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NASA/RSS SMAP Salinity Version 4.0 Validation Analysis

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SMAP Salinity Validation Analysis; Data Version 4.0

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1. Introduction

The purpose of this report is to document the Soil Moisture Active Passive (SMAP) sea surface salinity (SSS) measurement uncertainty characteristics, including residual errors in the latest version (**V4.0**) of the SMAP data, which was released 23 August 2019. We document the improvement from V3.0 to V4.0 by comparing each version of SMAP data with in situ data. It should be noted that the matchup statistics (e.g., Section 4, 7 and 8) between SMAP and in situ observations not only include SMAP SSS uncertainty, but also the sampling differences in sampling (e.g., spatial scales) between SMAP data (averaged over SMAP footprint) and the point-wise-in-situ measurements. "SMAP salinity data are produced by Remote Sensing Systems (RSS) and sponsored by the NASA Ocean Salinity Science Team. They are available at www.remss.com."

Here we use 46 months of data for V3.0 and V4.0 (from April 2015 to Jan 2019) for validation analysis. The rain flag is included in both V3.0 and V4.0. Although considerable improvements have been achieved since V2.1 (results not shown here), there remain a number of issues affecting the quality of the V4.0 data. These are detailed in the report and summarized in the last section (**Summary, Conclusions and Cautions).**

Readers of this document are assumed to be familiar with the SMAP mission and sensor design, sampling pattern, and salinity remote sensing principles as described by [1], [2] and [3]. The L1B TA is resampled onto a fixed 0.25 earth grid with Backus-Gilbert type optimum interpolation (OI). Based on the spatial resolution, there are 40-km and 70-km products. The 40-km product uses 39 km and 47 km elliptical footprint. The target of the 70-km product is a circle whose diameter is about 75 km. The results in this document are based on the standard (70-km) products. It should be noted that for V4.0, the 70-km product is derived using simple-neighbor averaging from the 40-km product instead of using BG OI in V3.0. The differences between the BG OI in V3.0 70-km product and the smoothed V4.0 product are small in the open ocean. More details are described in [2].

The SMAP V3.0 and V4.0 Level-2C salinity retrieval algorithm have been adapted from Aquarius V5.0 salinity retrieval algorithm to facilitate a continuous data record of SSS. The ancillary SSS data have been derived from the US Navy HYbrid Coordinate Ocean Model (HYCOM) daily averaged data-assimilative analysis ([4] and Appendix A). The operational data are produced by the U.S. Naval Oceanographic Office (NAVO), and the digital output is distributed by Florida State University. The HYCOM global mean salinity over the open ocean has been used as an ocean calibration target for the sensor.

The SMAP SSS project produces three data sets: Level 1a (raw data), Level 2 (science data in swath coordinates and matching ancillary data), and Level 3 (gridded ¼ degree 1-day running, 8-day running average, monthly salinity with and without rain filtered and wind speed maps,). This validation analysis will start with Level 2 data evaluation followed by Level 3 on rain filtered monthly average. Salinity measurements are on the practical salinity scale (PSS-78), technically a dimensionless number, but in some figures labeled as practical salinity units (psu).

The near-surface in situ salinity data used here are from Argo floats from US Global Ocean Data Assimilation Experiment (GODAE, http://www.usgodae.org/argo/argo.html [7]). The shallowest sampling depths of the Argo data are generally 3-5 meters below the surface. Under most conditions (e.g., moderate to high winds) the surface ocean mixed layer extends much deeper, and the floats provides an accurate measure of the 1-2 cm surface layer that emits the microwave signal seen by the satellite. However, under persistently rainy conditions (especially under low winds when vertical mixing is small), there are often vertical gradients between the surface and the buoy measurement depth. Argo floats rise to the surface once every 10 days and remain at the surface for a few hours. The data are collected randomly at any time of the day.

2. Methodology for the Matchup

2.1 Level 2 (swath) data

2.1.1 Satellite-centered

"Satellite-centered" match-up indicate the time window centered on the satellite data. The goal of the satellite-centered Level 2 validation in this document is to include more biases in the SMAP SSS, such as the daily biases and ascending and descending differences. The results are useful for the cal/val team to examine thoroughly the biases in the SMAP SSS. Detailed steps for SMAP Level 2 satellite-centered validation processes are as followed:

1) Gather one orbit (day 0) of SMAP Level 2 data, including both forward (for) and backward (aft) look.
2) Apply the flags to the SMAP data as described in Section 3.
3) Retrieve all the in situ (Argo) data within the ±4-day time window.
4) For each in situ observation obtain from the last step, we search for all the SMAP data gathered in step 1 that are within the 50 km search radius, regardless the look direction.
5) If there are SMAP footprints found within the search radius, we average all the SMAP salinity for the matchup. These SMAP salinity will come from the same orbit because we only used one orbit of SMAP data in step 1.
6) We exclude the matchup if the time differences between the Argo and SMAP are more than 3.5 days. It should be noted that the SMAP revisit time (2-3 days) is smaller than the orbit repeat (approx. 8 days). Hence, over counting possible.
7) Then we move to the next SMAP orbit, and repeat the processes (step 1 to 6). Therefore, the same in situ observation may be used for matchup again for the different orbits of SMAP.

2.1.2 In situ-centered

"In situ-centered" match-up indicate the time window centered on the in-situ data. The goal of the in situ-centered Level 2 validation in this document is to estimate the salinity data quality of SMAP SSS with greater temporal and spatial averages. The results are useful for the general users to examine and compare the salinity data quality from different satellite observations.

1) Gather one day (day 0) of in situ (Argo) data.
2) Retrieve all the SMAP data within the ±4-day time window.
3) Apply the flags to the SMAP data as described in Section 3.
4) For each in situ observation obtain from Step 1, we search for all the SMAP data gathered in step 3 that are within the 50 km search radius, regardless the look direction.
5) We exclude the matchup if the time differences between the Argo and SMAP are more than 3.5 days.
6) For all the SMAP footprints found within the search radius, we average all the SMAP salinity for the matchup. SMAP data from salinity will come from several orbits within the 7-day time window.
7) Then we move to the next day of the in-situ data and repeat the processes (step 1 to 6). Therefore, the same in situ observation will only be used once for match-up because we search one Argo report at a time with in-situ centered method.

2.2 Level 3 (gridded) data

The detailed steps for SMAP Level 3 validation processes are as followed:

1) Download one month of SMAP Level-3 0.25° × 0.25° gridded salinity map
2) Retrieve all the in situ (Argo) data within the 1-month time window.
3) For each grid cell on the SMAP salinity maps, we search for the in-situ data from step 2 and find the in-situ data that are within the 50 km search radius. The average of the individual Argo floats is used instead of using the Level gridded Argo data to mitigate the biases induced by the gridding algorithm with sparse in situ data in certain regions.
4) For that SMAP cell and the salinity value averaged from all the in-situ data within the 50 km search radius are used as a match-up.
5) Then we repeat the validation with each monthly gridded map.

3. Quality Control (Q/C) Flags

Flag #0	no valid radiometer observation in cell
Flag #1	problem with OI
Flag #2	strong land contamination
Flag #3	strong ice contamination
Flag #4	MLE in SSS retrieval algo has not converged
Flag #5	sun glint angle < 50° and azimuthal look angle between 30° and 50°
Flag #6	moon glint angle < 15°
Flag #7	high reflected galaxy
Flag #8	moderate land contamination (*gland* >0.04 or *fland* >0.001)
Flag #9	moderate ice contamination (*gice* >0.003)
Flag #10	high residual of MLE in SSS retrieval algo

Flag #11 low SST (*surtep*-273.15<5°C)
Flag #12 high wind speed (*winspd* > 15 m/s)
Flag #13 light land contamination (*gland* > 0.001)
Flag #14 light ice contamination (*gice*> 0.001)
Flag #15 rain flag (IMERG rain rate > 0.1 mm/h)

All the flags above except Flag #13 and #14 are used for Level 2 validation in the document. In Section 5, only Flag #0-7 and Flag #10 are used for the sensitivity tests. In Level 3 files, flags #0 to #10 and #15 are applied and wind speed larger than 20 m/s are excluded.

4. Matchup Maps and Differences

4.1 Global maps of the salinity biases

We start with global maps comparing the SMAP Level 2 samples with in situ data. **Figure 1** shows the SMAP retrieved salinity at the in-situ matchup points for 46 months of V3.0 and V4.0 observations. In situ salinity data at the same matchup points are also shown. The correspondence is visibly quite clear with SMAP Level 2 data resolving the salient large-scale ocean features. V3.0 SSS is too fresh in the Mediterranean Sea and Arabian Sea.

