillValue = -999.f ;
float LONGITUDE_Satellite_product(N_prof) ;
LONGITUDE_Satellite_product:long_name = ”Satellite product longitude at marine mammal location” ;
LONGITUDE_Satellite_product:units = ”degrees_east” ;
LONGITUDE_Satellite_product:valid_min = -180. ;
LONGITUDE_Satellite_product:valid_max = 180. ;
LONGITUDE_Satellite_product:standard_name = ”longitude” ;
LONGITUDE_Satellite_product:_FillValue = -999.f ;
float SSS_Satellite_product(N_prof) ;
SSS_Satellite_product:long_name = ”Satellite product SSS at marine mammal location” ;
SSS_Satellite_product:units = ”1” ;
SSS_Satellite_product:salinity_scale = ”Practical Salinity Scale(PSS-78)” ;
SSS_Satellite_product:standard_name = ”sea_surface_salinity” ;
SSS_Satellite_product:_FillValue = -999.f ;
float SST_Satellite_product(N_prof) ;
SST_Satellite_product:long_name = ”Satellite product SST at marine mammal location” ;
SST_Satellite_product:units = ”degree Celsius” ;
SST_Satellite_product:standard_name = ”sea_surface_temperature” ;

SST_Satellite_product:_FillValue = -999.f ;
float Spatial_lags(N_prof) ;
Spatial_lags:long_name = ”Spatial lag between marine mammal location and satellite SSS product pixel center” ;
Spatial_lags:units = ”km” ;
Spatial_lags:_FillValue = -999.f ;
float Time_lags(N_prof) ;
Time_lags:long_name = ”Temporal lag between marine mammal time and satellite SSS product central time” ;
Time_lags:units = ”days” ;
Time_lags:_FillValue = -999.f ;
float ROSSBY_RADIUS_at_MAMMAL(N_prof) ;
ROSSBY_RADIUS_at_MAMMAL:long_name = ”Baroclinic Rossby radius of deformation (Chelton et al., 1998) at marine mammal location” ;
ROSSBY_RADIUS_at_MAMMAL:units = ”km” ;
ROSSBY_RADIUS_at_MAMMAL:_FillValue = -999.f ;
float Ascat_daily_wind_at_MAMMAL(N_prof) ;
Ascat_daily_wind_at_MAMMAL:long_name = ”Daily Ascat wind speed module at marine mammal location” ;
Ascat_daily_wind_at_MAMMAL:units = ”m/s” ;
Ascat_daily_wind_at_MAMMAL:_FillValue = -999.f ;
float CMORPH_3h_Rain_Rate_at_MAMMAL(N_prof) ;
CMORPH_3h_Rain_Rate_at_MAMMAL:long_name = ”3-hourly CMORPH rain rate at marine mammal location” ;
CMORPH_3h_Rain_Rate_at_MAMMAL:units = ”mm/3h” ;
CMORPH_3h_Rain_Rate_at_MAMMAL:_FillValue = -999.f ;
float Ascat_10_prior_days_wind_at_MAMMAL(N_prof, N_DAYS_WIND) ;
Ascat_10_prior_days_wind_at_MAMMAL:long_name = ”Prior 10 days time series of Ascat wind speed module at marine mammal location” ;
Ascat_10_prior_days_wind_at_MAMMAL:units = ”m/s” ;
Ascat_10_prior_days_wind_at_MAMMAL:_FillValue = -999.f ;
float CMORPH_10_prior_days_Rain_Rate_at_MAMMAL(N_prof, N_3H_RAIN) ;
CMORPH_10_prior_days_Rain_Rate_at_MAMMAL:long_name = ”Prior 10 days times series of 3-hourly CMORPH Rain Rate at marine mammal location” ;
CMORPH_10_prior_days_Rain_Rate_at_MAMMAL:units = ”mm/3h” ;
CMORPH_10_prior_days_Rain_Rate_at_MAMMAL:_FillValue = -999.f ;
float SSS_ISAS_at_MAMMAL(N_prof) ;
SSS_ISAS_at_MAMMAL:long_name = ”ISAS SSS (5m depth) at marine mammal location” ;
SSS_ISAS_at_MAMMAL:units = ”1” ;
SSS_ISAS_at_MAMMAL:salinity_scale = ”Practical Salinity Scale(PSS-78)” ;
SSS_ISAS_at_MAMMAL:standard_name = ”sea_water_salinity” ;
SSS_ISAS_at_MAMMAL:_FillValue = -999.f ;
float SSS_PCTVAR_ISAS_at_MAMMAL(N_prof) ;
SSS_PCTVAR_ISAS_at_MAMMAL:long_name = ”Error on ISAS SSS (5m depth) at marine mammal location (% variance)” ;
SSS_PCTVAR_ISAS_at_MAMMAL:units = ”%” ;
SSS_PCTVAR_ISAS_at_MAMMAL:_FillValue = -999.f ;
float SSS_WOA13_at_MAMMAL(N_prof) ;

SSS_WOA13_at_MAMMAL:long_name = ”Annual WOA 2013 (DECAV-1deg) SSS (0m depth) at marine mammal location” ;
SSS_WOA13_at_MAMMAL:units = ”1” ;
SSS_WOA13_at_MAMMAL:salinity_scale = ”Practical Salinity Scale(PSS-78)” ;
SSS_WOA13_at_MAMMAL:standard_name = ”sea_surface_salinity” ;
SSS_WOA13_at_MAMMAL:_FillValue = -999.f ;
float SSS_STD_WOA13_at_MAMMAL(N_prof) ;
SSS_STD_WOA13_at_MAMMAL:long_name = ”Annual WOA 2013 (DECAV-1deg) SSS STD (0m depth) at marine mammal location ” ;
SSS_STD_WOA13_at_MAMMAL:units = ”1” ;
SSS_STD_WOA13_at_MAMMAL:_FillValue = -999.f ;
float SSS_ISAS15_at_MAMMAL(N_prof) ;
SSS_ISAS15_at_MAMMAL:long_name = ”Monthly ISAS-15 SSS (5m depth) at marine mammal location” ;
SSS_ISAS15_at_MAMMAL:units = ”1” ;
SSS_ISAS15_at_MAMMAL:salinity_scale = ”Practical Salinity Scale (PSS-78)” ;
SSS_ISAS15_at_MAMMAL:standard_name = ”sea_water_salinity” ;
SSS_ISAS15_at_MAMMAL:_FillValue = -999.f ;
float SSS_PCTVAR_ISAS15_at_MAMMAL(N_prof) ;
SSS_PCTVAR_ISAS15_at_MAMMAL:long_name = ”Error on monthly ISAS-15 SSS (5m depth) at marine mammal location (% variance)” ;
SSS_PCTVAR_ISAS15_at_MAMMAL:units = ”%” ;
SSS_PCTVAR_ISAS15_at_MAMMAL:_FillValue = -999.f ;
float SSS_WOA18_at_MAMMAL(N_prof) ;
SSS_WOA18_at_MAMMAL:long_name = ”Monthly WOA 2018 (DECAV-1deg) SSS (0m depth) at marine mammal location” ;
SSS_WOA18_at_MAMMAL:units = ”1” ;
SSS_WOA18_at_MAMMAL:salinity_scale = ”Practical Salinity Scale (PSS-78)” ;
SSS_WOA18_at_MAMMAL:standard_name = ”sea_surface_salinity” ;
SSS_WOA18_at_MAMMAL:_FillValue = -999.f ;
float SSS_STD_WOA18_at_MAMMAL(N_prof) ;
SSS_STD_WOA18_at_MAMMAL:long_name = ”Monthly WOA 2018 (DECAV-1deg) SSS STD (0m depth) at marine mammal location ” ;
SSS_STD_WOA18_at_MAMMAL:units = ”1” ;
SSS_STD_WOA18_at_MAMMAL:_FillValue = -999.f ;
float SEA_ICE_CONCENTRATION_at_MAMMAL(N_prof) ;
SEA_ICE_CONCENTRATION_at_MAMMAL:long_name = ”Daily sea ice area fraction (EUMETSAT OSI-SAF OSI-450) at marine mammal location (%)” ;
SEA_ICE_CONCENTRATION_at_MAMMAL:units = ”1” ;
SEA_ICE_CONCENTRATION_at_MAMMAL:standard_name = ”sea_ice_area_fraction” ;
SEA_ICE_CONCENTRATION_at_MAMMAL:_FillValue = -999.f ;
float CCMP_6h_Wind_Speed_at_MAMMAL(N_prof) ;
CCMP_6h_Wind_Speed_at_MAMMAL:long_name = ”6-hourly CCMP wind speed at marine mammal location” ;
CCMP_6h_Wind_Speed_at_MAMMAL:units = ”m s-1” ;
CCMP_6h_Wind_Speed_at_MAMMAL:standard_name = ”wind_speed” ;
CCMP_6h_Wind_Speed_at_MAMMAL:_FillValue = -999.f ;
float CCMP_10_prior_days_Wind_Speed_at_MAMMAL(N_prof, N_DAYS_WIND_CCMP) ;
CCMP_10_prior_days_Wind_Speed_at_MAMMAL:long_name = ”Prior 10 days time series

