Match-up database Analyses Report

SMOS SSS L4 OI v342 - Weekly
(CMEMS-CATDS-LOPS)

Moorings

Global Ocean

prepared by the Pi-MEP Consortium

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Contents

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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 and merged into a single file available here for the below pair of Satellite/*in situ* SSS data:

- SSS satellite product (SSS_{SAT}): SMOS SSS L4 OI v342 - Weekly (CMEMS-CATDS-LOPS)

- *In situ* dataset (SSS_{Insitu}): Moorings (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 (**??**)

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

- Time-series of mooring and satellite salinity (3.1)

- Time-series of mooring and models/*in situ* analyses salinity (3.2)

- Power spectrum of SSS for each mooring (3.3)

- Average of all mooring power spectra (3.4)

All analyses are conducted over the full satellite SSS product period. Original figures appearing in this report can be downloaded here as PNG files.

2 The MDB file datasets

2.1 Satellite SSS product

2.1.1 SMOS SSS L4 OI v342 - Weekly (CMEMS-CATDS-LOPS)

The base products, for all the CATDS-PDC (Centre Aval de Traitement des Données SMOS - Production & Dissemination Center) processing chains, are the SMOS L1B products from ESA (European Space Agency).

From these, brightness temperatures at various incidence angles are reconstructed. The Sea Surface Salinity (SSS) are retrieved from multi-angular brightness temperatures through a maximum likelihood Bayesian approach in which measured Tb and Tb simulated using a forward direct model are compared (see **?** for a general description of the retrieval method, and $pro_contableforasummaryofthesimilarities/differenceswithrespecttoESAlevel2oceansalinityprocessing$).

The L4OS SMOS-OI product contains global Level 4 analyses of the of the Sea Surface Salinity (SSS), Sea Surface Density (SSD) and Sea Surface Spiciness (SSSp), along with Sea Surface Absolute Salinity (SSA), Conservative Temperature (SCT), surface thermal expansion coefficient (alpha) and haline contraction coefficient (beta). The SSS product is obtained using an optimal interpolation (OI) algorithm, that combines ISAS in situ SSS OI analyses and Soil Moisture Ocean Salinity (SMOS) satellite image to reduce large scale and temporally varying bias. The SSS L4 product outcome is then combined with satellite SST products to compute thermodynamic sea water parameters using TEOS-10 (**?**).

Products from reprocessing RE07 are available for the period 01/2011 - 05/2021. Products from operational (OPER) processing are available since 06/2021. Reprocessed products and operational products are derived using the same algorithm and configuration, hence ensuring the temporal continuity.

These products are generated with a delay of about 1 month after the end of the period.

Table 1: Satellite SSS product characteristics

SMOS SSS L4 OI v342 - Weekly (CMEMS-CATDS-LOPS)	
Spatial resolution	0.25°
Temporal resolution	Weekly
Temporal coverage	From 2010-12-27 to present
Production center	CATDS-PDC at Ifremer, Brest, France
Version	342
Data Provider	CMEMS
Release Date	2022-09-19
Data access	MULTIOBS_GLO_PHY_SSS_L4_MY_015_015
Quality report	CMEMS-MOB-QUID-015-015.pdf
User manual	CMEMS-MOB-PUM-015-015.pdf
DOI	https://doi.org/10.12770/639a918e-0711-4eff-965d-15a728acb27d
Acknowledgements	CATDS (CNES, IFREMER, LOPS).
References	**?** height

2.2 *In situ* SSS dataset

The Pi-MEP collects data from the Global Tropical Moored Buoy Array (GTMBA), a multinational effort to provide data in real-time for climate research and forecasting. Major compo-

nents include the TAO/TRITON array in the Pacific, PIRATA in the Atlantic, and RAMA in the Indian Ocean. Data collected within TAO/TRITON, PIRATA and RAMA come primarily from ATLAS and TRITON moorings. These two mooring systems are functionally equivalent in terms of sensors, sample rates, and data quality. The data are directly downloaded from ftp.pmel.noaa.gov every day and stored in the Pi-MEP. Only salinity data measured at 1 or 1.5 meter depth with standard (pre-deployment calibration applied) and highest quality (pre/post calibration in agreement) are considered. A careful filtering of suspiciously erroneous mooring salinity data when compared with all satellite data has also been performed (cf. presentation). The Pi-MEP project acknowledges the GTMBA Project Office of NOAA/PMEL for providing the data. Data from the Ocean Station PAPA are also added to the Pi-MEP *in situ* database.

