Changes to calculations of the World Ocean Atlas 2013 for version 2

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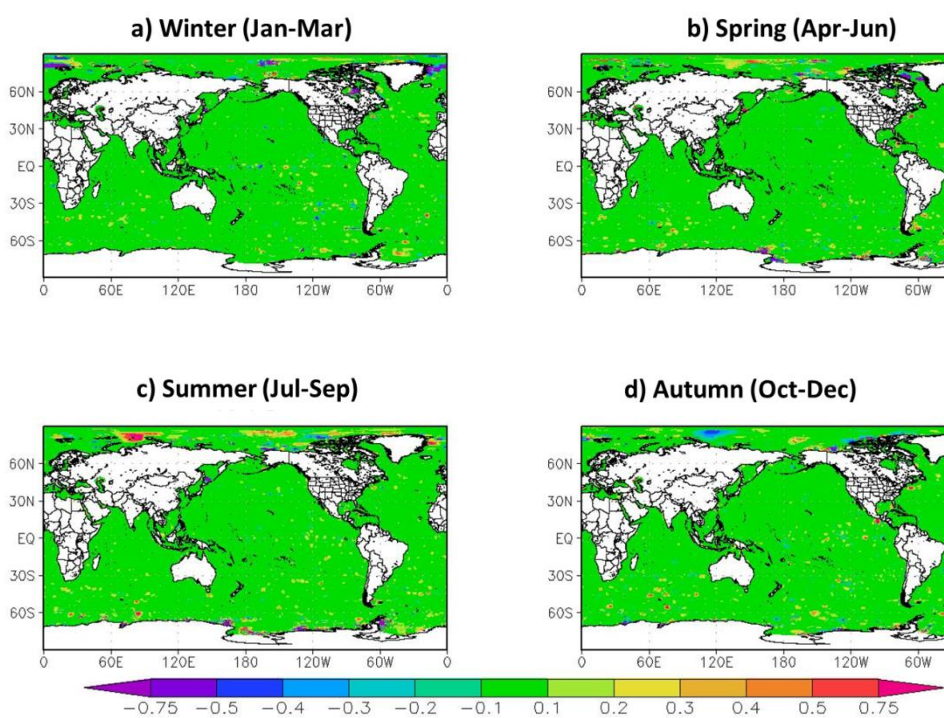
Introduction: The World Ocean Atlas 2013 (WOA13) represents the ocean state variables of temperature and salinity with more detail and less uncertainty than previous iterations in the World Ocean Atlas series due to large increases in data holdings and better temporal and spatial coverage coupled with refined analysis and quality control techniques. WOA13 expanded on previous releases with increased vertical resolution (3x in the upper ocean, 2x below 1500 m.), increased spatial resolution (16x), and the release of the decadal climatologies which were used to calculate the final 1955-2012 long-term climatological mean fields. This expansion greatly increased the burden on the calculation methodology and the quality control procedures. In order to improve upon the initial release of WOA13 (hereafter WOA13v1), an update, WOA13v2 has been prepared. This version addresses both methodology concerns and, to a lesser extent, quality control concerns which have surfaced since the initial release of WOA13. Below is an accounting of each of the methodology modifications found in WOA13v2 as well as the few quality control adjustments. Each of the changes has some effect on the resultant fields from local to global. The initial WOA13 fields are still of great utility and the updates detailed below do not preclude use of these initial WOA13 fields. Differences between WOA13v1 and WOA13v2 for temperature (Figure 1 a-d) and for salinity (Figure 1 e-g) are small over most of the ocean. However, for the regions specifically described further in the text, the WOA13v2 provides a more realistic representation of the temperature and salinity fields.