of CCMP wind speed at marine mammal location" ;
CCMP_10_prior_days_Wind_Speed_at_MAMMAL:units = "m s-1" ;
CCMP_10_prior_days_Wind_Speed_at_MAMMAL:standard_name = "wind_speed" ;
CCMP_10_prior_days_Wind_Speed_at_MAMMAL:_FillValue = -999.f ;
float CDM_GLOBCOLOUR_at_MAMMAL(N_prof) ;
CDM_GLOBCOLOUR_at_MAMMAL:long_name = "8-day Coloured dissolved and detrital organic materials - mean of the binned pixels at marine mammal location" ;
CDM_GLOBCOLOUR_at_MAMMAL:units = "m-1" ;
CDM_GLOBCOLOUR_at_MAMMAL:standard_name = "volume_absorption_coefficient_of_radiative_flux_in_sea_
;
CDM_GLOBCOLOUR_at_MAMMAL:_FillValue = -999.f ;
float CHL1_GLOBCOLOUR_at_MAMMAL(N_prof) ;
CHL1_GLOBCOLOUR_at_MAMMAL:long_name = "8-day Chlorophyll concentration - mean of the binned pixels at marine mammal location" ;
CHL1_GLOBCOLOUR_at_MAMMAL:units = "mg m-3" ;
CHL1_GLOBCOLOUR_at_MAMMAL:standard_name = "mass_concentration_of_chlorophyll_a_in_sea_water"
;
CHL1_GLOBCOLOUR_at_MAMMAL:_FillValue = -999.f ;
float EVAPORATION_OAFLUX_at_MAMMAL(N_prof) ;
EVAPORATION_OAFLUX_at_MAMMAL:long_name = "Daily mean evaporation rate (OAFlux) at marine mammal location" ;
EVAPORATION_OAFLUX_at_MAMMAL:units = "cm year-1" ;
EVAPORATION_OAFLUX_at_MAMMAL:_FillValue = -999.f ;
float SSS_SCRIPPS_at_MAMMAL(N_prof) ;
SSS_SCRIPPS_at_MAMMAL:long_name = "Argo gridded monthly mean SSS (0m depth) from SCRIPPS (Roemmich-Gilson) at marine mammal location" ;
SSS_SCRIPPS_at_MAMMAL:units = "1" ;
SSS_SCRIPPS_at_MAMMAL:salinity_scale = "Practical Salinity Scale (PSS-78)" ;
SSS_SCRIPPS_at_MAMMAL:standard_name = "sea_water_salinity" ;
SSS_SCRIPPS_at_MAMMAL:_FillValue = -999.f ;
float SSS_IPRC_at_MAMMAL(N_prof) ;
SSS_IPRC_at_MAMMAL:long_name = "Argo gridded monthly mean SSS (0m depth) from IPRC at marine mammal location" ;
SSS_IPRC_at_MAMMAL:units = "1" ;
SSS_IPRC_at_MAMMAL:salinity_scale = "Practical Salinity Scale (PSS-78)" ;
SSS_IPRC_at_MAMMAL:standard_name = "sea_water_salinity" ;
SSS_IPRC_at_MAMMAL:_FillValue = -999.f ;
float SST_AVHRR_at_MAMMAL(N_prof) ;
SST_AVHRR_at_MAMMAL:long_name = "Daily OI AVHRR-only v2 SST (Reynolds et al., 2007) at marine mammal location" ;
SST_AVHRR_at_MAMMAL:units = "degree Celsius" ;
SST_AVHRR_at_MAMMAL:standard_name = "sea_water_temperature" ;
SST_AVHRR_at_MAMMAL:_FillValue = -999.f ;
float U_EKMAN_GLOBCURRENT_at_MAMMAL(N_prof) ;
U_EKMAN_GLOBCURRENT_at_MAMMAL:long_name = "15m depth Ekman current velocity: zonal component at marine mammal location" ;
U_EKMAN_GLOBCURRENT_at_MAMMAL:units = "m s-1" ;
U_EKMAN_GLOBCURRENT_at_MAMMAL:_FillValue = -999.f ;
float V_EKMAN_GLOBCURRENT_at_MAMMAL(N_prof) ;

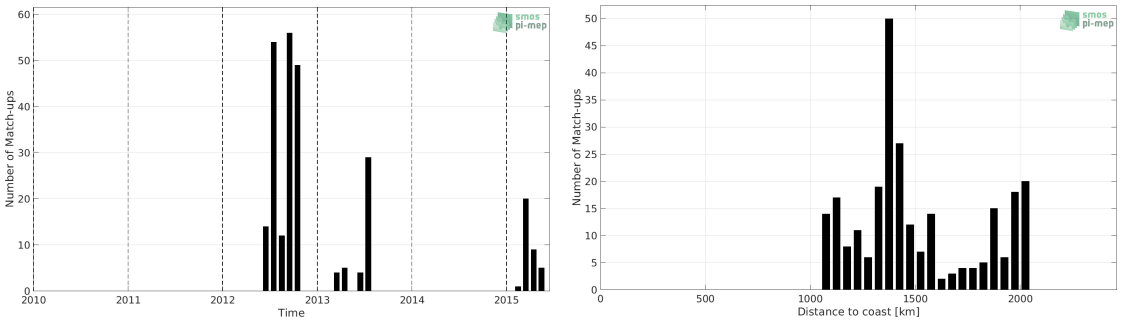
V_EKMAN_GLOBCURRENT_at_MAMMAL:long_name = ”15m depth Ekman current velocity: meridian component at marine mammal location” ;
V_EKMAN_GLOBCURRENT_at_MAMMAL:units = ”m s-1” ;
V_EKMAN_GLOBCURRENT_at_MAMMAL:_FillValue = -999.f ;
float U_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL(N_prof) ;
U_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:long_name = ”Absolute geostrophic velocity: zonal component at marine mammal location” ;
U_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:units = ”m s-1” ;
U_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:_FillValue = -999.f ;
float V_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL(N_prof) ;
V_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:long_name = ”Absolute geostrophic velocity: meridian component at marine mammal location” ;
V_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:units = ”m s-1” ;
V_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:_FillValue = -999.f ;

// global attributes:
:Conventions = ”CF-1.6” ;
:title = ”Marine Mammals Match-Up Database” ; :Satellite_product_name = ”Aquarius SSS L4 OI v5 - Monthly (IPRC)” ;
:Satellite_product_spatial_resolution = ”0.5 deg” ;
:Satellite_product_temporal_resolution = ”Monthly” ;
:Satellite_product_filename = ” v5/glb/monthly/SSS_OI_MO_2011_09_V50.nc” ;
:Match-Up_spatial_window_radius_in_km = 27.5;
:Match-Up_temporal_window_radius_in_days = 15;
:start_time = ”20100114T000005Z” ;
:stop_time = ”20100118T235026Z” ;
:northernmost_latitude = 77.676f ;
:sourthenmost_latitude = -66.423f ;
:westernmost_longitude = -179.219f ;
:easternmost_longitude = 179.199f ;
:geospatial_lat_units = ”degrees north” ;
:geospatial_lat_resolution = ”0.5 deg” ;
:geospatial_lon_units = ”degrees east” ;
:geospatial_lon_resolution = ”0.5 deg” ;
:institution = ”ESA-IFREMER-ODL-OCEANSCOPE” ;
:project_name = ”SMOS Pilot-Mission Exploitation Platform (Pi-MEP) for salinity” ;
:project_url = ”https://www.salinity-pimep.org” ;
:license = ”Pi-MEP data use is free and open” ;
:product_version = ”1.0” ;
:keywords = ”Oceans > Ocean Salinity > Sea Surface Salinity” ;
:acknowledgment = ”Please acknowledge the use of these data with the following statement: These data were provided by the SMOS Pilot-Mission Exploitation Platform (Pi-MEP) for salinity” ;
:source = ” v5/glb/monthly/SSS_OI_MO_2011_09_V50.nc” ;
:references = ”https://www.salinity-pimep.org” ;
:history = ”Processed on 2018-04-18 using MDB_generator” ;
:date_created = ”2018-04-18 17:09:30” ;
}

2.5 MDB characteristics for the particular *in situ*/satellite pairs

2.5.1 Number of paired SSS data as a function of time and distance to coast

Figure 1 shows the time (a) and distance to coast (b) distributions of the match-ups between Sea mammals and Aquarius SSS L4 OI v5 - Monthly (IPRC) for the Atlantic Ocean Pi-MEP region and for the full satellite product period.

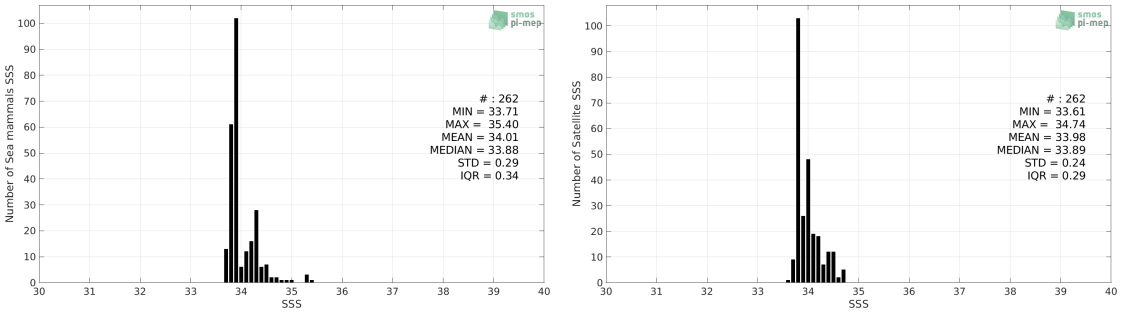


(a) (b)

Figure 1: Number of match-ups between Sea mammals and Aquarius SSS L4 OI v5 - Monthly (IPRC) SSS as a function of time (a) and as function of the distance to coast (b) over the Atlantic Ocean Pi-MEP region and for the full satellite product period.

2.5.2 Histograms of the SSS match-ups

Figure 2 shows the SSS distribution of Sea mammals (a) and Aquarius SSS L4 OI v5 - Monthly (IPRC) (b) considering all match-up pairs per bins of 0.1 over the Atlantic Ocean Pi-MEP region and for the full satellite product period.