From the Upper Ocean Processes Group at Woods Hole Oceanographic Institution (WHOI), several moorings data are also included in the Pi-MEP. Namely, delayed mode surface mooring salinity records under the stratus cloud deck in the eastern tropical Pacific (Stratus), in the trade wind region of the northwest tropical Atlantic (NTAS), 100 km north of Oahu at the WHOI Hawaii Ocean Time-series Site (WHOTS), in the salinity maximum region of the subtropical North Atlantic (SPURS-1) and in the Pacific intertropical convergence zone (SPURS-2).

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 to the measurements, to get an estimate of the geophysical concomitant condition and history. As discussed in **?**, 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 areas, among others. 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 ISAS

The In Situ Analysis System (ISAS), as described in **?** is a data based re-analysis 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 used are the INSITU_GLO_PHY_TS_OA_MY_013_052 for the period 2010 to 2021 and the INSITU_GLO_PHY_TS_OA_NRT_013_002 for the Near-Real Time (2022-2023) 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/). 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 (?). 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 $1/2°\text{x}1/2°$ boxes.

2.3.2 Mercator

The Operational Mercator global ocean analysis and forecast system at 1/12 degree is providing 10 days of 3D global ocean forecasts updated daily. The time series start on December 27, 2006 and is aggregated in time in order to reach a two full year's time series sliding window.This product includes daily and monthly mean files of temperature, salinity, currents, sea level, mixed layer depth and ice parameters from the top to the bottom over the global ocean. It also includes hourly mean surface fields for sea level height, temperature and currents. The global ocean output files are displayed with a 1/12 degree horizontal resolution with regular longitude/latitude equirectangular projection. 50 vertical levels are ranging from 0 to 5500 meters.

The high resolution global analysis and forecasting system PSY4V3R1 uses version 3.1 of NEMO ocean model (?). The physical configuration is based on the tripolar ORCA grid type (?) with a horizontal resolution of 9 km at the equator, 7 km at Cape Hatteras (mid-latitudes) and 2 km toward the Ross and Weddell seas. The 50-level vertical discretization retained for this system has 1 m resolution at the surface decreasing to 450 m at the bottom, and 22 levels within the upper 100 m. The bathymetry used in the system is a combination of interpolated ETOPO1 (?) and GEBCO8 (?) databases. ETOPO1 datasets are used in regions deeper than 300 m and GEBCO8 is used in regions shallower than 200 m with a linear interpolation in the 200-300 m layer. The atmospheric fields forcing the ocean model are taken from the ECMWF (European Centre for Medium-Range Weather Forecasts) Integrated Forecast System. A 3 h sampling is used to reproduce the diurnal cycle. The system does not include tides. "Partial cells" parametrization (?) is chosen for a better representation of the topographic floor (?) and the momentum advection term is computed with the energy and enstrophy conserving scheme proposed by ?. The advection of the tracers (temperature and salinity) is computed with a total variance diminishing (TVD) advection scheme (Lévy et al., 2001; ?). The high frequency gravity waves are filtered out by a free surface (?). A laplacian lateral isopycnal diffusion on tracers and a horizontal biharmonic viscosity for momentum are used. In addition, the vertical mixing is parametrized according to a turbulent closure model (order 1.5) adapted by ?, the lateral friction condition is a partial-slip condition with a regionalisation of ano-slip condition (over the Mediterranean Sea) and the Elastic-Viscous-Plastic rheology formulation for the LIM2 ice model (hereafter called LIM2_EVP, ?) has been activated (?). Instead of being constant, the depth of light extinction is separated in Red-Green-Blue bands depending on the chlorophyll data

distribution from mean monthly SeaWIFS climatology. Altimeter data, *in situ* temperature and salinity vertical profiles and satellite sea surface temperature are jointly assimilated to estimate the initial conditions for numerical ocean forecasting.Moreover, satellite sea ice concentration is now assimilated in the PSY4V3R1 system in a monovariate/monodata mode.

