Summary of Changes to "Aquarius sea surface salinity optimal interpolation analysis"

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The purpose of this note is to describe the changes made to the Aquarius sea surface salinity optimum interpolation analysis (OI SSS) between the release of version V4.0 and V5.0 of the Aquarius SSS data.

Briefly, the changes can be listed as follows.

- 1) V5.0 (end-of mission) version of Aquarius Level-2 (swath) SSS data are used as input data for the OI SSS analysis.
- 2) The source of the first guess fields has changed from the APDRC Argo-derived SSS product to the average of four different in-situ based SSS products.
- 3) The bias correction algorithm has changed to adjust SSS retrievals for large-scale systematic biases on a repeat-track basis.
- 4) New, less restrictive thresholds are implemented to filter observations for land and ice contamination. The goal is to improve coverage in the coastal areas and semi-enclosed seas.
- 5) Level-2 RFI masks for descending and ascending satellite passes (flag 23) are used to discard observations in specific geographic zones where excessive ascending descending differences are observed due to contamination from undetected RFI. In those zones, the OI SSS analysis uses data from only ascending or descending passes, accordingly.

Aquarius SSS data

The satellite observations of SSS are obtained from Level-2 version 5.0 Aquarius data produced by the NASA Goddard Space Flight Center's Aquarius Data Processing System (ADPS). The Level-2 data files are distributed by the Physical Oceanography Distributed Active Archive Center (PO.DAAC) of the Jet Propulsion Laboratory (JPL), <u>ftp://podaac-ftp.jpl.nasa.gov/allData/aquarius/</u>.

First guess

In the previous version of the OI SSS analysis the first guess fields were derived from monthly mean SSS fields produced by the APDRC (Asia-Pacific Data Research Center, University of Hawaii) with variational interpolation of Argo buoy measurements. In the new analysis, the average of four in-situ based salinity products is used to derive the first guess fields. These products are:

- APDRC of the University of Hawaii Argo-derived salinity product (<u>http://apdrc.soest.hawaii.edu/projects/Argo/data/gridded/On_standard_levels/ind</u> <u>ex-1.html</u>);
- (2) Scripps Institution of Oceanography Argo-derived salinity product (<u>http://sio-argo.ucsd.edu/RG_Climatology.html</u>; Roemmich, D. and J. Gilson, 2009);
- (3) Met Office Hadley Center objective analysis from the profile data, version EN.4.2.1 (http://hadobs.metoffice.com/en4/index.html; Good et al., 2013); and
- (4) ISAS-15 salinity gridded fields (<u>http://www.seanoe.org/data/00412/52367/;</u> Kolodziejczyk et al., 2017)

The average of the four products is assume to better represent the ground truth (at large spatial scales) provided that the mapping errors of the products are not correlated.

Bias correction

In the OI SSS analysis, satellite biases are corrected relative to in-situ salinity data. In the new analysis, the bias fields are constructed on a repeat track basis. To construct the bias fields, satellite observations along each repeat track are averaged over a 3-year period from September 2011 through August 2014 and compared to in-situ salinity averaged over the same period. The in-situ salinity, which we regard as the "ground truth" at large spatial scales, is the compilation of the four Argo-based products, as described in section "First guess", interpolated into the ground track locations. Thus, there are two bias fields, one for ascending and one for descending ground tracks. They are shown in Figure 1 (note that the bias fields are constructed on a specific (irregular) grid, which corresponds to the ground track segments).

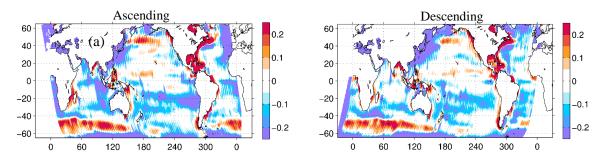


Figure 1. Mean spatial bias correction fields (psu) for Aquarius ascending (a) and descending (b) data.

As in the previous version of the OI SSS analysis, only systematic, time averaged biases (Figure 1) are taken into account. Correcting for the large-scale satellite biases on a repeat track basis separately for each of the three Aquarius beams helps eliminate residual interbeam biases which otherwise persist even after applying a multi-year average.

Coastal areas, RFI contamination, and global OI SSS fields

The following thresholds for data quality have been changed compared to the previous version of OI SSS analysis.

- Land fraction: from 0.005 in V4.0 to 0.01 in V5.0.
- Sea ice fraction: from 0.005 in V4.0 to 0.01 in V5.0.
- Cold water: from 5° C in V4.0 to 2.5° C in V5.0.

These changes helped to improve coverage in the coastal areas in high latitudes (Figure 2). In addition, Level-2 RFI masks for descending and ascending satellite passes have been used to discard observations in specific geographic zones indicated by the radiometer flag 23 (Aquarius User Guide, Dataset Version 5.0). In those zones, the OI SSS analysis may use data from only ascending or descending passes, accordingly.

Figure 2 presents an example map of the global SSS distribution for the week September 17-23, 2011.

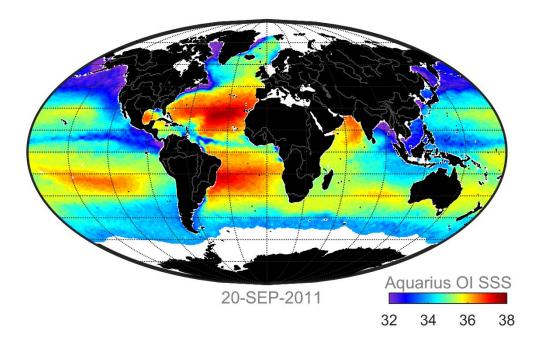


Figure 2. Aquarius V5.0 OI SSS field for the week 17-23 September 2011.