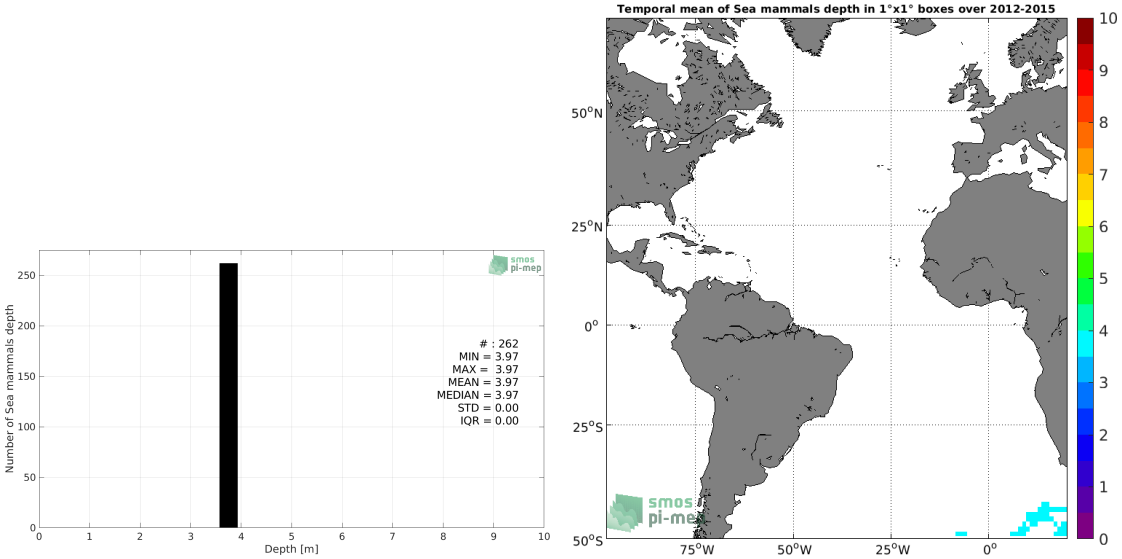


(a) (b)

Figure 2: Histograms of SSS from Sea mammals (a) and Aquarius SSS L4 OI v5 - Monthly (IPRC) (b) considering all match-up pairs per bins of 0.1 over the Atlantic Ocean Pi-MEP region and for the full satellite product period.

2.5.3 Distribution of *in situ* SSS depth measurements

Figure 3 shows the depth distribution of the upper level SSS measurements from Sea mammals in the Match-up DataBase for the Atlantic Ocean Pi-MEP region (a) and temporal mean spatial distribution of pressure of the *in situ* SSS data over 1°x1° boxes and for the full satellite product period (b).



(a) (b)

Figure 3: Histograms of the depth of the upper level SSS measurements from Sea mammals in the Match-up DataBase for the Atlantic Ocean Pi-MEP region (a) and temporal mean spatial distribution of pressure of the *in situ* SSS data over 1°x1° boxes and for the full satellite product period (b).

2.5.4 Spatial Distribution of Match-ups

The number of SSS match-ups between Sea mammals SSS and the Aquarius SSS L4 OI v5 - Monthly (IPRC) SSS product for the Atlantic Ocean Pi-MEP region over 1°x1° boxes and for the full satellite product period is shown in Figure 4.

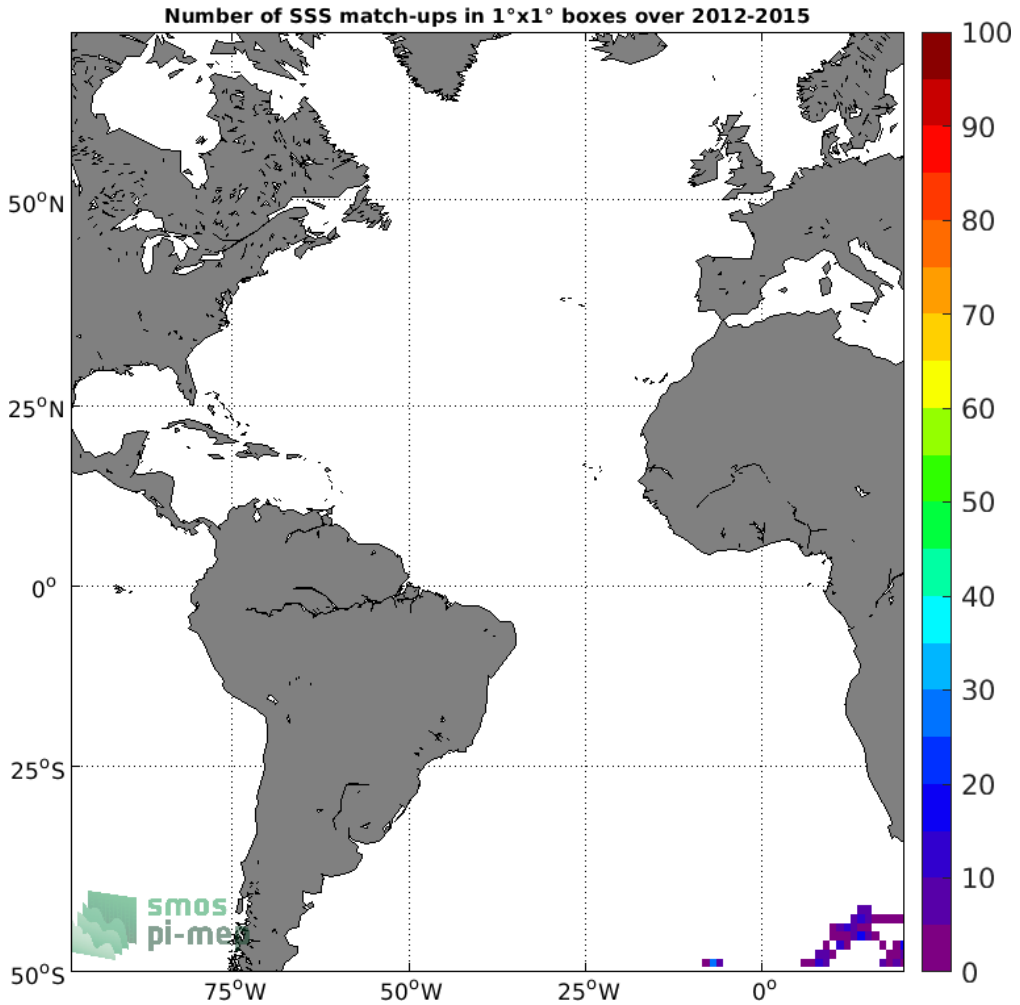
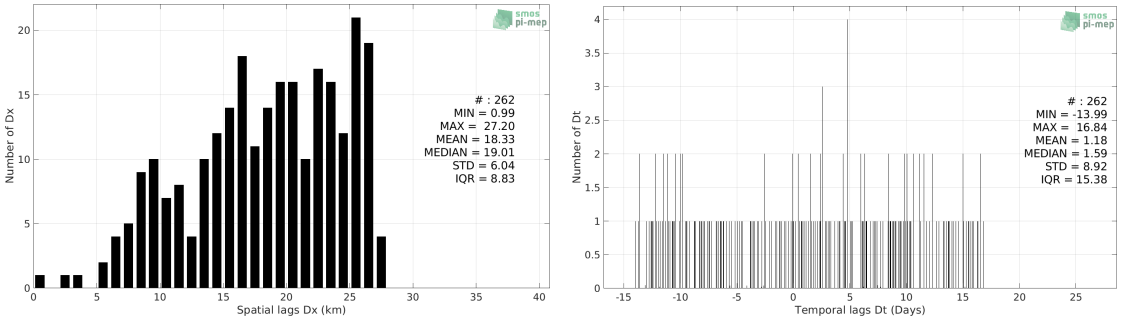


Figure 4: Number of SSS match-ups between Sea mammals SSS and the Aquarius SSS L4 OI v5 - Monthly (IPRC) SSS product for the Atlantic Ocean Pi-MEP region over 1°x1° boxes and for the full satellite product period.

2.5.5 Histograms of the spatial and temporal lags of the match-ups pairs

Figure 5 reveals the spatial (left) and temporal (right) lags between the location/time of the Sea mammals measurement and the position/date of the corresponding Aquarius SSS L4 OI v5 - Monthly (IPRC) SSS pixel of all match-ups pairs.



(a) (b)

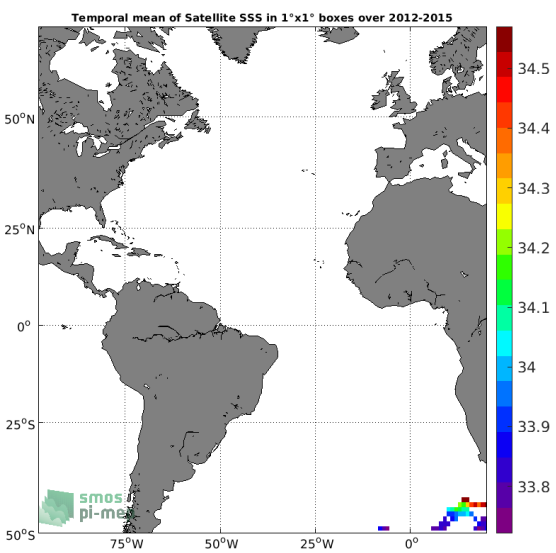
Figure 5: Histograms of the spatial (a) and temporal (b) lags between the location/time of the Sea mammals measurement and the date of the corresponding Aquarius SSS L4 OI v5 - Monthly (IPRC) SSS pixel.