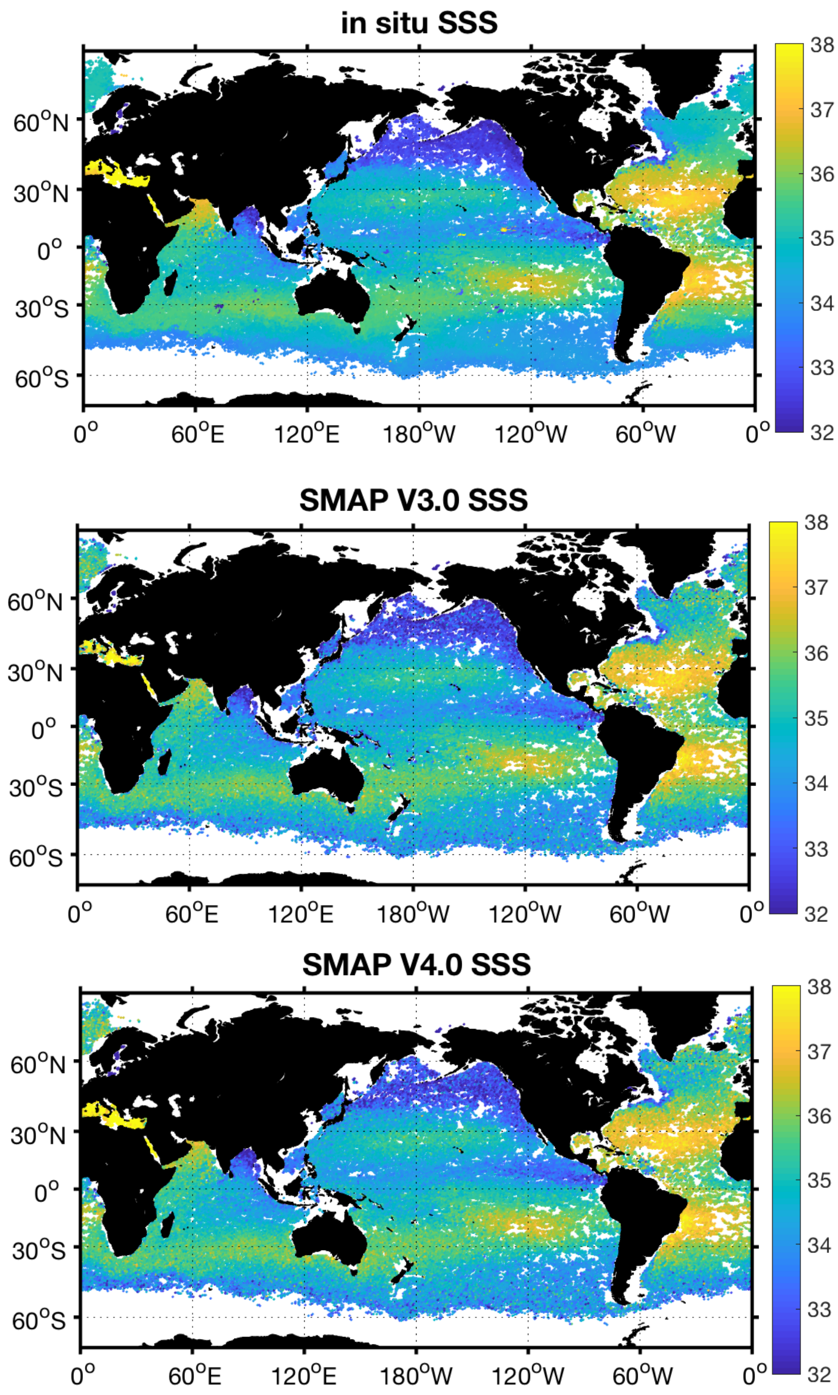

Figure 1. In situ and SMAP co-located salinity data.

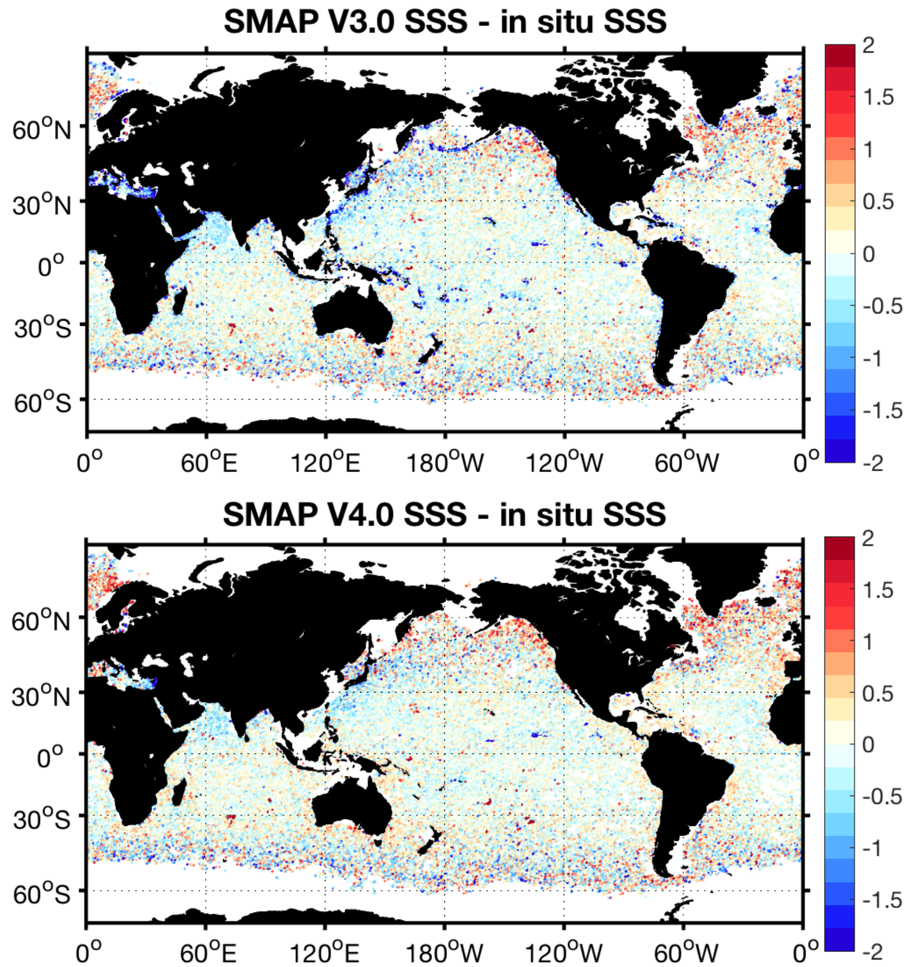

Figure 2. Global maps of SSS differences defined as the SMAP (a) V3.0 and (b) V4.0 data minus the co-located in situ salinity (satellite-centered).

Based on **Figure 1, Figure 2** shows the SMAP – in situ differences with the same match-ups for V3.0 and V4.0. The negative biases near the coastal regions in V3.0 are greatly reduced in V4.0. On the other hand, stronger positive biases in the high latitude in the Northern Hemisphere are observed in the V4.0. These are the caused by the problematic SSS data in the first few months of SMAP mission, possibly related to the instrument calibration. The actual cause for the biases is still unknown. These positive biases in the Northern Hemisphere are not shown in V2.0 (not shown) and more investigations are needed to understand the sources of the errors.

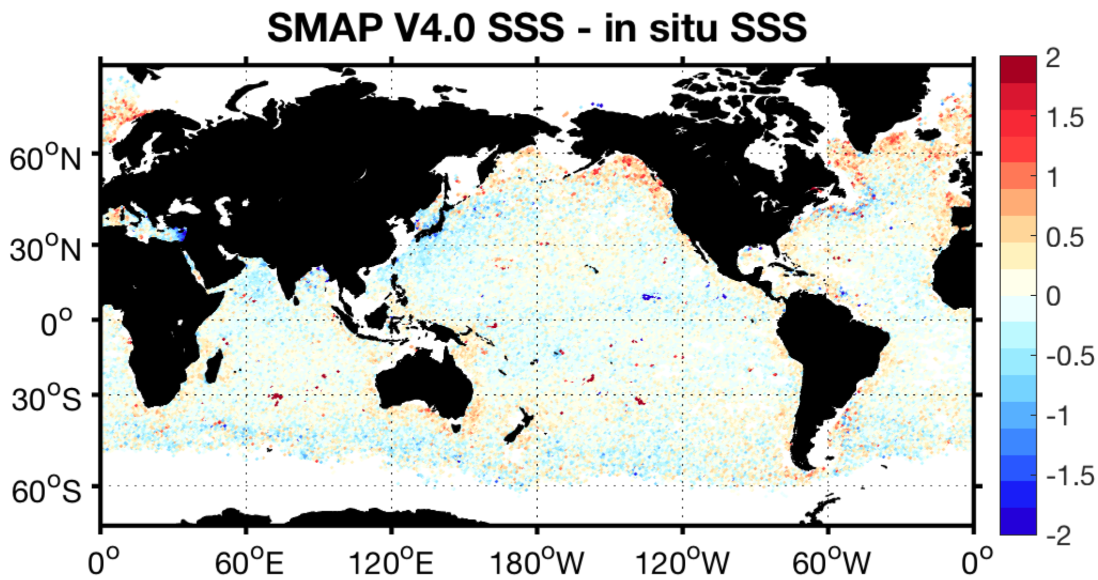

Figure 3. Global maps of SSS differences defined as the SMAP V4.0 data minus the co-located in situ salinity (in situ-centered).

Figure 3 shows the SMAP – in situ differences for SMAP V4.0 with "in situ-centered" matchup. Variations of the salinity differences are greatly reduced globally compared to the satellite centered matchup, especially in the Southern Ocean. Whereas, strong positive biases in the high latitude in the Northern Hemisphere are still observed in the V4.0.

4.2 Comparisons between HYCOM and Argo SSS

The top layer salinity in the HYbrid Coordinate Ocean Model (HYCOM) are used as a salinity reference in SMAP Level 2 data (sss_ref) [4], [5] and [6]. The HYCOM surface salinity is interpolated to the time and location of SMAP footprint. Here, in **Figure 4**, these reference salinity data are evaluated against the Argo measurements with the same matchup processing as SMAP Level 2 data for the whole SMAP mission time period. In other words, the HYCOM data are collocated and compared with the in-situ data. The one-to-one match between HYCOM and Argo are also calculated but similar results are obtained with smoothed or not-smoothed HYCOM data. It is clear that there are regional long-term systematic biases between HYCOM salinity and the in-situ data. HYCOM is biased positively relative to the Argo floats in the Antarctic Circumpolar current, tropics, Bay of Bengal and North Pacific. Over much of the mid-latitudes the bias is slightly negative, and larger biases in Gulf Stream and east coast of South America. These differences exist even though most of the in-situ data we are using here are assimilated by HYCOM and therefore not fully independent data. It should be noted that SMAP is calibrated on HYCOM, but only on the global averages, which are very close between Argo and HYCOM (Figure 4b).