The Pi-MEP uses daily salinity fields at the surface (GLOBAL_ANALYSIS_FORECAST_PHY_001_024) provided by the Copernicus Marine environment monitoring service (CMEMS) and freely available here. For more information, please refer to the user manual (CMEMS-GLO-PUM-001-024.pdf) and quality information document (CMEMS-GLO-QUID-001-024.pdf)

2.3.3 Hycom

Pi-MEP uses daily HYCOM+NCODA Global 1/12° Analysis product interpolates on a uniform 0.08 degree lat/lon grid between 80.48S and 80.48N (GLBu0.08). HYCOM is a data-assimilative hybrid isopycnal-sigma-pressure (generalized) coordinate ocean model (called HYbrid Coordinate Ocean Model). It uses the Navy Coupled Ocean Data Assimilation (NCODA) system (?, ?) for data assimilation. NCODA uses the model forecast as a first guess in a 3D variational scheme and assimilates available satellite altimeter observations (along track obtained via the NAVOCEANO Altimeter Data Fusion Center) satellite and *in situ* Sea Surface Temperature (SST) as well as available *in situ* vertical temperature and salinity profiles from XBTs, ARGO floats and moored buoys. MODAS synthetics are used for downward projection of surface information (?).

2.3.4 ECCO

Version 4 Release 3 (V4r3), covering the period 1992-2015, represents the latest ocean state estimate of the Consortium for Estimating the Circulation and Climate of the Ocean (ECCO) (?; ?) that synthesizes nearly all modern observations with an ocean circulation model (MITgcm, originally described by ?) into coherent, physically consistent descriptions of the ocean's time-evolving state covering the era of satellite altimetry. Among its characteristics, Version 4 (?) is the first multidecadal ECCO estimate that is truly global, including the Arctic Ocean. Unlike previous versions, the model uses a nonlinear free surface formulation and real freshwater flux boundary condition, permitting a more accurate simulation of sea level change. In addition to estimating forcing and initial conditions as done in earlier analyses, the Version 4 estimate also adjusts the model's mixing parameters that enables an improved fit to observations (?). The Version 4 synthesis also incorporates a diffusion operator in evaluating model-data misfits (?) and controls (?), accounting for some of the spatial correlation that exist among these elements. The Release 3 edition includes improvements in time-period (1992-2015), model (e.g., sea-ice), observations (e.g., GRACE, Aquarius), and constraints (e.g., correlated errors).

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 Moorings *in situ* dataset using the quality flags as described in 2.2 so that only valid salinity data remains in the produced match-ups.

For high-temporal resolution *in situ* SSS measurements such as moorings, an additional temporal-filtering step is performed on the *in situ* data that will be in fine compared to the satellite SSS products. A running median filtered is applied with a window width of D, the period over which the composite product was built. Both the original and the filtered 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 other auxiliary SSS sources which are included in the final match-up files. The collocation is done for each *in situ* SSS measurement contained in the match-up files as follows:

For the given day of the *in situ* data, we select the Hycom and Mercator SSS field of the same day than t_{insitu} found at the closest grid node from the *in situ* data location.

For the given month of the *in situ* data, we select the ISAS and ECCO fields for the same month and take the SSS analysis 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.

The resulting match-ups files are serialized as NetCDF-4 files and merged into a single file available here whose structure is described on section 2.4.4.

2.4.4 Content of the Match-Up NetCDF files

The content of the Match-Up NetCDF files for Moorings is described here.

3 MDB file Analyses

3.1 Time-series of mooring and satellite salinity

In Figure 1, time series of SSS from Moorings (black curve) and SMOS SSS L4 OI v342 - Weekly (CMEMS-CATDS-LOPS) (red curve) satellite SSS product at each mooring location is shown. To switch from a mooring location to another, you can play with the arrows between the plot and the caption.

Figure 1: Time series of SSS from Moorings and SMOS SSS L4 OI v342 - Weekly (CMEMS-CATDS-LOPS) satellite SSS product.