3 MDB file Analyses

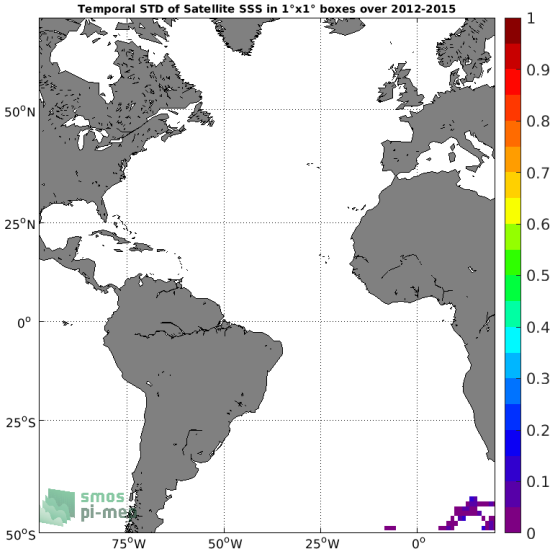
3.1 Spatial Maps of the Temporal mean and Std of *in situ* and satellite SSS and of the difference (ΔSSS)

In Figure 6, we show maps of temporal mean (left) and standard deviation (right) of the Aquarius SSS L4 OI v5 - Monthly (IPRC) (top) and of the Sea mammals *in situ* dataset at the collected Pi-MEP match-up pairs. The temporal mean and std are gridded over the full satellite product period and over spatial boxes of size 1°x1°.

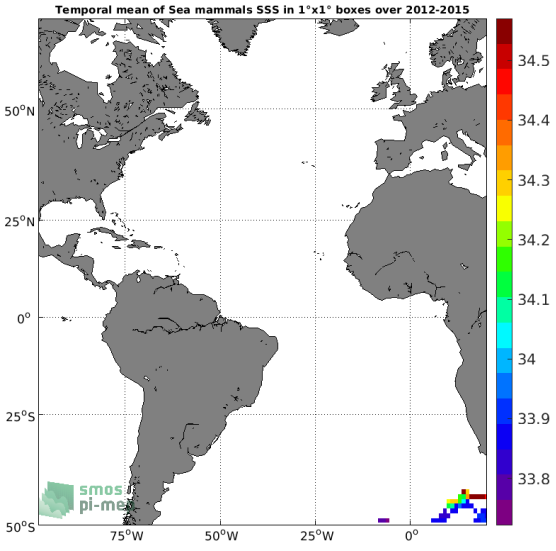
At the bottom of Figure 6, the temporal mean (left) and standard deviation (right) of the differences between the satellite SSS product and *in situ* data found at match-up pairs, namely ΔSSS(Satellite -Sea mammals), is also gridded over the full satellite product period and over spatial boxes of size 1°x1°.



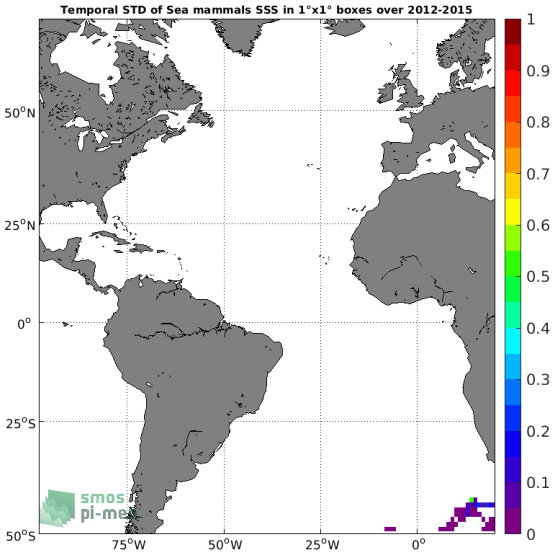
(a) MEAN(Satellite SSS)



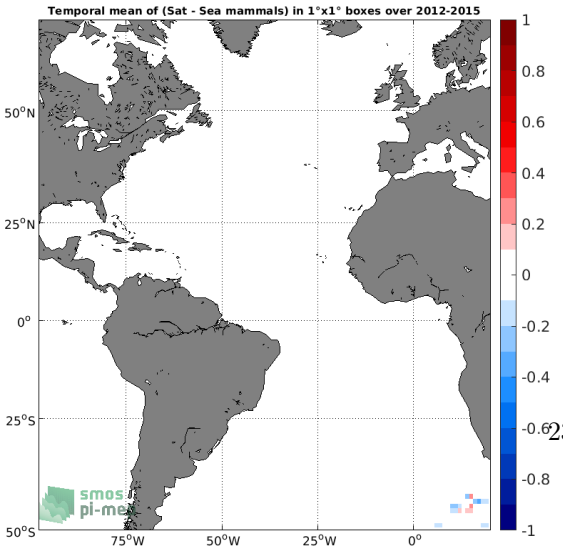
(b) Std(Satellite SSS)



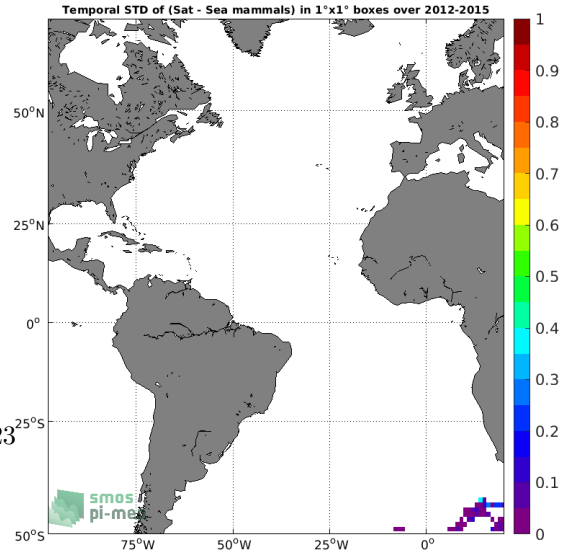
(c) MEAN(Sea mammals SSS)



(d) Std(Sea mammals SSS)



(e) MEAN(ΔSSS) (Satellite - Sea mammals)



(f) Std(ΔSSS) (Satellite - Sea mammals)

Figure 6: Temporal mean (left) and Std (right) of SSS from Aquarius SSS L4 OI v5 - Monthly (IPRC) (top), Sea mammals (middle), and of ΔSSS (Satellite - Sea mammals). Only match-up pairs are used to generate these maps.

3.2 Time series of the monthly median and Std of *in situ* and satellite SSS and of the difference (ΔSSS)

In the top panel of Figure 7, we show the time series of the monthly median SSS estimated over the full Atlantic Ocean Pi-MEP region for both Aquarius SSS L4 OI v5 - Monthly (IPRC) satellite SSS product (in black) and the Sea mammals *in situ* dataset (in blue) at the collected Pi-MEP match-up pairs.

In the middle panel of Figure 7, we show the time series of the monthly median of ΔSSS (Satellite - Sea mammals) for the collected Pi-MEP match-up pairs and estimated over the full Atlantic Ocean Pi-MEP region.

In the bottom panel of Figure 7, we show the time series of the monthly standard deviation of ΔSSS (Satellite - Sea mammals) for the collected Pi-MEP match-up pairs and estimated over the full Atlantic Ocean Pi-MEP region.

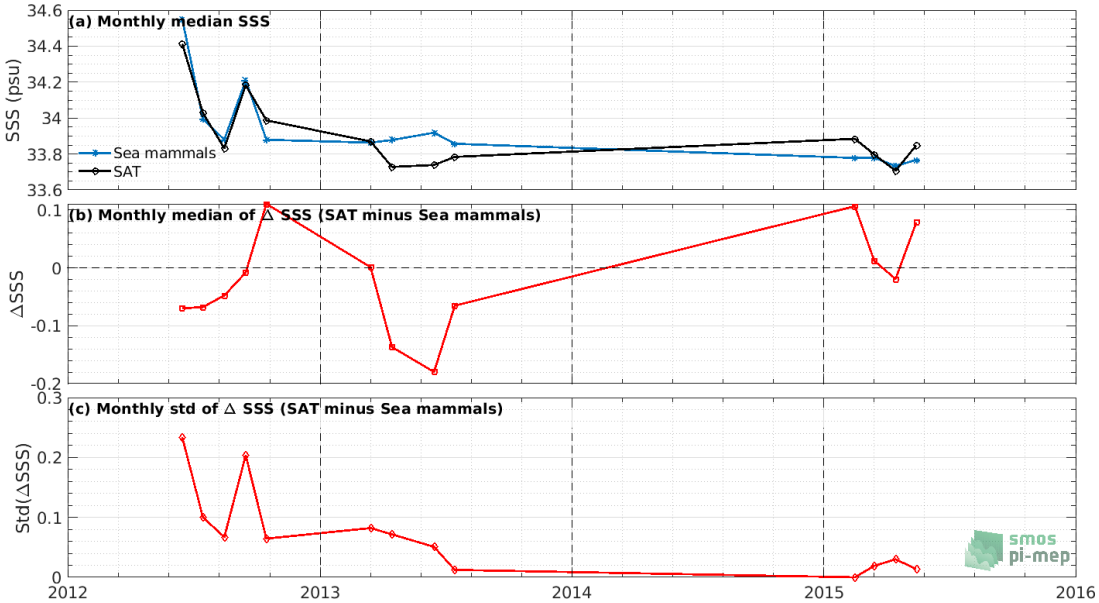


Figure 7: Time series of the monthly median SSS (top), median of ΔSSS (Satellite - Sea mammals) and Std of ΔSSS (Satellite - Sea mammals) over the Atlantic Ocean Pi-MEP region considering all match-ups collected by the Pi-MEP.