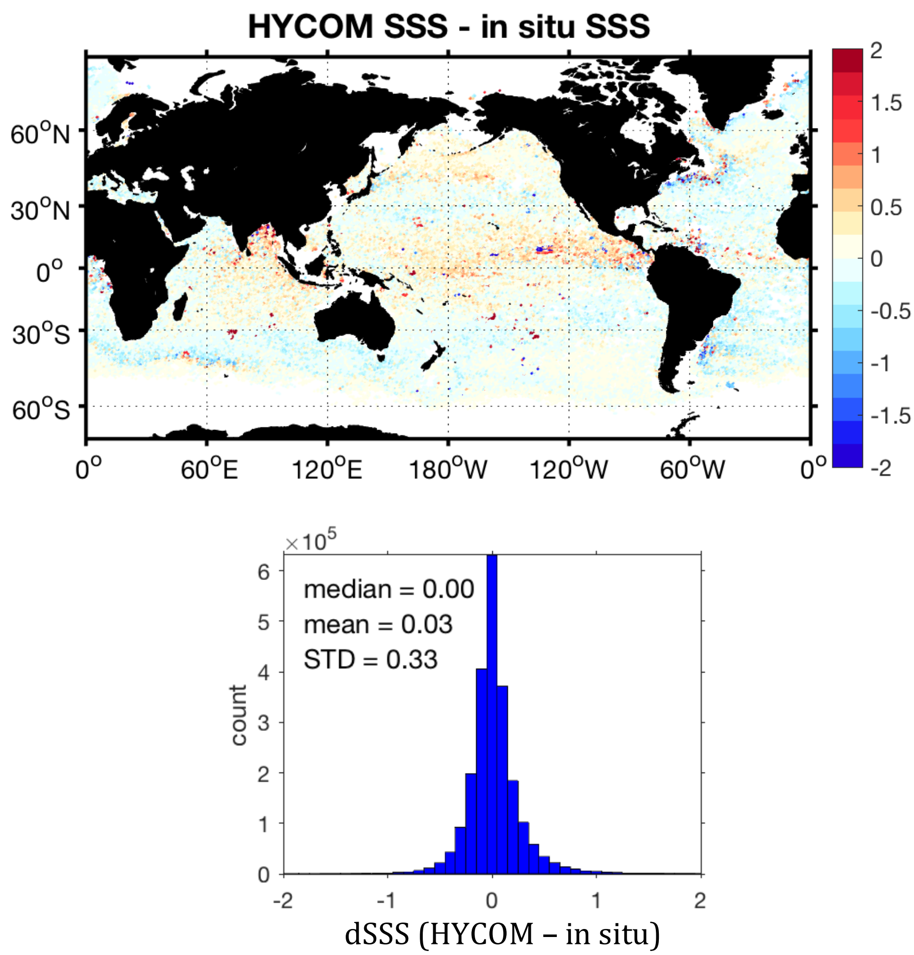

Figure 4. Salinity differences between co-located HYCOM and in situ.

4.3 Latitudinal variations of the salinity biases

Figure 5a and 5b show the in-situ difference statistics in discrete latitude bands for V3.0 and V4.0 data using satellite-centered matchup. Blue lines are the medians of the salinity biases and red lines are the standard deviations (STD) of the salinity biases. V4.0 shows smaller standard deviations (~ 0.7) in the Northern Hemisphere, especially around 60°N than V3.0 (~1.7). However, around 60°N, larger positive biases (~0.3 psu) are observed in V4.0 than V3.0 (~0.1 psu).

Figure 5c is the same as **Figure 5b** but for in situ-centered matchup. The median of the salinity differences is almost the same using either matchup method, but the STD is generally smaller using the in situ-centered matchup, including the high latitudinal regions.

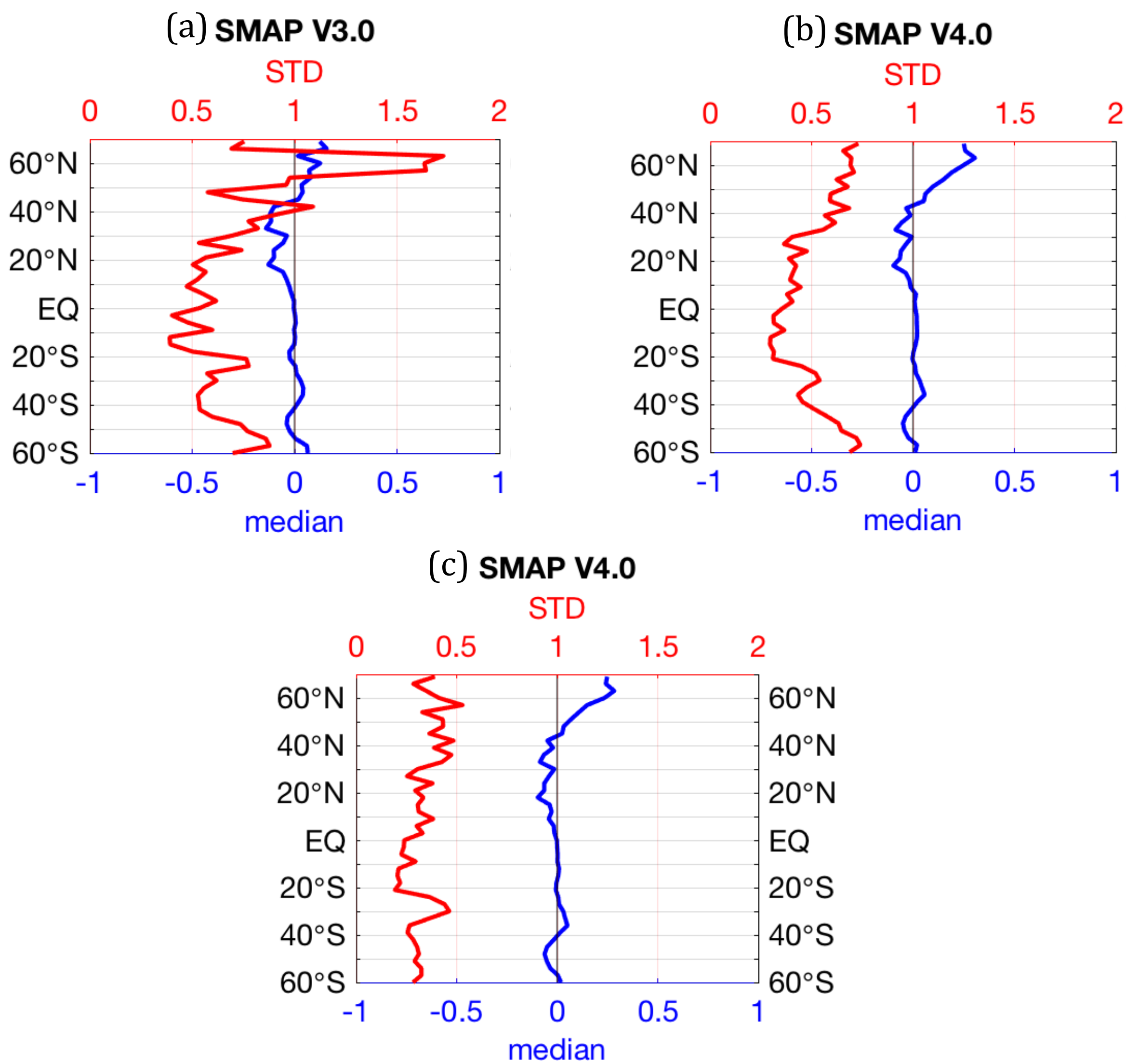

Figure 5. Differences of SMAP (a) V3.0 and (b) V4.0 L2c data and in situ salinity with satellite-centered matchup and (c) V4.0 with in situ-centered matchup by latitude bands.

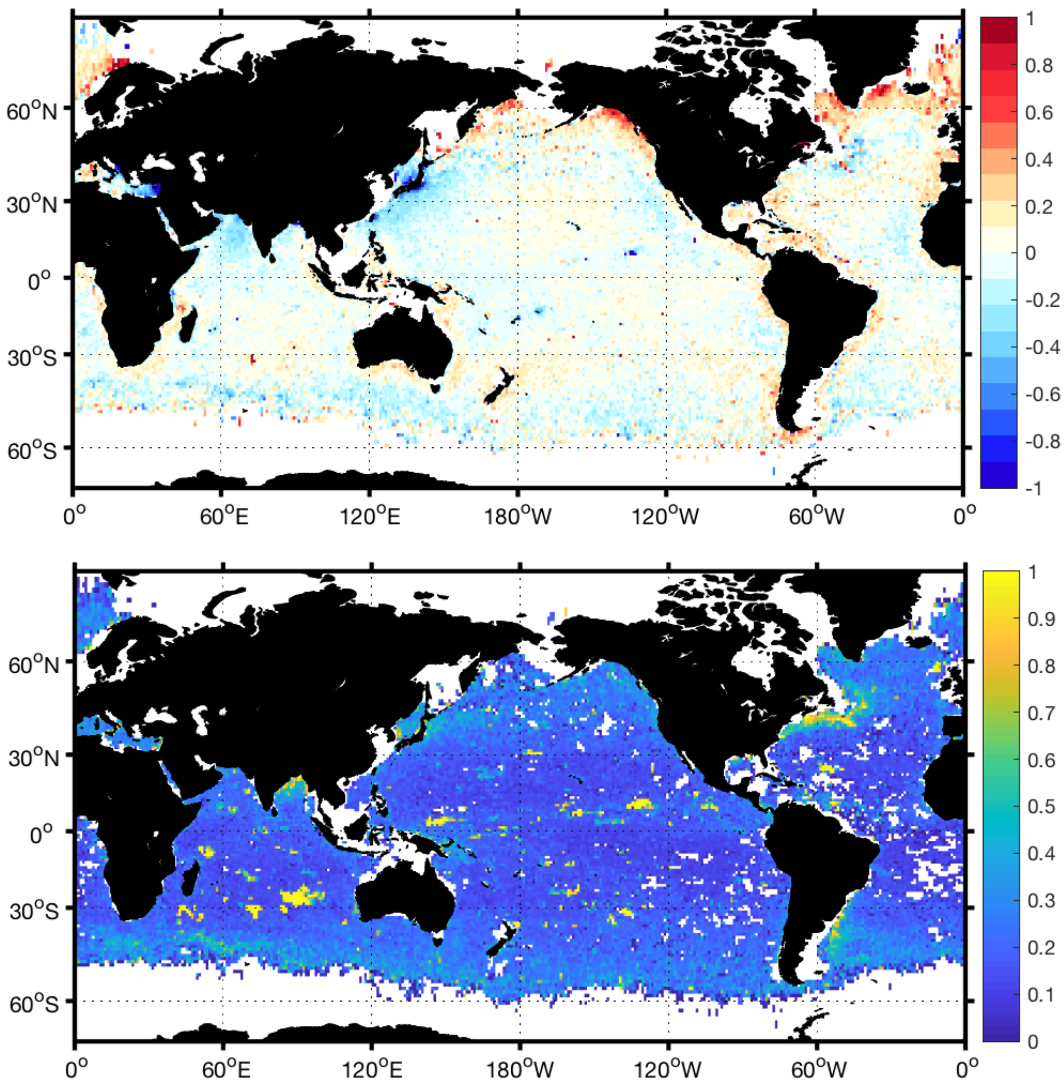

Figure 6. Global in-situ difference statistics on each grid cell. (upper) median and (below) STD of the salinity differences of SMAP minus in situ.