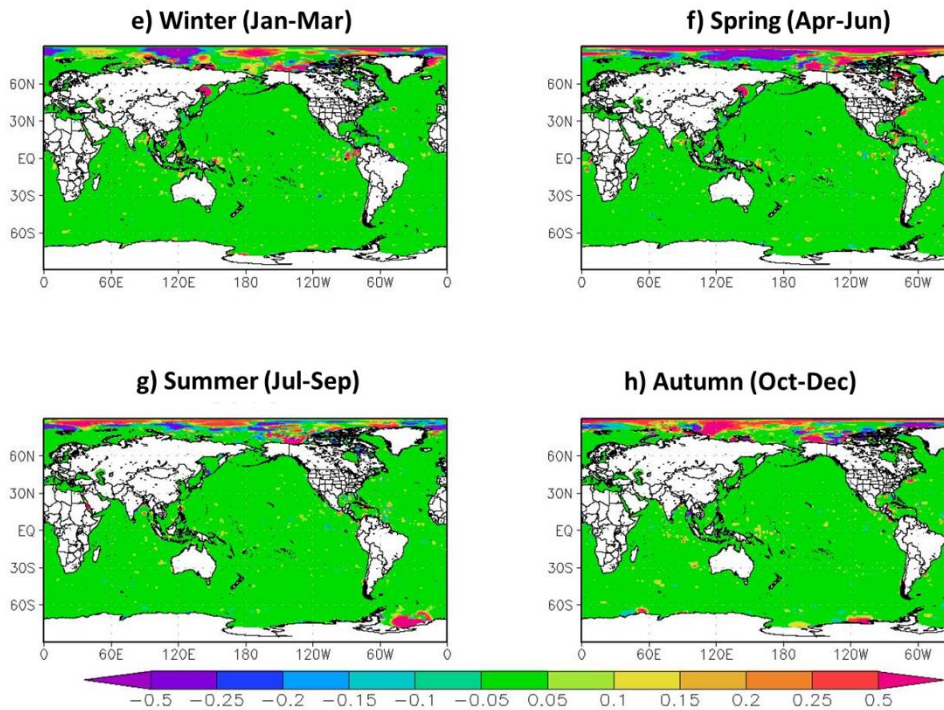


Figure 1: Difference between WOA13v1and WOA13v2 2005-2012 time period for temperature in Boreal a) Winter (Jan-Mar), b) Spring (Apr-Jun), c) Summer (Jul-Sep), d) Autumn (Oct-Dec) (°C) and for salinity in Boreal e) Winter (Jan-Mar), f) Spring (Apr-Jun), g) Summer (Jul-Sep), h) Autumn (Oct-Dec) (unitless, on Practical Salinity Scale 1978)

All-data first-guess field: The first-guess field for the analysis is the initial value assigned to each grid-box. The first-guess field is most important in data sparse areas where there are few data to alter the initial values. Prior to WOA09 release, the first-guess field for the annual mean was the zonal average using all available data. The first-guess field for each season was set to the analyzed annual mean field. The first-guess field for each month was set to the analyzed seasonal mean. WOA09 and WOA13 releases followed this procedure to create an initial all-data set of climatological mean fields. This initial all-data climatological mean field set was then used as a first-guess field for each of the analyzed decadal analyzed fields. These decadal fields were then averaged to calculate the final climatological mean field for the time period 1955-2006 (WOA09) and 1955-2012 (WOA13). The procedure as outlined was altered for the one-degree WOA13 fields to allow for the large amount of additional data added since the publication of WOA09. The first-guess field for each decade for WOA13 one-degree fields was the zonal average for the annual field, the analyzed annual field for each season and the analyzed seasonal field for the monthly fields only for that decades data. In this way data from any particular time period in data sparse areas would not influence the decadal mean for a decade which had few data in a region. In version 2, the procedure returned to the techniques used in WOA09, where the all-data analyzed fields were used as first-guess for the appropriate analysis.
Reason: Despite the increase in data used for the analysis, there are still time-periods and geographic areas, such as 2005-2012 (Figure 2a) in the Arctic, where data are too sparse to resolve known features (e.g. low near-coastal salinity values in some months). There are many more data when using values regardless of year (Figure 2b), providing a more representative first-guess field. While there are changes between version 1 (Figure 2c) and version 2 (Figure 2d), they are nearly identical outside high latitudes.