3.3 Zonal mean and Std of *in situ* and satellite SSS and of the difference (ΔSSS)

In Figure 8 left panel, we show the zonal mean SSS considering all Pi-MEP match-up pairs for both Aquarius SSS L4 OI v5 - Monthly (IPRC) satellite SSS product (in black) and the Sea mammals *in situ* dataset (in blue). The full satellite SSS product period is used to derive the mean.

In the right panel of Figure 8, we show the zonal mean of ΔSSS (Satellite - Sea mammals) for all the collected Pi-MEP match-up pairs estimated over the full satellite product period.

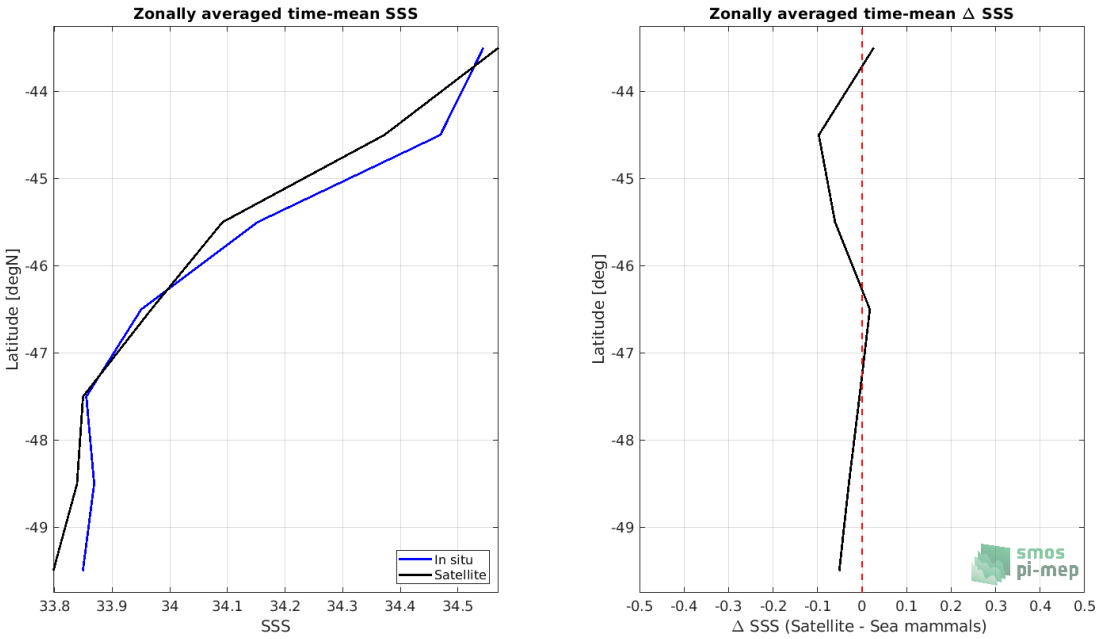
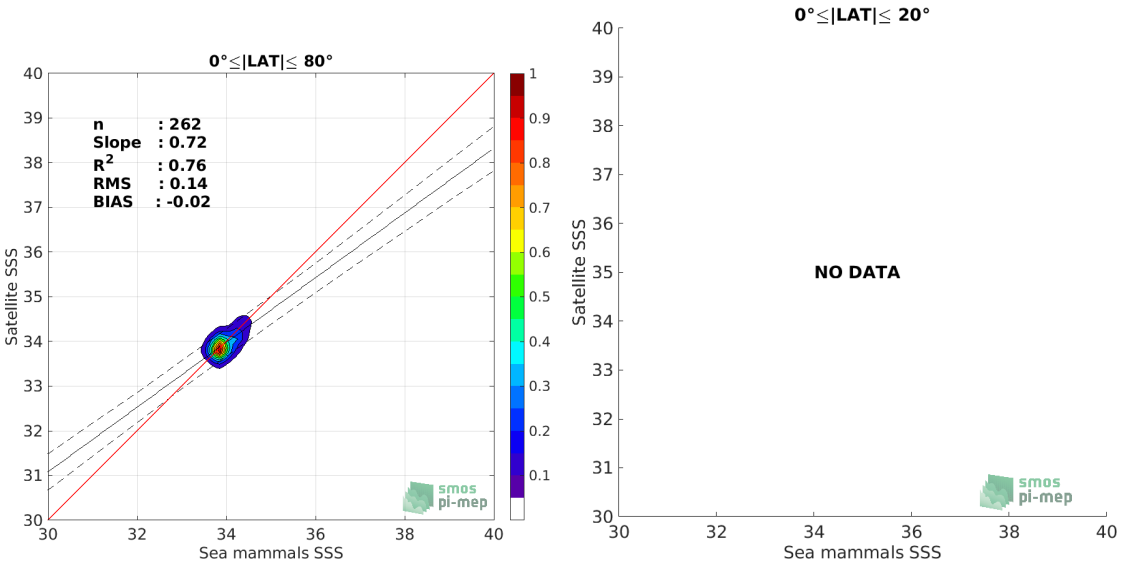


Figure 8: Left panel: Zonal mean SSS from Aquarius SSS L4 OI v5 - Monthly (IPRC) satellite product (black) and from Sea mammals (blue). Right panel: Zonal mean of ΔSSS (Satellite - Sea mammals) for all the collected Pi-MEP match-up pairs estimated over the full satellite product period.

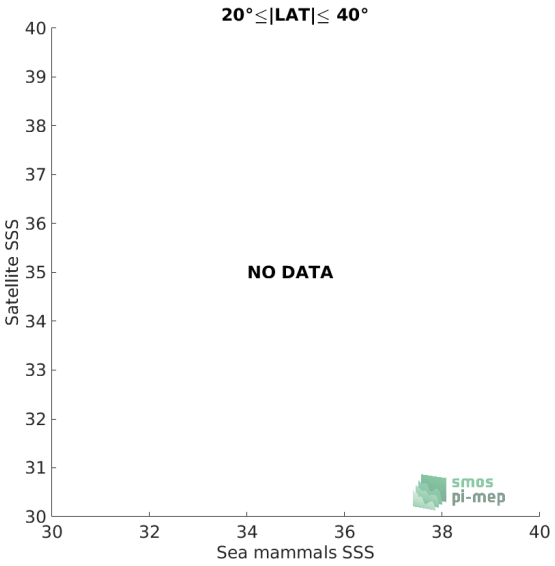
3.4 Scatterplots of satellite vs *in situ* SSS by latitudinal bands

In Figure 9, contour maps of the concentration of Aquarius SSS L4 OI v5 - Monthly (IPRC) SSS (y-axis) versus Sea mammals SSS (x-axis) at match-up pairs for different latitude bands: (a) 80°S-80°N, (b) 20°S-20°N, (c) 40°S-20°S and 20°N-40°N and (d) 60°S-40°S and 40°N-60°N. For each plot, the red line shows x=y. The black thin and dashed lines indicate a linear fit through the data cloud and the ±95% confidence levels, respectively. The number match-up pairs n, the slope and R^2 coefficient of the linear fit, the root mean square (RMS) and the mean bias between satellite and *in situ* data are indicated for each latitude band in each plots.