Figure 6 shows the global mission-long salinity differences statistics for 1-degree grid cell for SMAP V4.0 data using satellite-centered matchup method. For each gird cell, we aggregate all available in-situ salinity data for the mission (April 2015 to January 2019), then calculate the statistics (average and STD) from the salinity differences (SMAP minus in situ). Consistent with **Figure 5b**, **Figure 6a** shows that positive biases appear in the high latitude around 60°N, especially near the coastal regions. Negative biases are observed around 30°N, near Japan, eastern Mediterranean Sea, and Arabian Sea. In Southern Hemisphere positive biases show up near the coastal regions, including South America, Australia, New Zealand and east coast of Africa. **Figure 6b** shows that higher STD around the islands and Gulf Stream.

One thing to notice is the negative differences and higher STD in the Southern Ocean, especially south of the Indian Ocean, where the Antarctic Circumpolar Current (ACC) is the strongest. The salinity differences are likely due to the large salinity variations that are not captured by the insufficient observations of in-situ data. In other words, the differences could be the real salinity signals that are captured by the satellite observations but not by the in situ.

5. Sensitivity Tests

Figure 7 shows the salinity differences of SMAP and in in situ averaged with different SST, wind speed and land fraction. White lines show the salinity differences and red lines show the standard deviations of the salinity differences. In both V3.0 and V4.0, STD of the salinity differences are larger in cold water (SST<5°C) and in warm water (SST>30°C) regions, which are usually excluded after the flags applied. The high STD are also observed in the high wind speed (>15 m/s) regions. One thing to notice is that the salinity biases are much improved near the coastal regions in SMAP V4.0.

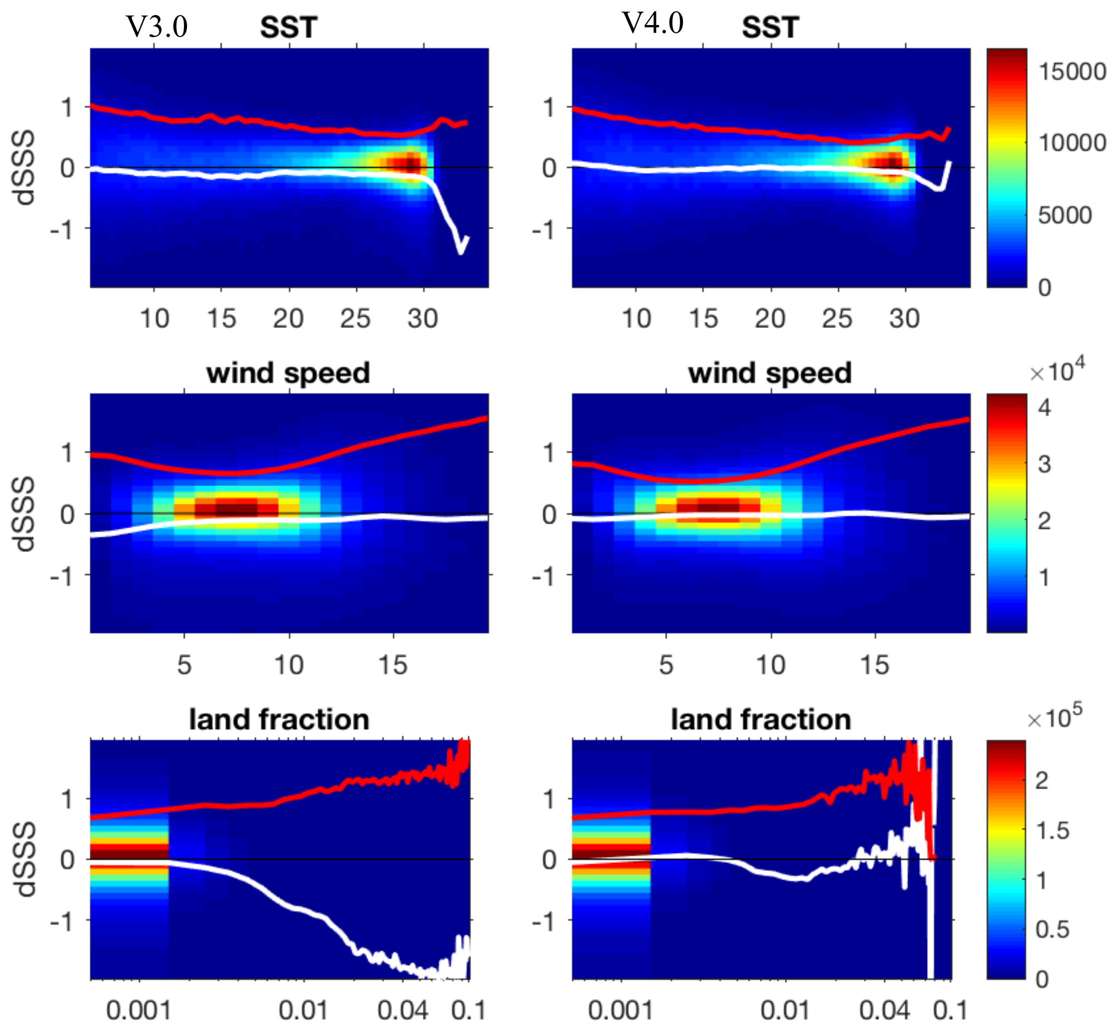

Figure 7. Differences of SMAP L2c data and in situ salinity compared with (upper) different sea surface temperature in °C (middle), wind speed in m/s and (bottom) and land fraction in V3.0 (left) and V4.0 (right). White lines show the salinity biases and red line shows the standard deviation.

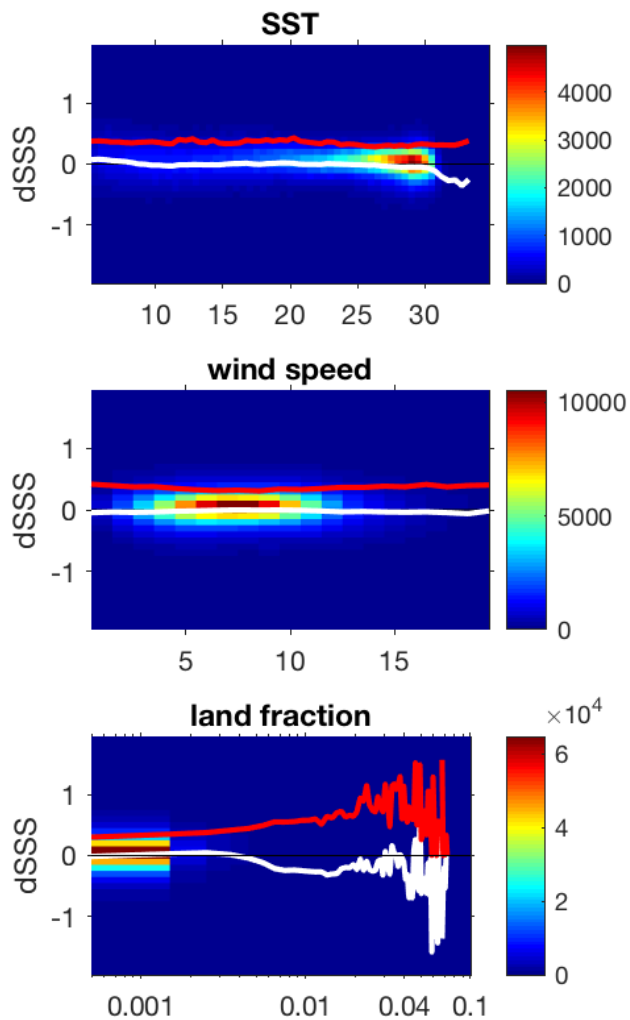

Figure 8. Same as Figure 7, but with V4.0 "in situ-centered" matchup.

Figure 8 shows that the median of the salinity differences in the in cold water (SST < 5°C), in warm water (SST > 30°C) and in high wind (wind speed > 15 m/s) regions are similar with satellite-centered and in situ-centered matchup. Whereas, the STD of the salinity differences in these particular regions are greatly reduced with the in situ-centered matchup, suggesting that the regional salinity variations are averaged out in the in situ-centered matchup. This is consistent with the purposes of different matchup methodology. "Satellite centered" is useful for cal/val team to understand the comprehensive salinity variations in the Level 2 data and "in situ-centered" is useful for general users to examine the best quality that comes out of the satellite observations with further averages.

6. Triple Point Analysis of Aquarius, SMAP and In Situ Data

For the triple point analysis, we use the "in situ-centered matchup". For each in situ data, we average all the Aquarius/SMAP Level 2 data within the ± 3.5 days and 50 km search radius for match up.

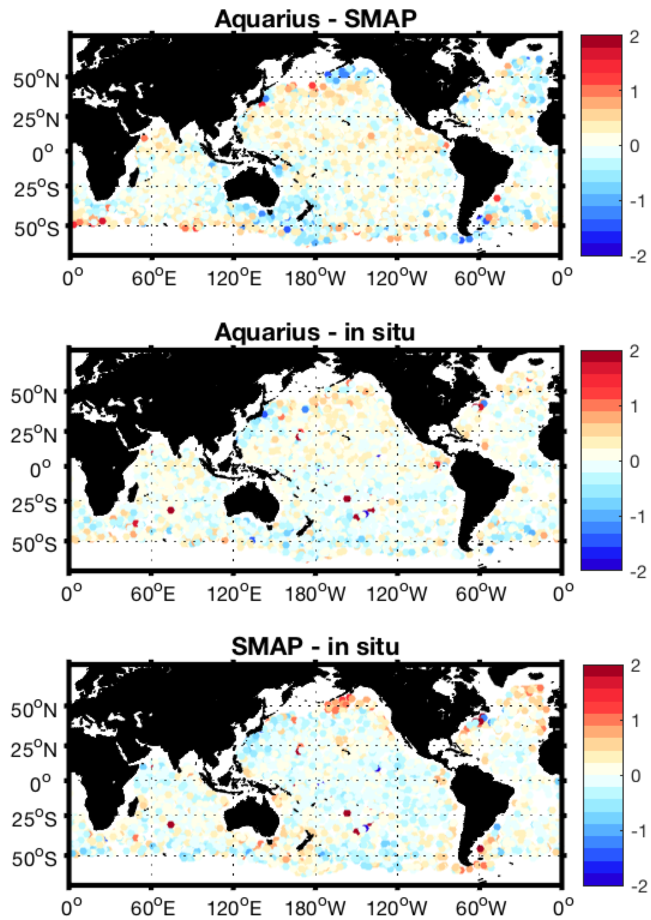

Figure 9. Global maps of (a) Aquarius minus SMAP, (b) Aquarius minus in situ and (c) SMAP minus in situ at the triple point co-locations.