Validation

Argo buoy observations of salinity in the near-surface layer are used to estimate the error statistics for the OI SSS analysis version V5.0. The Argo buoy network provides quasi-random geographical distribution of about 1100 in-situ salinity measurements for each week. Only measurements shallower than 6 m depth and flagged as good from each Argo profile are used for the analysis. The error statistics for the OI SSS analysis are calculated by comparing buoy measurements for a given week with SSS values at the same locations obtained by interpolating the corresponding OI SSS maps.

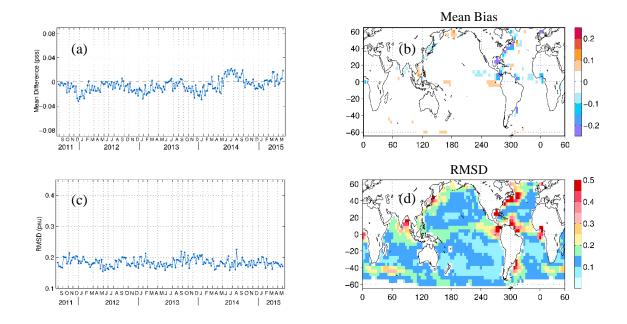


Figure 3. (a) Weekly mean differences (psu), (b) mean spatial bias (psu), (c) weekly RMSD (psu), and (d) geographical distribution of RMSD (psu) between Argo buoy observations and the Aquarius V5.0 OI SSS product. The error statistics were computed by comparing Argo buoy measurements for a given week with SSS values at the same locations obtained by interpolation of the corresponding OI SSS maps. The geographical distributions in (b) and (d) are computed in 8°-longitude by 8°-latitude bins.

The error statistics for the OI SSS analysis version 5.0 are presented in Figure 3. The product yields the time-series of the global bias oscillating around zero (Figure 3a). The time-mean global bias is smaller than 0.01 psu. The standard deviation of the weekly biases is 0.011 psu. The geographical distribution of the time-mean (static) bias is shown in Figure 3b. Over most of the ocean, the mean bias is smaller than 0.05 psu. Some residual biases (up to 0.2 psu locally) are observed along the continental boundary of North America in the Atlantic and in the eastern Tropical Pacific. The latter can be related to the difference in measurement depth between Aquarius (ocean surface) and Argo (~5 m depth) often observed in rainy conditions (Drucker and Riser, 2014).

The RMSD between the weekly OI SSS analysis and concurrent buoy data (Figure 3c) is smaller than 0.2 psu for nearly all weeks over the nearly 4-year period of comparison. The mean RMSD over the period September 2011 to June 2015 is 0.183 psu. The geographical distribution of the RMSD for the weekly OI SSS analysis is shown in Figure 3d. The RMSD are computed in 8°-longitude by 8°-latitude bins to ensure an adequate number of collocations (>100) in each bin. Over most of the ocean, the RMSD between weekly OI SSS maps and collocated buoy data do not exceed 0.15 psu. Figure 3d also demonstrates that the largest RMSD, exceeding 0.2 psu, are found in the regions of strong variability in SSS (see, e.g., Figure 4a in Melnichenko et al., 2016), such as along the North Pacific and North Atlantic ITCZ, the North Pacific sub-polar front, the Gulfstream, and near outflows of major rivers such as the Amazon in the tropical North Atlantic. In this regard, the observed relatively large RMSD between the Aquarius and buoy data in some areas are not necessarily due to errors in Aquarius measurements, but may rather reflect the sampling error (due to unresolved small-scale variability) and/or the difference in measurement depth between Aquarius (ocean surface) and Argo (~5 m depth).

The utility of the OI SSS product is further illustrated by Figure 4a, which shows the histogram distribution of the differences between the buoy data and OI SSS analysis. The OI SSS estimates have an overall good agreement with the buoy data such that the histogram of the differences is very narrow, with ~58% of the differences smaller than 0.1 psu and ~84% smaller than 0.2 psu. The number of outliers, defined in this particular case as the differences larger than 1 psu, is less than 0.3%. Their geographical distribution is shown in Figure 4b. Consistent with Figure 3d, the majority of 'outliers' are located in the areas of strong variability in SSS, contributing to large RMSD.

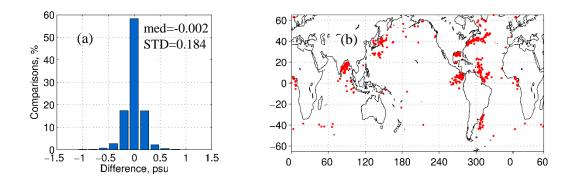


Figure 4. (a) Statistics of the differences between Argo buoy data and Aquarius OI SSS analysis. (b) Locations of 'outliers', defined as the differences large than 1 psu. The error statistics are computed by comparing Argo buoy measurements for a given week with SSS values at the same locations obtained by interpolation of the corresponding OI SSS maps.

Access to the data

The Aquarius OI SSS analysis can be accessed from the APDRC webpage <u>http://apdrc.soest.hawaii.edu/</u> either through the Live Access Server or OPeNDAP.

Digital data of the weekly OI SSS analysis (netCDF files) are also available at <u>http://iprc.soest.hawaii.edu/users/oleg/oisss/glb/OISSS_V5.0_weekly/</u>. Figures are here: <u>http://iprc.soest.hawaii.edu/users/oleg/oisss/glb/OISSS_PNG_V5.0_weekly/</u>.

Digital data of the monthly mean SSS fields can be downloaded from <u>http://iprc.soest.hawaii.edu/users/oleg/oisss/glb/OISSS_V5.0_monthly/</u>. Figures are here: <u>http://iprc.soest.hawaii.edu/users/oleg/oisss/glb/OISSS_PNG_V5.0_monthly/</u>

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