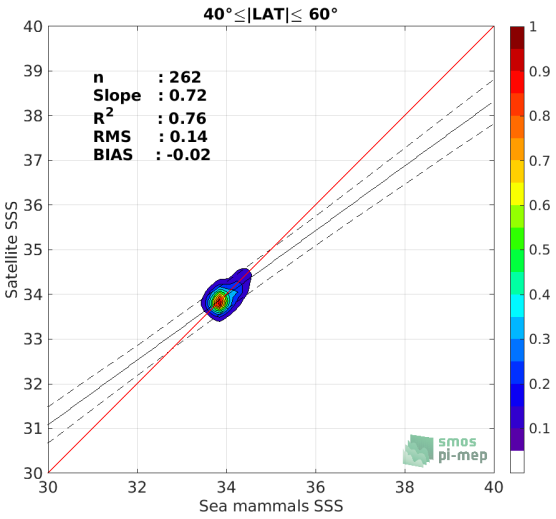


(a) $0° \leq |\text{LAT}| \leq 80°$

(b) $0° \leq |\text{LAT}| \leq 20°$



(c) $20° \leq |\text{LAT}| \leq 40°$

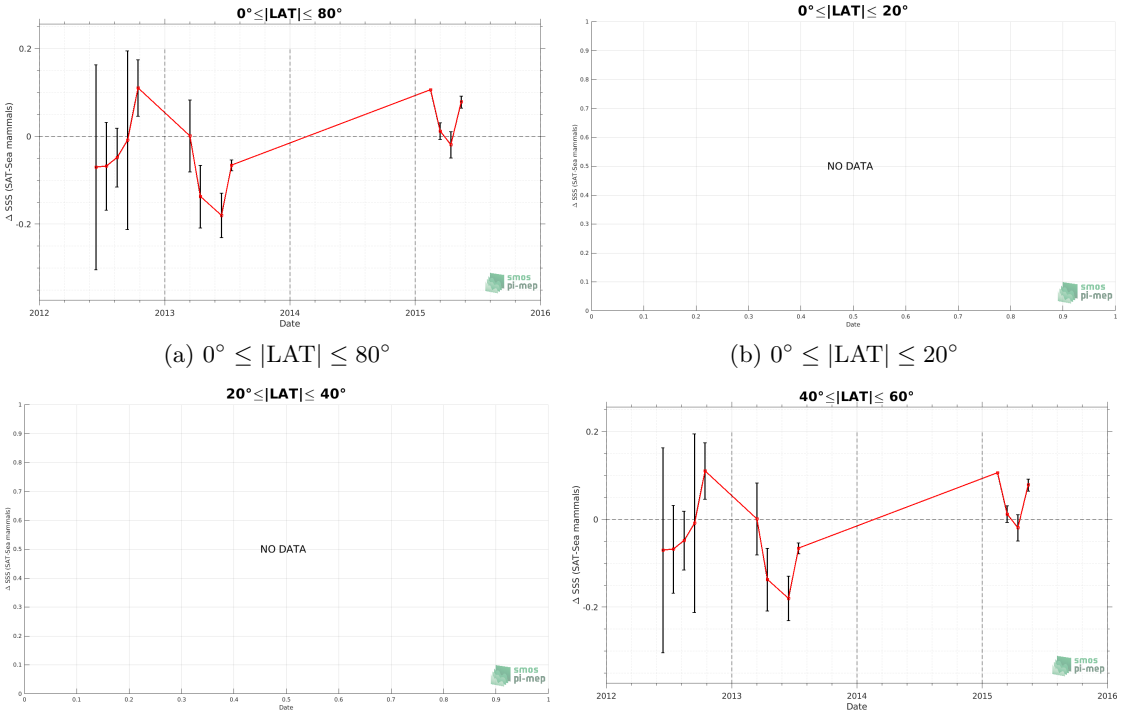


(d) $40° \leq |\text{LAT}| \leq 60°$

Figure 9: Contour maps of the concentration of Aquarius SSS L4 OI v5 - Monthly (IPRC) SSS (y-axis) versus Sea mammals SSS (x-axis) at match-up pairs for different latitude bands. For each plot, the red line shows x=y. The black thin and dashed lines indicate a linear fit through the data cloud and the ±95% confidence levels, respectively. The number match-up pairs n, the slope and R^2 coefficient of the linear fit, the root mean square (RMS) and the mean bias between satellite and *in situ* data are indicated for each latitude band in each plots.

3.5 Time series of the monthly median and Std of ΔSSS sorted by latitudinal bands

In Figure 10, time series of the monthly median (red curves) of ΔSSS (Satellite - Sea mammals) and ±1 Std (black vertical thick bars) as function of time for all the collected Pi-MEP match-up pairs estimated over the Atlantic Ocean Pi-MEP region and for the full satellite product period are shown for different latitude bands: (a) 80°S-80°N, (b) 20°S-20°N, (c) 40°S-20°S and 20°N-40°N and (d) 60°S-40°S and 40°N-60°N.



(a) 0° ≤ |LAT| ≤ 80°

(b) 0° ≤ |LAT| ≤ 20°

(c) 20° ≤ |LAT| ≤ 40°

(d) 40° ≤ |LAT| ≤ 60°

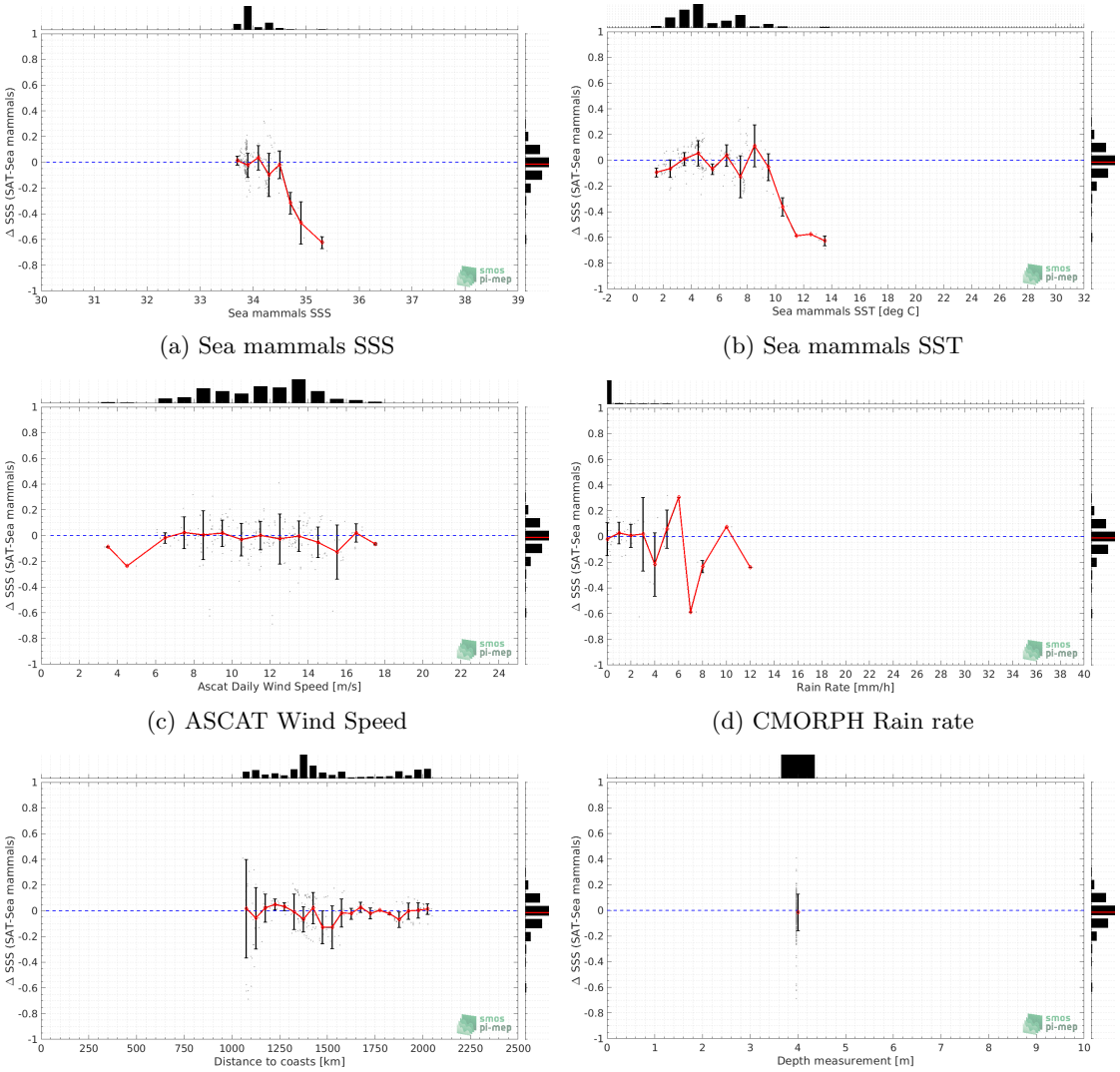
Figure 10: Monthly median (red curves) of ΔSSS (Satellite - Sea mammals) and ±1 Std (black vertical thick bars) as function of time for all the collected Pi-MEP match-up pairs estimated over the Atlantic Ocean Pi-MEP region and for the full satellite product period are shown for different latitude bands: (a) 80°S-80°N, (b) 20°S-20°N, (c) 40°S-20°S and 20°N-40°N and (d) 60°S-40°S and 40°N-60°N.

3.6 ΔSSS sorted as function of geophysical parameters

In Figure 11, we classify the match-up differences ΔSSS (Satellite - *in situ*) between Aquarius SSS L4 OI v5 - Monthly (IPRC) and Sea mammals SSS as function of the geophysical conditions at match-up points. The median and std of ΔSSS (Satellite - Sea mammals) is thus evaluated as function of the

- *in situ* SSS values per bins of width 0.2,
- *in situ* SST values per bins of width 1°C,
- ASCAT daily wind values per bins of width 1 m/s,

- CMORPH 3-hourly rain rates per bins of width 1 mm/h, and,
- distance to coasts per bins of width 50 km.
- *in situ* measurement depth (if relevant).



(a) Sea mammals SSS

(b) Sea mammals SST

(c) ASCAT Wind Speed

(d) CMORPH Rain rate

(e) Distance to coast

(f) *In situ* measurement Depth

Figure 11: ΔSSS (Satellite - Sea mammals) sorted as function of Sea mammals SSS values a), Sea mammals SST b), ASCAT Wind speed c), CMORPH rain rate d), distance to coast (e) and *in situ* measurement depth (f). In all plots the median and Std of ΔSSS for each bin is indicated by the red curves and black vertical thick bars (±1 Std)

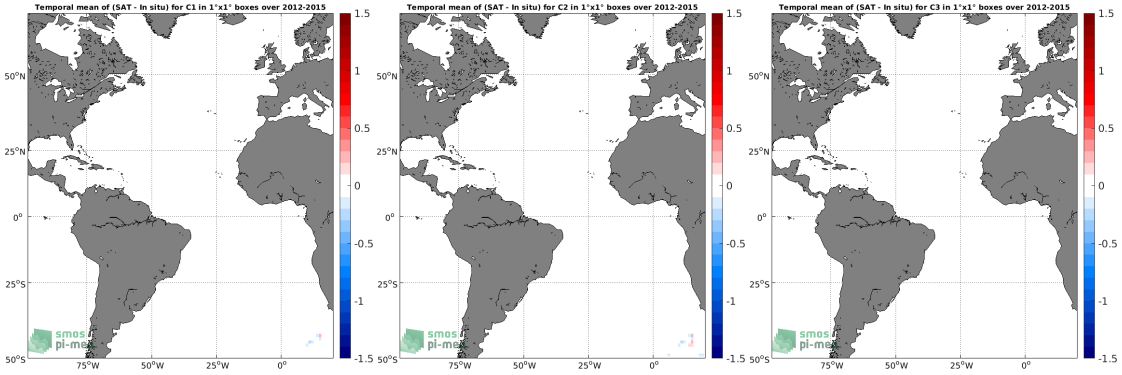
3.7 ΔSSS maps and statistics for different geophysical conditions

In Figures 12 and 13, we focus on sub-datasets of the match-up differences ΔSSS (Satellite - *in situ*) between Aquarius SSS L4 OI v5 - Monthly (IPRC) and Sea mammals for the following