Figure 9 shows the global maps of triple-point matchup for Aquarius V5.0 minus SMAP V4.0, Aquarius V5.0 minus in situ, and SMAP V4.0 minus in situ (at the in-situ locations) during the period when Aquarius and SMAP overlap from April 5, 2015 to May 30, 2015. The analysis period does not start on April 1st because the analysis is in situ centered. For April 5th, the in-situ data are compared with SMAP from April 1st to April 9th.

Figure 10 gives the triple-point matchup statistics. The root-mean-square deviation (RMSD) is defined as RMSD=sqrt(bias^2+STD^2). From **Figure 10,** Aquarius-SMAP RMSD is calculated ~0.31. The RMSD for Aquarius-in situ and SMAP-in situ are 0.53 and 0.54, respectively. The co-located statistics allow us to estimate the root-mean-square error (RMSE) of each of the three measurements (See Appendix B). The results of the co-located matchup points are given in **Table 1**. The Aquarius RMSE is ~0.21 and the SMAP and in situ RMSE are ~0.23 and ~0.49, respectively. Higher RMSE in the in situ indicates the differences caused by the sub-footprint variations and the vertical stratifications [8]. Directly computed monthly statistics for the satellite data are not this small, as will be discussed in a later section.

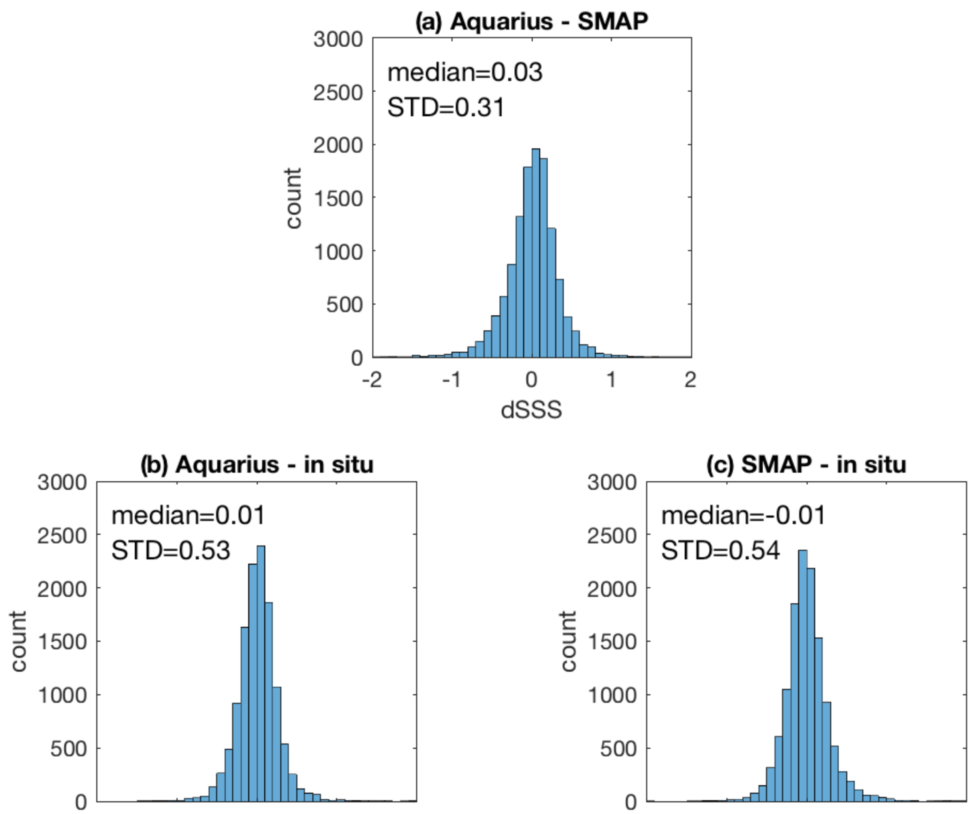

Figure 10. Co-located difference histograms for (a) Aquarius - SMAP, (b) Aquarius - in situ and (c) SMAP - in situ.

Table 1. Estimated Root Mean Square Error (RMSE) for each data type based on the triple point analysis co-located point measurements.

Aquarius RMSE	0.21
SMAP RMSE	0.23
In situ RMSE	0.49

7. In Situ Matchup Time Series and Histograms

Figure 11 and **Figure 12** show the statistics of the global salinity biases for V3.0 and V4.0 using satellite-centered matchup. Small negative biases are observed in V3.0 in the global average from 2015 to 2017, but are removed in V4.0. Larger STD in the beginning few months of the SMAP mission period. Slight increase of the STD is also observed since 2018 in both versions.

Histograms of the matchup salinity differences are reported in **Figure 11** and **Figure 12**. In these statistics, we excluded the colocations that introduced considerable noise and skewness to the data (SST < 5°C, wind speed > 15 m/s, and gain-weighted land fraction >0.04 and ice fractions >0.003). The root-mean-square difference (RMSD), which is the root sum square (RSS) of the bias and standard deviation, is reduced from ~**0.72** in V3.0 to ~**0.50** in V4.0. These are the ensemble statistics for the 46-month data.

Figure 13 show the statistics of the global salinity biases for V4.0 using in situ-centered matchup. Daily variations and STD are greatly reduced from the further averaging of the satellite data. The RMSD has dropped to **0.34** with the in situ-centered matchup.

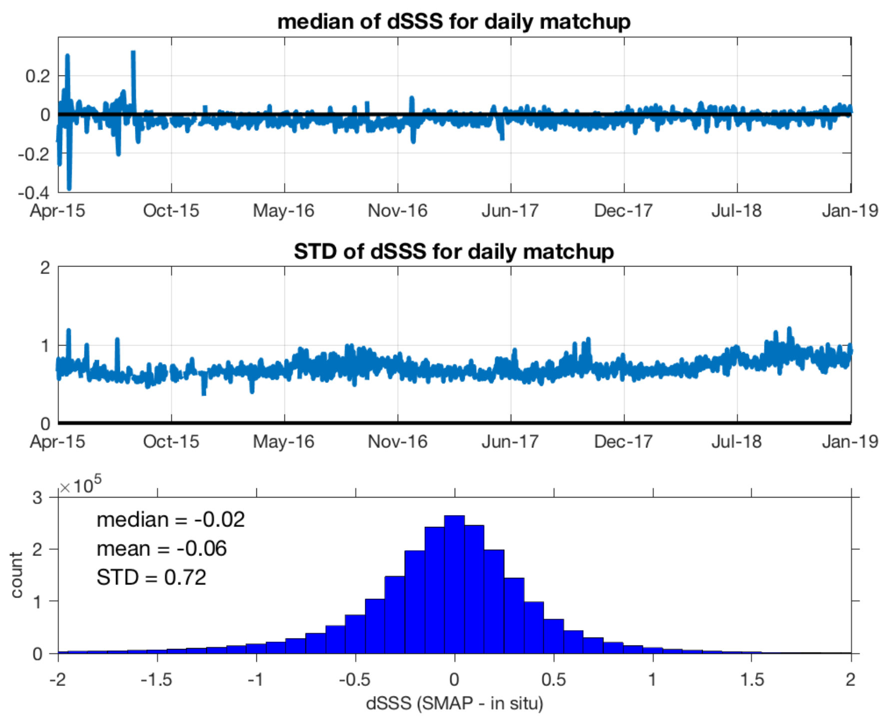

Figure 11. Statistics of the salinity differences for SMAP V3.0. (a) Time series of daily median of the differences (b) time series of daily STD of the differences and (c) histogram of the differences.

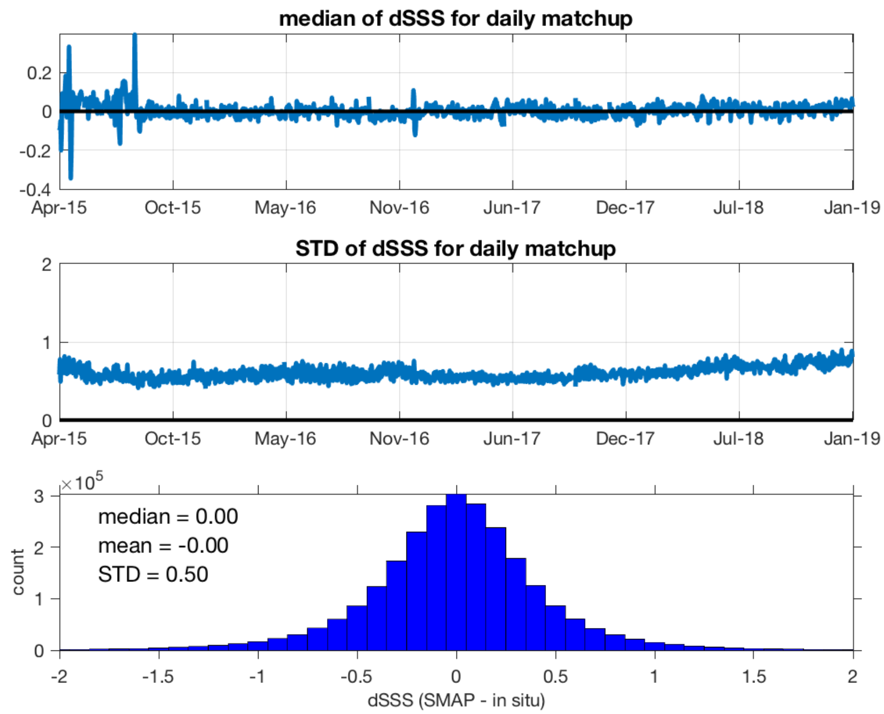

Figure 13. Same as Figure 11, but for SMAP V4.0 with satellite-centered matchup.