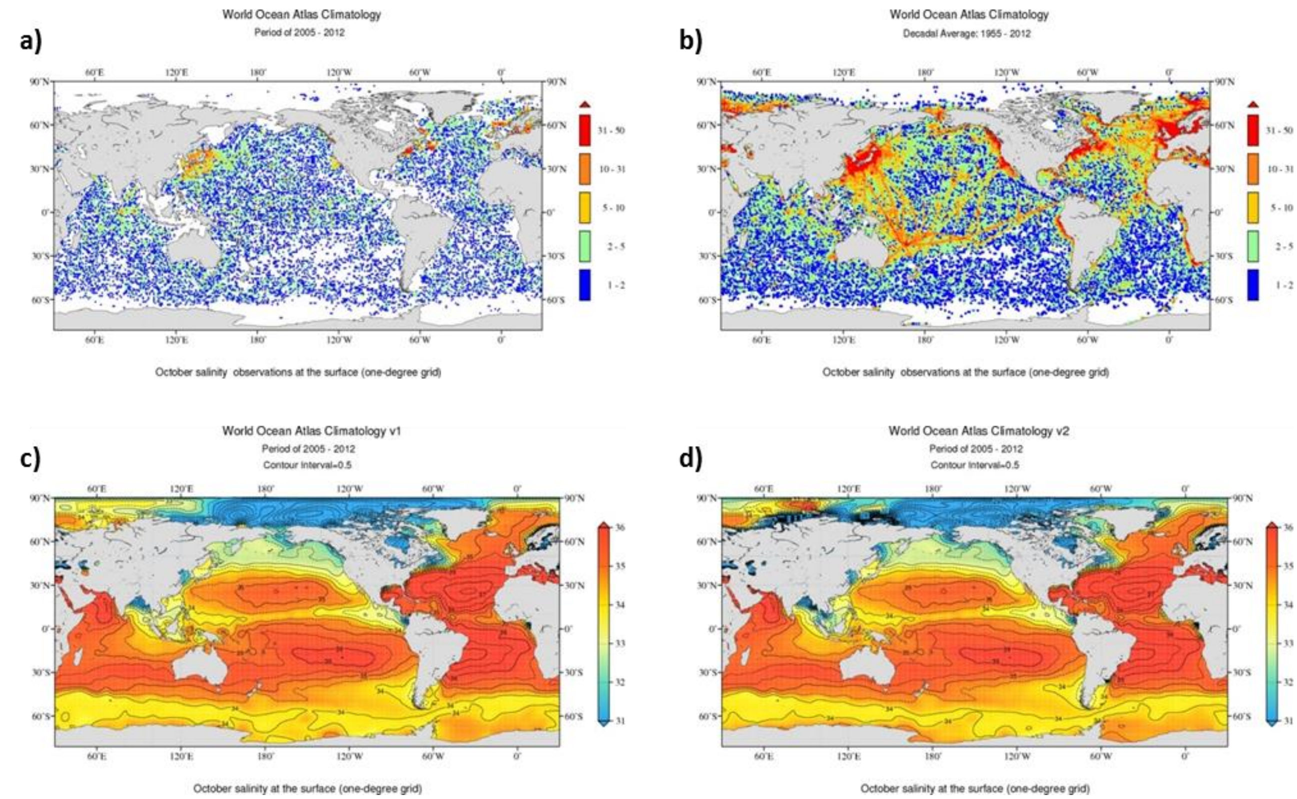


Figure 2: October surface salinity a) number of observations for 2005-2012, b) number of observations for 1955-2012, c) climatological mean from WOA13v1, d) climatological mean from WOA13v2. Colors for a, b correspond to number of observations in a one-degree grid box. Colors for c, d correspond to the Practical Salinity Scale 1978.

Salinity only stabilization: For any grid box where analyzed temperature is < 0.0°C in the top 400m, the stabilization routine will only alter salinity values, not temperature.

Reason: Stratification regimes at high latitudes are complex. Salinity in particular is highly locally variable in space and time, depending on ice freezing (high salinity) and melt (low salinity) and freshwater from runoff or rivers. The stabilization routine attempts to create a density-stable water column by changing temperature or salinity to achieve stability. However, at temperatures near the freezing point, density depends mostly on salinity and the stabilization routine can produce unrealistic results. This situation can be exacerbated in grid boxes where a shallow oceanographic cast with salinity and temperature is combined with a deeper cast with temperature only, leading to many cases where, if temperature is changed in the upper water column in this grid box based on the stabilization algorithm, the resultant temperature values are unrealistically high. It should be noted also that the correction is limited to waters close to their freezing point (<0.0C); there are high latitude areas, such as where North Atlantic waters make their highest penetration north of Norway, with relatively warm waters at depth and the standard stabilization routine is used in these cases.