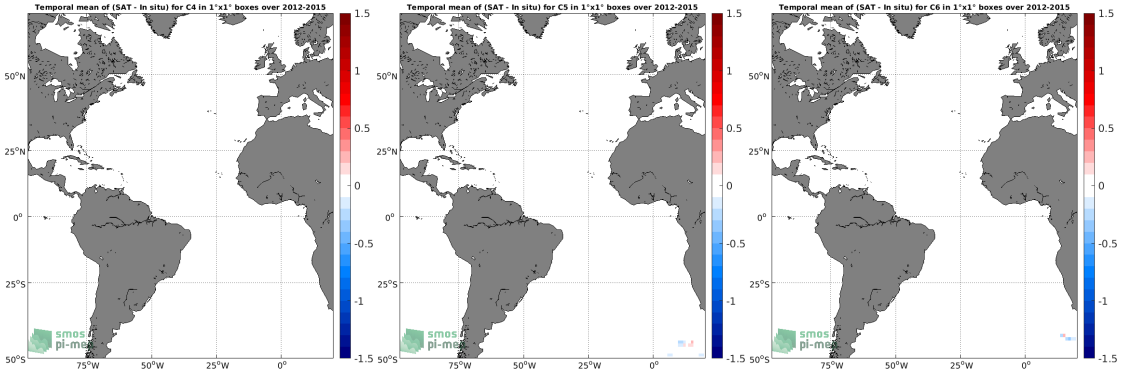
specific geophysical conditions:

- **C1**:if the local value at *in situ* location of estimated rain rate 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.
- **C2**:if the local value at *in situ* location of estimated rain rate is zero, mean daily wind is in the range [3, 12] m/s.
- **C3**:if the local value at *in situ* location of estimated rain rate is high (ie. > 1 mm/h) and mean daily wind is low (ie. < 4 m/s).
- **C4**:if the mixed layer is shallow with depth <20m.
- **C5**:if the *in situ* data is located where the climatological SSS standard deviation is low (ie. above < 0.2).
- **C6**:if the *in situ* data is located where the climatological SSS standard deviation is high (ie. above > 0.2).

For each of these conditions, the temporal mean (gridded over spatial boxes of size 1°x1°) and the histogram of the difference ΔSSS (Satellite - *in situ*) are presented.

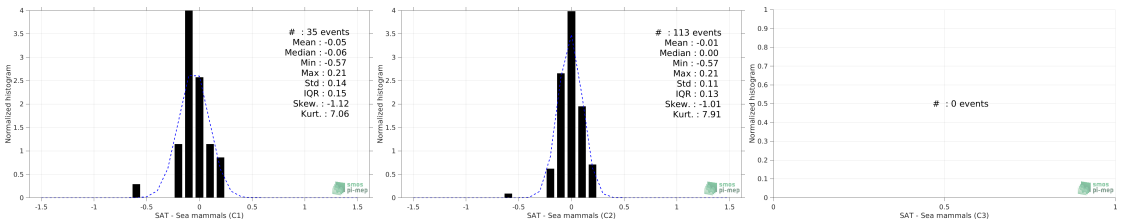


(a) RR=0 mm/h, 3< U_{10} <12 m/s, SST>5°C, distance to coast > 800 km (b) RR=0 mm/h, 3< U_{10} <12 m/s (c) RR>1mm/h and U_{10} <4m/s



(d) MLD<20m (e) WOA2013 SSS Std<0.2 (f) WOA2013 SSS Std>0.2

Figure 12: Temporal mean gridded over spatial boxes of size 1°x1° of ΔSSS (Aquarius SSS L4 OI v5 - Monthly (IPRC) - Sea mammals) for 6 different subdatasets corresponding to:RR=0 mm/h, 3< U_{10} <12 m/s, SST>5°C, distance to coast > 800 km (a), RR=0 mm/h, 3< U_{10} <12 m/s (b), RR>1mm/h and U_{10} <4m/s (c),MLD<20m (d),WOA2013 SSS Std<0.2 (e),WOA2013 SSS Std>0.2 (f).



(a) RR=0 mm/h, 3< U_{10} <12 m/s, SST>5°C, distance to coast > 800 km (b) RR=0 mm/h, 3< U_{10} <12 m/s (c) RR>1mm/h and U_{10} <4m/s

(d) MLD<20m (e) WOA2013 SSS Std<0.2 (f) WOA2013 SSS Std>0.2

Figure 13: Normalized histogram of ΔSSS (Aquarius SSS L4 OI v5 - Monthly (IPRC) - Sea mammals) for 6 different subdatasets corresponding to: RR=0 mm/h, 3< U_{10} <12 m/s, SST>5°C, distance to coast > 800 km (a), RR=0 mm/h, 3< U_{10} <12 m/s (b), RR>1mm/h and U_{10} <4m/s (c), MLD<20m (d), WOA2013 SSS Std<0.2 (e), WOA2013 SSS Std>0.2 (f).

4 Summary

► Table 1 shows the mean, median, standard deviation (Std), root mean square (RMS), interquartile range (IQR), correlation coefficient (r^2) and robust standard deviation (Std*) of the match-up differences ΔSSS (Satellite - *in situ*) between Aquarius SSS L4 OI v5 - Monthly (IPRC) and Sea mammals derived over the Atlantic Ocean Pi-MEP region and for the full satellite product period and for the following conditions:

- all: All the match-up pairs satellite/*in situ* SSS are used to derive the statistics
- C1: only pairs where RR=0 mm/h, 3< U_{10} <12 m/s, SST>5°C, distance to coast > 800 km
- C2: only pairs where RR=0 mm/h, 3< U_{10} <12 m/s
- C3: only pairs where RR>1mm/h and U_{10} <4m/s
- C4: only pairs where MLD<20m
- C5: only pairs where WOA2013 SSS Std<0.2
- C6: only pairs at WOA2013 SSS Std>0.2
- C7a: only pairs where distance to coast is < 150 km.
- C7b: only pairs where distance to coast is in the range [150, 800] km.
- C7c: only pairs where distance to coast is > 800 km.
- C8a: only pairs where *in situ* SST is < 5°C.

- C8b: only pairs where *in situ* SST is in the range [5, 15]°C.
- C8c: only pairs where *in situ* SST is > 15°C.
- C9a: only pairs where *in situ* SSS is < 33.
- C9b: only pairs where *in situ* SSS is in the range [33, 37].
- C9c: only pairs where *in situ* SSS is > 37.

Table 1: Statistics of ΔSSS (Satellite - Sea mammals)

Condition	#	Median	Mean	Std	RMS	IQR	r^2	Std*
all	262	-0.01	-0.02	0.14	0.14	0.14	0.760	0.10
C1	35	-0.06	-0.05	0.14	0.15	0.15	0.755	0.11
C2	113	0.00	-0.01	0.11	0.11	0.13	0.770	0.10
C3	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C4	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C5	214	-0.02	-0.02	0.10	0.10	0.13	0.592	0.09
C6	48	0.03	-0.05	0.26	0.26	0.21	0.500	0.14
C7a	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C7b	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C7c	262	-0.01	-0.02	0.14	0.14	0.14	0.760	0.10
C8a	163	0.00	0.01	0.09	0.09	0.14	0.182	0.09
C8b	99	-0.06	-0.08	0.19	0.21	0.21	0.632	0.15
C8c	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C9a	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C9b	262	-0.01	-0.02	0.14	0.14	0.14	0.760	0.10
C9c	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN

► Table 2 presents statistics of ΔSSS (Satellite - ISAS) using only ISAS SSS values with PCTVAR<80%.

Table 2: Statistics of ΔSSS (Satellite - ISAS)

Condition	#	Median	Mean	Std	RMS	IQR	r^2	Std*
all	262	0.03	0.04	0.07	0.08	0.08	0.921	0.06
C1	35	0.00	0.02	0.06	0.06	0.05	0.959	0.01
C2	113	0.02	0.03	0.06	0.07	0.08	0.914	0.05
C3	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C4	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C5	214	0.02	0.03	0.06	0.07	0.08	0.777	0.05
C6	48	0.08	0.06	0.08	0.10	0.13	0.847	0.08
C7a	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C7b	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C7c	262	0.03	0.04	0.07	0.08	0.08	0.921	0.06
C8a	163	0.04	0.04	0.07	0.08	0.09	0.509	0.06
C8b	99	0.03	0.04	0.07	0.08	0.08	0.929	0.06
C8c	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C9a	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C9b	262	0.03	0.04	0.07	0.08	0.08	0.921	0.06
C9c	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN

► Numerical values can be downloaded as csv files for Table 1 and Table 2.