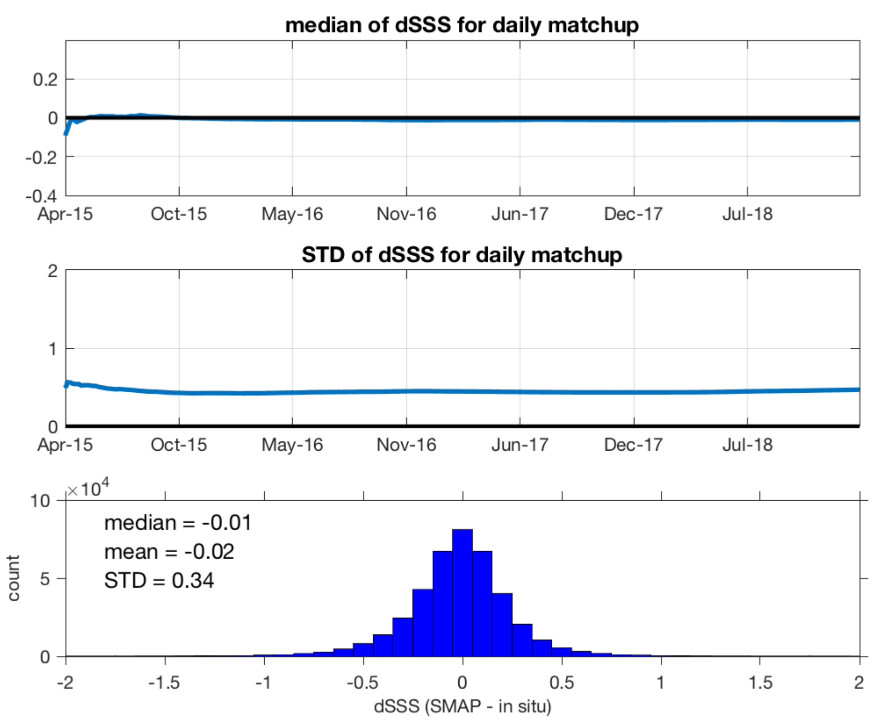

Figure 12. Same as Figure 12, but for SMAP V4.0 with in situ-centered matchup.

Scatter plots between the in-situ data and V3.0 and V4.0 of SMAP data are shown in **Figure 14**. The color contours represent the density of points, and fit is quite linear over the open ocean salinity dynamic range. It is evident that SMAP salinity observations are more concentrated to the 1:1: ratio line using the in situ-centered matchup, indicating the smaller biases with further averaging. **Figure 13** also shows that he correlation coefficients between in situ and SMAP data are 0.76 in V3.0 and improve to 0.88 in V4.0 using satellite-centered matchup. The correlation coefficient is 0.92, which is higher with SMAP V4.0 in situ-centered matchup as expected.

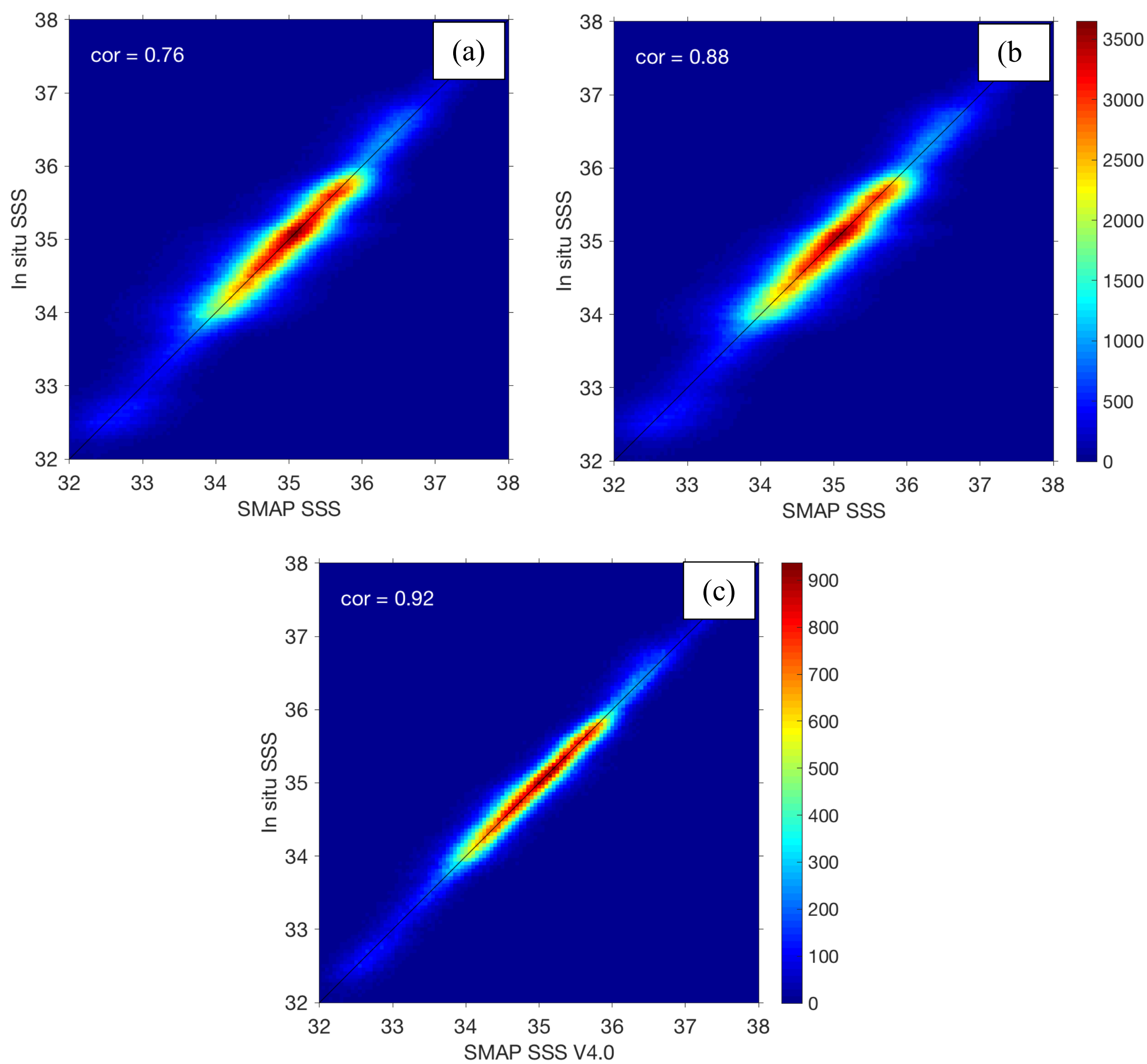

Figure 14. Scatter plots of SMAP Level-2 (abscissa) and co-located in situ data (ordinate). (a) SMAP V3.0 satellite-centered matchup, (b) SMAP V4.0 satellite-centered matchup and (c) SMAP V4.0 in situ-centered matchup.

8. Level 3 Monthly in situ Matchup

Next, we examine in situ difference statistics of monthly ¼ × ¼ degree Level 3 salinity data maps with rain filtered. The Level 3 maps are generated from Level 2 salinity data by averaging all valid L2C observations within each grid cell without any added adjustment for climatology, reference model output or in situ data. The standard SMAP Level 3 data produced by the RSS use the criterion for gain weighted land fraction *gland* set to 0.001 and the land fraction in the 3-dB footprint *fland* set to 0.001 to include more salinity information near the coastal regions. The flag of gain weighted sea ice fraction *gice* is set to 0.003. *Therefore, when using the RSS/SMAP Level-3 mapped data, the users should be careful when analyzing the salinity data near the coasts.* The wind speed exceeds 20 m/s are also excluded. For additional information see Section 3 in this document or Section 6 in SMAP V4.0 release note [2]. More details about the biases in the monthly maps will be discussed in **Figure 15**. The results shown here are computed using a 50 km radius. The radius is the same as what we used for Level 2, which is chosen based on the sensitivity tests (not shown here). The RSS/SMAP monthly Level 3 data used in this document is filtered with rain masks and is available on RSS website (http://data.remss.com/smap/SSS/V04.0/FINAL/L3/monthly_RF/). The folder is named "monthly_RF" and the data files are labeled as "RSS_smap_SSS_L3_monthly_RF_*year_month*_FNL_v04.0.nc". The salinity data are discarded if the IMERG rain rate, resampled to 40 km, exceeds 0.1 mm/h.

8.1 SMAP – in situ monthly difference statistics

Table 2 shows the results of Level 3 monthly validation for SMAP V4.0. The tabulated monthly standard deviations range from 0.279 to 0.376 from April 2015 to March 2018.

Table 2. SMAP V4.0 - in situ monthly difference statistics (Level 3 maps from RSS SMAP data with rain filtered) from April 2015 to March 2018. Each panel represents one year (April-March) beginning April 2015.

	SMAP – in situ	
	Bias	STD
Apr-15	0.002	0.376
May-15	0.038	0.369
Jun-15	0.022	0.350
Jul-15	0.007	0.350
Aug-15	0.020	0.304
Sep-15	-0.007	0.312
Oct-15	-0.010	0.336
Nov-15	0.000	0.310
Dec-15	0.010	0.329
Jan-16	0.014	0.329
Feb-16	0.009	0.302
Mar-16	0.014	0.308

	SMAP – in situ	
	Bias	STD
Apr-16	0.004	0.321
May-16	0.008	0.327
Jun-16	0.011	0.328
Jul-16	0.002	0.332
Aug-16	-0.012	0.318
Sep-16	-0.014	0.314
Oct-16	-0.025	0.332
Nov-16	-0.006	0.330
Dec-16	-0.008	0.345
Jan-17	0.009	0.304
Feb-17	0.003	0.283
Mar-17	0.000	0.279

	SMAP – in situ	
	Bias	STD
Apr-17	-0.002	0.290
May-17	0.008	0.309
Jun-17	0.003	0.326
Jul-17	-0.004	0.304
Aug-17	-0.015	0.313
Sep-17	-0.020	0.286
Oct-17	-0.023	0.298
Nov-17	-0.009	0.321
Dec-17	-0.009	0.321
Jan-18	-0.014	0.298
Feb-18	0.002	0.319
Mar-18	0.001	0.316

8.2 Global maps of salinity monthly biases

The maps of SMAP V4.0 monthly biases for the first year of observations (April 2015 to March 2016) are shown in **Figure 15**. Positive biases are observed in the coastal regions in the higher latitudes in both Northern and Southern Hemisphere from April 2015 to August 2015. This is consistent with the **Figure 12** that larger STD showed up during the first few months of SMAP mission. Negative biases are observed under the intertropical convergence zone, partly due to the vertical stratification.