3.2 Time-series of mooring and models/*in situ* analyses salinity

In Figure 2, time series of SSS from Moorings (black curve), models (Hycom in cyan, Mercator in blue and ECCO in magenta) and in situ analyses ISAS (red curve) at each mooring location is shown. To switch from a mooring location to another, you can play with the arrows between the plot and the caption.

Figure 2: Time series of SSS from Moorings, models (Hycom, Mercator, ECCO) and monthly Argo *in situ* analyses (ISAS).

3.3 Power spectrum of SSS for each mooring

In Figure 3, we estimate the frequency averaged power spectrum with geophysical normalization after trend has been removed, using a Blackman-Harris window for each individual mooring/satellite match-up time series. Numerical values can be downloaded as a NetCDF file here.

Figure 3: Power spectrum of SSS from Moorings (black), SMOS SSS L4 OI v342 - Weekly (CMEMS-CATDS-LOPS) satellite SSS product (red), ISAS (blue) and Mercator (pink) for each individual mooring/satellite match-up time series.

3.4   Average of all mooring power spectra

In Figure 4, we average all power spectra calculated previously for mooring (black), satellite (red), ISAS (blue) and Mercator (dashed magenta) time series.
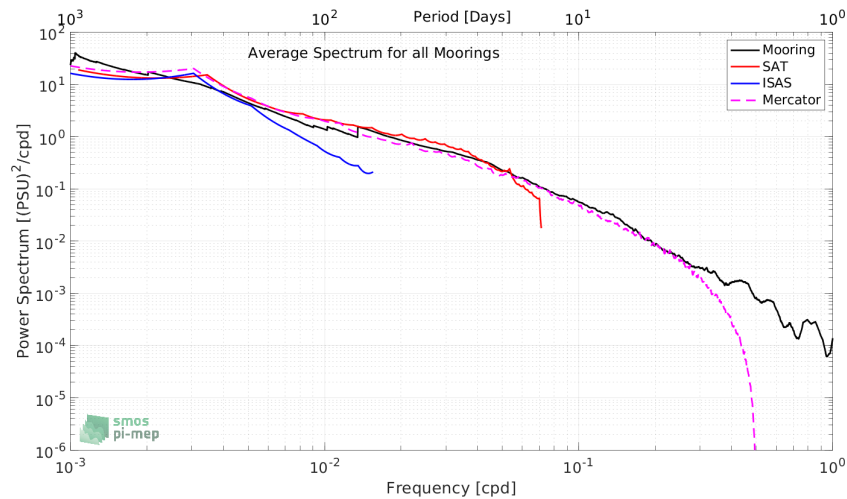

Figure 4: Average of all mooring (black), satellite (red), ISAS (blue) and Mercator (dashed magenta) SSS power spectra.

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$_{filtered}$*) between SMOS SSS L4 OI v342 - Weekly (CMEMS-CATDS-LOPS) SSS satellite product and filtered Moorings for the full satellite product period. Same statistical values are also shown for different ΔSSS: (Satellite - *in situ*), (Satellite - ISAS), (Satellite - Mercator), (ISAS - Mooring), (Mercator - Mooring) and (ISAS - Mercator).

Table 1: Statistics of ΔSSS

Condition	#	Median	Mean	Std	RMS	IQR	r^2	Std*
Satellite - Mooring (filtered)	36274	0.02	0.02	0.26	0.26	0.30	0.93	0.23
Satellite - Mooring	36904	0.02	0.03	0.27	0.27	0.31	0.93	0.23
Satellite - ISAS	92554	0.00	0.00	0.25	0.25	0.29	0.93	0.22
Satellite - Mercator	92554	0.03	0.04	0.29	0.29	0.32	0.90	0.24
ISAS - Mooring	7042742	0.00	0.02	0.25	0.25	0.23	0.93	0.17
Mercator - Mooring	7057110	-0.02	-0.02	0.23	0.23	0.18	0.94	0.14
ISAS - Mercator	17814874	0.01	0.03	0.25	0.26	0.23	0.92	0.17

Numerical values of Table 1 can be downloaded as a csv file here.

References