5 More Comparison/Validation Materials

5.1 Comparisons with other satellite products

▶ Table 1 shows the mean, median, standard deviation (Std), root mean square (RMS), interquartile range (IQR), correlation coefficient (r^2) and robust standard deviation (Std*) of the match-up differences ΔSSS (Satellite - Sea mammals) between different satellite products and **Sea mammals** derived over the Atlantic Ocean Pi-MEP region considering all match-up pairs satellite/*in situ* SSS values to derive the statistics:

Table 1: Statistics of ΔSSS (Satellite - Sea mammals) - All

Satellite products	#	Median	Mean	Std	RMS	IQR	r^2	Std*
smos-l2-v700	171	-0.48	-0.52	1.94	2.00	2.11	0.091	1.61
smap-l2-jpl-v5.0	13	0.73	0.87	1.92	2.04	2.58	0.007	2.09
aquarius-l2-or-v5	112	0.27	0.12	0.67	0.68	0.79	0.045	0.62
aquarius-l2-jpl-v5	115	0.29	0.26	0.85	0.88	0.90	0.048	0.66
smos-l3-catds-cpdc-v321-l2q	107	0.22	0.23	1.64	1.65	1.83	0.052	1.57
smos-l3-catds-cpdc-v317-10d-25km	633	-0.06	-0.14	1.11	1.12	1.26	0.195	0.93
smos-l3-catds-cpdc-v317-1m-25km	724	-0.01	-0.15	1.14	1.15	1.00	0.278	0.76
smos-l3-catds-locean-v5-9d	1149	-0.32	-0.40	0.65	0.77	0.68	0.393	0.51
smos-l3-catds-locean-v5-18d	1149	-0.21	-0.23	0.36	0.43	0.39	0.767	0.30
smos-l3-bec-v2-9d	256	0.05	0.04	0.35	0.35	0.46	0.203	0.37
smos-l3-icdc-v3-1m	250	-0.12	-0.04	0.75	0.75	1.06	0.107	0.79
smap-l3-rss-v4-8dr	16	-0.01	0.06	0.22	0.22	0.14	0.007	0.11
smap-l3-rss-v4-1m	16	0.32	0.29	0.12	0.31	0.17	0.236	0.11
smap-l3-jpl-v5.0-8dr	5	1.23	0.97	0.47	1.05	0.55	0.125	0.27
smap-l3-jpl-v5.0-1m	16	0.80	0.75	0.17	0.76	0.23	0.349	0.21
aquarius-l3-or-v5-7dr	240	0.12	0.09	0.34	0.36	0.49	0.128	0.37
aquarius-l3-or-v5-1m	244	0.18	0.12	0.21	0.24	0.26	0.512	0.14
aquarius-l3-or-v5-7dr-rain-mask	240	0.12	0.09	0.34	0.35	0.49	0.146	0.37
aquarius-l3-or-v5-1m-rain-mask	244	0.18	0.12	0.22	0.25	0.26	0.473	0.15
aquarius-l3-jpl-v5-7dr	244	0.27	0.18	0.35	0.40	0.48	0.243	0.31
aquarius-l3-jpl-v5-1m	244	0.21	0.18	0.26	0.32	0.44	0.427	0.28
cci-l4-esa-merged-oi-v3.2-7dr	657	-0.07	-0.10	0.30	0.32	0.26	0.869	0.19
cci-l4-esa-merged-oi-v3.2-30dr	741	-0.07	-0.10	0.29	0.31	0.25	0.885	0.18
smap-l4-iprc-oi-v1-7d	256	-0.02	-0.03	0.19	0.19	0.25	0.601	0.19
smap-l4-iprc-oi-v1-1m	256	-0.04	-0.04	0.15	0.16	0.13	0.733	0.10
aquarius-l4-iprc-v5-1w	262	-0.01	-0.03	0.17	0.17	0.24	0.668	0.16
aquarius-l4-iprc-v5-1m	262	-0.01	-0.02	0.14	0.14	0.14	0.760	0.10

▶ Table 2 is similar to Table 1 but considering only match-up pairs where RR=0 mm/h, 3< U_{10} <12 m/s, SST>5°C, distance to coast > 800 km.

Table 2: Statistics of ΔSSS (Satellite - Sea mammals) - C1

Satellite products	#	Median	Mean	Std	RMS	IQR	r^2	Std*
smos-l2-v700	27	-0.93	-1.13	2.33	2.55	2.17	0.034	1.84
smap-l2-jpl-v5.0	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
aquarius-l2-or-v5	11	-0.21	-0.22	0.46	0.49	0.51	0.151	0.39
aquarius-l2-jpl-v5	13	-0.02	0.00	0.63	0.60	0.48	0.001	0.37
smos-l3-catds-cpdc-v321-l2q	22	0.65	0.44	1.55	1.58	1.50	0.012	1.17
smos-l3-catds-cpdc-v317-10d-25km	53	0.23	0.15	0.84	0.85	1.52	0.080	1.10
smos-l3-catds-cpdc-v317-1m-25km	53	0.17	0.14	0.46	0.48	0.75	0.310	0.60
smos-l3-catds-locean-v5-9d	75	-0.29	-0.25	0.52	0.57	0.80	0.002	0.58
smos-l3-catds-locean-v5-18d	75	-0.20	-0.16	0.29	0.33	0.48	0.306	0.32
smos-l3-bec-v2-9d	34	-0.06	-0.05	0.37	0.37	0.53	0.175	0.43
smos-l3-icdc-v3-1m	38	-0.34	-0.21	0.64	0.67	0.97	0.266	0.72
smap-l3-rss-v4-8dr	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
smap-l3-rss-v4-1m	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
smap-l3-jpl-v5.0-8dr	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
smap-l3-jpl-v5.0-1m	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
aquarius-l3-or-v5-7dr	33	-0.07	-0.11	0.31	0.32	0.43	0.245	0.28
aquarius-l3-or-v5-1m	33	0.10	0.06	0.22	0.22	0.30	0.528	0.18
aquarius-l3-or-v5-7dr-rain-mask	33	-0.12	-0.15	0.31	0.34	0.46	0.228	0.34
aquarius-l3-or-v5-1m-rain-mask	33	0.10	0.05	0.23	0.23	0.22	0.468	0.17
aquarius-l3-jpl-v5-7dr	33	0.09	0.08	0.28	0.28	0.29	0.325	0.25
aquarius-l3-jpl-v5-1m	33	0.15	0.09	0.25	0.26	0.34	0.556	0.28
cci-l4-esa-merged-oi-v3.2-7dr	53	-0.11	-0.12	0.15	0.19	0.18	0.786	0.13
cci-l4-esa-merged-oi-v3.2-30dr	51	-0.10	-0.12	0.15	0.19	0.18	0.798	0.14
smap-l4-iprc-oi-v1-7d	34	-0.10	-0.11	0.15	0.19	0.15	0.718	0.12
smap-l4-iprc-oi-v1-1m	34	-0.10	-0.10	0.16	0.19	0.14	0.693	0.11
aquarius-l4-iprc-v5-1w	35	-0.05	-0.06	0.15	0.16	0.15	0.719	0.13
aquarius-l4-iprc-v5-1m	35	-0.06	-0.05	0.14	0.15	0.15	0.755	0.11

► Numerical values can be downloaded as csv files for Table 1 and Table 2.
► Figures using numerical values of Table 1 sorted by MEDIANS, MEANS, IQR, RMS, STD, R2 are also provided.
► Figures using numerical values of Table 2 sorted by MEDIANS, MEANS, IQR, RMS, STD, R2 are also provided.

Caution has to be made in the interpretation of the "ranking" between different satellite products in particular when looking at the dispersion parameters like the standard deviation (STD), or the interquartile range (IQR). Keep in mind that low spatial and/or temporal resolution satellite SSS products tend to have lower dispersions than products at higher resolutions. For example, a level 2 (swath) product of a specific sensor will always have more dispersion than level 3 or 4 products where spatial and temporal averaging tend to reduce the instrumental noise and potential small scale variability. In general, products at 1°x1° spatial resolution have lower dispersion than products at 0.25°x0.25°. Same result applies for monthly products compared to daily products.

5.2 Statistics derived for the different *in situ* databases

▶ Table 1 shows the mean, median, standard deviation (Std), root mean square (RMS), interquartile range (IQR), correlation coefficient (r^2) and robust standard deviation (Std*) of the match-up differences ΔSSS (Satellite - *in situ*) between **Aquarius SSS L4 OI v5 - Monthly (IPRC)** and all the available *in situ* datasets derived over the Atlantic Ocean Pi-MEP region and for the full satellite product period and considering all match-up pairs satellite/*in situ* SSS values to derive the statistics:

Table 1: Statistics of ΔSSS (Satellite - *in situ*)

***in situ* database**	**#**	**Median**	**Mean**	**Std**	**RMS**	**IQR**	**r^2**	**Std***
argo	84203	-0.01	-0.03	0.28	0.28	0.17	0.928	0.13
tsg-legos-dm	947751	0.01	0.13	0.69	0.70	0.23	0.778	0.17
tsg-gosud-research-vessel	659249	-0.01	0.09	1.00	1.00	0.25	0.560	0.18
tsg-gosud-sailing-ship	225309	-0.02	-0.03	0.68	0.68	0.28	0.770	0.19
tsg-samos	2700912	-0.14	-0.29	1.29	1.32	0.96	0.532	0.69
mammal	262	-0.01	-0.02	0.14	0.14	0.14	0.760	0.10
drifter	817208	-0.03	-0.02	0.21	0.21	0.12	0.934	0.09
tsg-polarstern	71572	-0.02	-0.02	0.14	0.14	0.15	0.970	0.11

▶ Table 2 is similar to Table 1 but considering only match-up pairs where RR=0 mm/h, 3< U_{10} <12 m/s, SST>5°C, distance to coast > 800 km.

Table 2: Statistics of ΔSSS (Satellite - *in situ*)

***in situ* database**	**#**	**Median**	**Mean**	**Std**	**RMS**	**IQR**	**r^2**	**Std***
argo	29558	-0.01	-0.01	0.15	0.15	0.14	0.977	0.10
tsg-legos-dm	60733	-0.01	-0.01	0.21	0.21	0.17	0.933	0.13
tsg-gosud-research-vessel	77253	-0.01	0.00	0.20	0.20	0.17	0.954	0.13
tsg-gosud-sailing-ship	52631	0.03	0.03	0.15	0.15	0.17	0.978	0.13
tsg-samos	177708	0.21	0.28	0.36	0.45	0.33	0.866	0.25
mammal	35	-0.06	-0.05	0.14	0.15	0.15	0.755	0.11
drifter	526592	-0.03	-0.03	0.11	0.12	0.11	0.944	0.08
tsg-polarstern	16092	-0.02	-0.01	0.12	0.12	0.15	0.979	0.11

▶ Numerical values can be downloaded as csv files for Table 1 and Table 2.

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