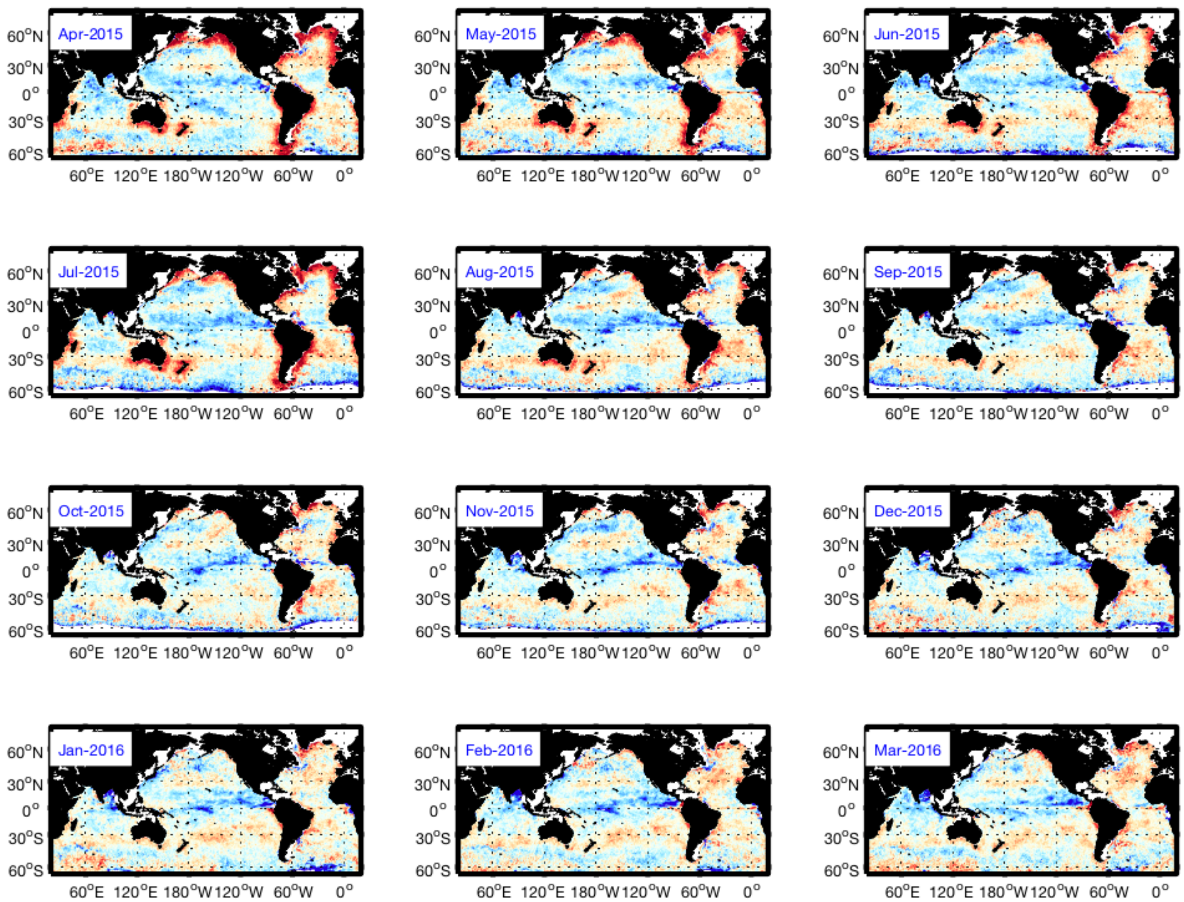

Figure 15 SMAP V4.0 monthly difference maps (with rain filtered) for the first year of observations.

8.3 Triple-Point Analysis of Monthly Level 3 Gridded Data

Here, we apply the triple-point approach (Appendix B) to assess the Aquarius and SMAP monthly root mean square error (RMSE). **Table 3** gives the month-by-month bias and standard deviation (STD) differences between the Aquarius and SMAP monthly Level 3 gridded data and in situ observations, respectively. From these, the root-mean-square-difference (RMSD) is obtained as the square-root of the ($bias^2 + STD^2$). The RMSD, of course, combines both the Aquarius/SMAP and in situ measurement errors, whereas our goal here is to isolate the Aquarius, SMAP and in situ RMSE.

Three data sets for the triple-point analysis are (1) the same monthly 1×1 degree Aquarius ADPS Level 3 salinity data maps, (2) SMAP monthly RF maps interpolated onto 1×1 maps, and (3) the in situ data set (un-gridded). Next, we find the RMSD of three data pairs: (1) Aquarius-in situ, (2) SMAP-in situ, and (3) Aquarius-SMAP. The process finds all the in-situ data points within the 50 km search radius for each grid cell on the mapped 1×1 boxes for each month, averages those, differences that from the gridded monthly value for that grid-box, and then computes the RMSD of all the matched 1×1 grid-boxes over the globe for that month. Aquarius-SMAP is simply the RMSD between the respective monthly 1×1 degree maps. The RMSD accumulations also ensure that only the 1×1 grid cell containing in situ samples are counted, to ensure common sampling. We also note that the standard Level 3 gridding masks and flags are applied, and thus cold regions (SST<5°C) and regions higher than the threshold for land contamination are omitted (See Table 1 in AQ-014-PS-0018_AquariusLevel2specification_DatasetVersion5.0 for Aquarius data quality flags and masks and see Section 7.1 in SMAP V4.0 release note [2] for SMAP Level 3 Q/C checks).

Table 3 shows the results of Level 3 monthly validation for Aquarius V5.0, SMAP V4.0 interpolated onto Aquarius spatial scale. The tabulated monthly standard deviations are 0.396 and 0.435 in April and May 2015 for Aquarius and 0.459 and 0.406 for SMAP. The STD in Table 3 are larger than the values calculated in Table 2. This could be because that that in Table 3 the SMAP is interpolated onto Aquarius spatial scale.

Table 3. Triple-point analysis: Monthly Bias and Standard Deviation (STD) differences for pairs Aquarius – in situ, SMAP – in situ and Aquarius - SMAP in April and May 2015.

	Aquarius – in situ		SMAP – in situ		Aquarius – SMAP	
	Bias	STD	Bias	STD	Bias	STD
April 2015	0.009	0.396	-0.005	0.459	0.012	0.340
May 2015	-0.008	0.435	0.031	0.406	-0.035	0.333

The difference statistics are quite similar in magnitude for the three pairs (**Table 3**). The triple-point analyses giving estimated RMSE of each measurement system (Aquarius, SMAP, in situ) are presented in **Table 4**. *Note that the largest RMSE belongs to the in-situ data. These are a combination of in situ sensor and representativeness errors. The latter include* *spatial and temporal variations of the in-situ observations within the 50 km search radius for each grid cell during the month, plus the salinity differences between the in-situ sampling depths and the surface.*

The Aquarius monthly RMSE estimates are 0.176 and 0.260 psu for April and May 2015. The Aquarius RMSE are larger than the calculations in the official Aquarius V5.0 validation report [9]. This could be related to the different search radius used for averaging the in situ, which is 150 km in [9] and 50 km in this report.

Table 4. Triple-point analysis: Monthly Root Mean Square Error (RMSE) differences for Aquarius, SMAP and in situ fields.

	Aquarius		SMAP		In situ	
	MSE	RMSE	MSE	RMSE	MSE	RMSE
April 2015	0.031	0.176	0.085	0.291	0.126	0.354
May 2015	0.067	0.260	0.044	0.211	0.122	0.349

8.4 Latitudinal distribution of zonally averaged and Longitudinal distribution of meridional averaged SAMP – in situ SSS differences

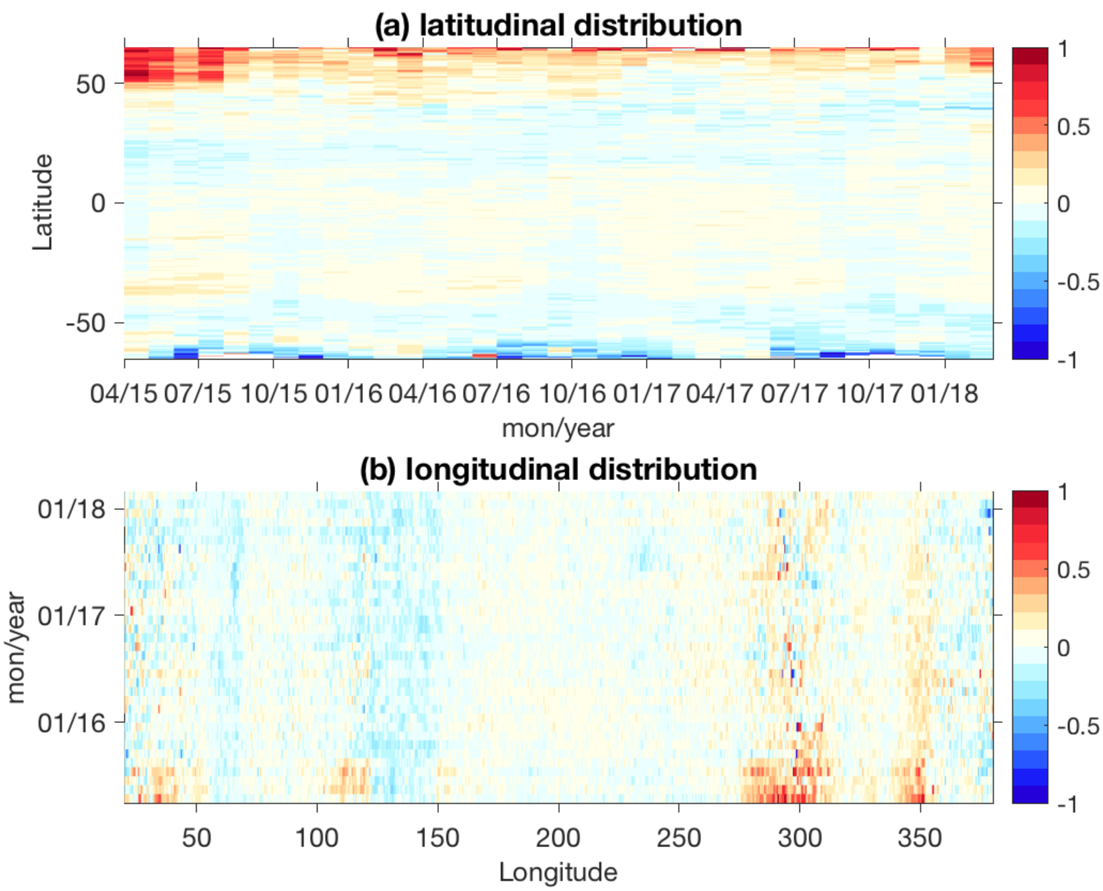

Figure 16 (a) Latitudinal distribution of zonally averaged and (b) longitudinal distribution of meridional averaged of SMAP - in situ SSS differences.

Figure 16 shows the in-situ difference statistics in discrete latitude bands for entire orbits for SMAP V4.0 Level 3 data. Strong positive biases (> 0.5 psu) are observed in the high latitude in the Northern Hemisphere (higher than 50°N) in the beginning of the first few months. Smaller positive biases continue around 60°N. Negative biases show up in the high latitude of the Southern Hemisphere, which was also seen in **Figure 6.** For the longitudinal distribution of the salinity differences (**Figure 16b**), the positive biases are consistent with the locations of the large variations in the high latitude of Northern Hemisphere during the early mission.

9. Summary, Conclusions and Cautions

This analysis documents the improvements from V3.0 to V4.0 science data processing and their effect on the SMAP salinity data. By various measures, the RMS errors are reduced in V4.0. In this document we also compared the satellite-centered and in situ-centered match-up for V4.0.

In this report, SMAP data Version 4.0 has been evaluated with multiple approaches. Regarding the data accuracy on monthly ¼ × ¼ degree scales, the results consistently demonstrate that V4.0 errors are around 0.22 psu. In Section 6, the triple-point analysis resolved SMAP RMSE 0.23 and Aquarius RMSE 0.21 for point comparisons (no monthly averaging). On monthly time scales, Section 8.3 triple-point analysis demonstrated a nominal RMSE ~0.24 for SMAP and ~0.22 for Aquarius.

9.1 Important achievement in each version

V3.0: The V3.0 use the geophysical model function (GMF) from Aquarius V5.0 release adapted to SMAP V4.0 (Meissner et al. 2017, 2018). Cross-Calibrated Multi-Platform (CCMP) product is used for near-real time ancillary wind speed and wind direction. V3.0 includes the NASA Global Precipitation Measurement (GPM) Integrated Multi-Satellite Retrievals for GPM (IMERG) rain rate for the atmospheric liquid cloud water correction and rain flags.

V4.0: The most important improvement in V4.0 is the land correction. The spatial resolution of the land tables is 1/2° in V3.0 and has been increased to 1/8° in V4.0. The land surface TB was based on a land surface emission model in V3.0 but is based on a monthly climatology of SMAP land TB measurements in V4.0. In V3.0, the sea-ice mask was from NCEP and is replaced with RSS AMSR-2 sea-ice maps in V4.0. The V4.0 salinity retrieval algorithm is using 40-km spatial Backus Gilbert Optimum Interpolation (OI). From the 40-km product, the smoothed 70-km product is derived using simple next-neighbor averaging. More details of the data updates are documented in [1].

9.2 Notes of Caution

<u>Note of Caution, during early mission:</u> Positive salinity biases are present in high latitude in the Northern Hemisphere in the early SMAP mission (around April to August in 2015). The actual cause is still unknown and further investigations are needed.

<u>Note of Caution, rain masks:</u> The rain-filtered (RF) are added in V3.0 for monthly Level 3 data. The data are discarded when the IMERG rain rate, resampled to 40 km, exceeds 0.1 mm/h. If the users are interested in the SMAP SSS under strong precipitation, the data without RF should be used. Otherwise, data with rain masks should be used for general studies. The users can tell if the data has been RF from the file titles.

Note of Caution, land fraction in the Level 3 mapped data: The RSS data uses *gland* > 0.04 and *fland* > 0.001 (moderate) for the criterion to include more data information near the coast. However, regions with *gland* between 0.04 and 0.001 are included in the mapped data with larger biases due to the land contaminations. The users should be aware the biases in these regions as discussed in Section 5.

Note of Caution, salinity differences around Antarctic Circumpolar Currents (ACC): As shown in Figure 6, negative differences and larger STD is observed around the Antarctic Circumpolar Currents. The salinity differences are more likely due to the salinity variations related to the ACC that are not captured by the low resolutions of the in-situ observations. More comparisons with other variables, such as sea surface temperature, surface wind speed and chlorophyll are needed to examine the ACC associated salinity variations in the SMAP data. Also, when the users are attempting to remove the high latitude biases in the SMAP data. Cautious should be used not to remove the ACC signals.

10. Reference

1. SMAP handbook. https://smap.jpl.nasa.gov/system/internal_resources/details/original/178_SMAP_Handbook_FINAL_1_JULY_2014_Web.pdf
2. Meissner, T., F.J. Wentz, A. Manaster, and R. Lindsley, 2019, NASA/RSS SMAP SSS V4.0 validated release (release notes, file and data formats, description of the algorithm, ATBD, validation).
3. Meissner, T., F.J. Wentz, and D.M. Le Vine, 2018, The Salinity Retrieval Algorithms for the NASA Aquarius Version 5 and SMAP Version 3 Releases. *Remote Sens*. **2018**, *10*, 1121
4. Chassignet, E.P., H.E. Hurlburt, E.J. Metzger, O.M. Smedstad, J. Cummings, G.R. Halliwell, R. Bleck, R. Baraille, A.J. Wallcraft, C. Lozano, H.L. Tolman, A. Srinivasan, S. Hankin, P. Cornillon, R. Weisberg, A. Barth, R. He, F. Werner, and J. Wilkin, 2009. U.S. GODAE: Global Ocean Prediction with the HYbrid Coordinate Ocean Model (HYCOM). Oceanography, 22(2), 64-75.
5. E.J. Metzger, O.M. Smedstad, P. Thoppil, H.E. Hurlburt, A.J. Wallcraft, D.S. Franklin, J.F. Shriver, and L.F. Smedstad, 2008: Validation Test Report for the Global Ocean Prediction System V3.0 – 1/12° HYCOM/NCODA: Phase I. NRL Memo. Report, NRL/MR/7320--08-9148.
6. E.J. Metzger, O.M. Smedstad, P.G. Thoppil, H.E. Hurlburt, D.S. Franklin, G. Peggion, J.F. Shriver, T.L. Townsend, and A.J. Wallcraft, 2008: Validation Test Report for the Global Ocean Prediction System V3.0 – 1/12° HYCOM/NCODA: Phase II. NRL/MR/7320--10-9236.
7. Argo (2019). Argo float data and metadata from Global Data Assembly Centre (Argo GDAC). SEANOE. https://doi.org/10.17882/42182
8. Boutin, J.; Chao, Y.; Asher, W.E.; Delcroix, T.; Drucker, R.; Drushka, K.; Kolodziejczyk, N.; Lee, T.; Reul, N.; Reverdin, G.; et al. Satellite and in situ salinity: Understanding near surface stratification and sub-footprint variability. *Bull. Am. Meteorol. Soc.* **2016**, *97*, 1391–1407.
9. Aquarius V5.0 Salinity data validation analysis (.pdf) [doi:10.5067/DOCUM-AQR02]

Appendix A: The NAVO/FSU HYCOM data are obtained from the global 1/12° data-assimilative HYCOM model along with the Navy Coupled Ocean Data Assimilation (NCODA) system at the Naval Oceanographic Office (NAVOCEANO). The HYCOM data are available from the HYCOM data server http://tds.hycom.org/thredds/GLBa0.08/expt_90.9.html?dataset=GLBa0.08/expt_90.9.

This HYCOM run assimilates available along track satellite altimeter observations, satellite and in situ sea surface temperature as well as in situ vertical temperature and salinity profiles from XBTs, ARGO floats, and moored buoys. In terms of near surface salinity forcing, HYCOM uses monthly climatology of river discharges (applied at the top 6 meters of the model) and relaxation to monthly SSS climatology (at 15 m) with a restoring time scale of 30 days, in addition to E-P forcing. Both the climatological river forcing and near surface salinity relaxation are intended to prevent the HYCOM simulation from drifting away from climatology, but at the same time they may suppress non-seasonal variations occurring in nature. The NCODA system is based on a multi-variate Optimal Interpolation (MVOI) scheme. Because of the assimilation of Argo floats and buoy data, the HYCOM analysis is not independent of Argo and buoys. Moreover, the nature of the assimilation could also introduce some level of correlation between the errors of the HYCOM analysis field and the errors of Argo and buoy SSS. More details of this HYCOM solution can be found in [4], [5] and [6].

Appendix B: Triple point uncertainty estimate of Aquarius, SMAP and validation data

The Aquarius salinity measurement S_A and the in-situ validation measurement S_V are defined by:

$$S_A = S \pm \varepsilon_A$$

$$S_S = S \pm \varepsilon_S$$

$$S_V = S \pm \varepsilon_V$$

where S is the true surface salinity averaged over the Aquarius footprint area and microwave optical depth in sea water (~ 1 cm). $\varepsilon_{A,}$ ε_S and ε_V are the respective Aquarius, SMAP satellite and in situ measurement errors relative to S. The mean square of the difference ΔS between S_S and S_V is given by:

$$<\Delta S_{AV}^2> = <\varepsilon_A^2> + <\varepsilon_V^2> \quad (1)$$

where < > denotes the average over a given set of paired Aquarius satellite and *in situ* measurements, and $<\varepsilon_A \varepsilon_V> = 0$.

Likewise, define SMAP salinity over the satellite footprint as $S_S = S \pm \varepsilon_S$, and mean square differences

$<\Delta S_{SV}{}^2> = <\varepsilon_S{}^2> + <\varepsilon_V{}^2>$ (2) SMAP vs in situ validation data

$<\Delta S_{AS}{}^2> = <\varepsilon_A{}^2> + <\varepsilon_S{}^2>$ (3) Aquarius vs SMAP

Equations (1)-(3) comprise three equations with three variables given by:

$<\varepsilon_A{}^2> = \{<\Delta S_{AV}{}^2> + <\Delta S_{AS}{}^2> - <\Delta S_{SV}{}^2>\} /2$ (4) Aquarius measurement error

$<\varepsilon_S{}^2> = \{<\Delta S_{SA}{}^2> + <\Delta S_{SV}{}^2> - <\Delta S_{AV}{}^2>\} /2$ (5) SMAP measurement error

$<\varepsilon_V{}^2> = \{<\Delta S_{AV}{}^2> + <\Delta S_{SV}{}^2> - <\Delta S_{AS}{}^2>\} /2$ (6) In situ validation measurement error

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