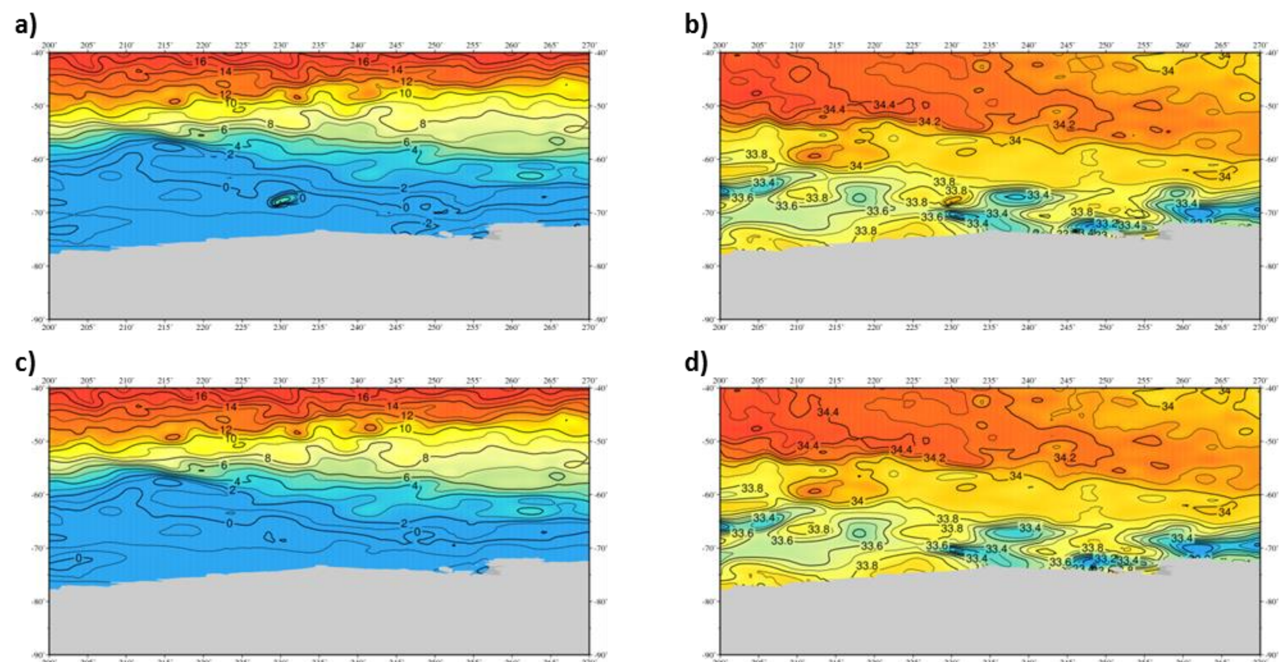


Figure 3: Quarter-degree gridded January mean for 2005-2012 at the surface for a) temperature WOA13v1, b) salinity WOA13v1, c) temperature WOA13v2, and d) salinity WOA13v2

Anomalously high sea surface temperatures are evident near 68S, 130W in the Southern Ocean for the quarter-degree gridded objectively analyzed January temperature field for time period 2005-2012 (Figure 3a) from WOA13v1. This feature is coupled with anomalously high salinities (Figure 3b). There are very few salinity data in this region for January for 2005-2012, as it out of the normal geographic range for Argo floats. In the upper twenty meters, the analyzed temperature before stabilization is close to 0.0°C (grey line in Figure 4a, same as black line in this case). The salinities before stabilization (grey curve in Figure 3b, same as turquoise curve in the upper 30 meters) are anomalously high, and exhibit an increase in the upper 20 meters which creates instability. The stabilization procedure aims to preserve as much of the original profile as possible, making changes to temperature and salinity at the fewest levels possible. In this case, that entails increasing the temperature unrealistically in the upper 30 meters of the water column (turquoise curve Figure 4a). Under the newly implemented restriction for cold water, the temperature remains unchanged (Figure 4a, black line), while the salinity alone is altered (Figure 4b, black line). This results in preserving the temperature values (Figure 3c), which are close to the freezing point, as expected, and moving the salinity values into more normal ranges for this part of the ocean (Figure 3d).

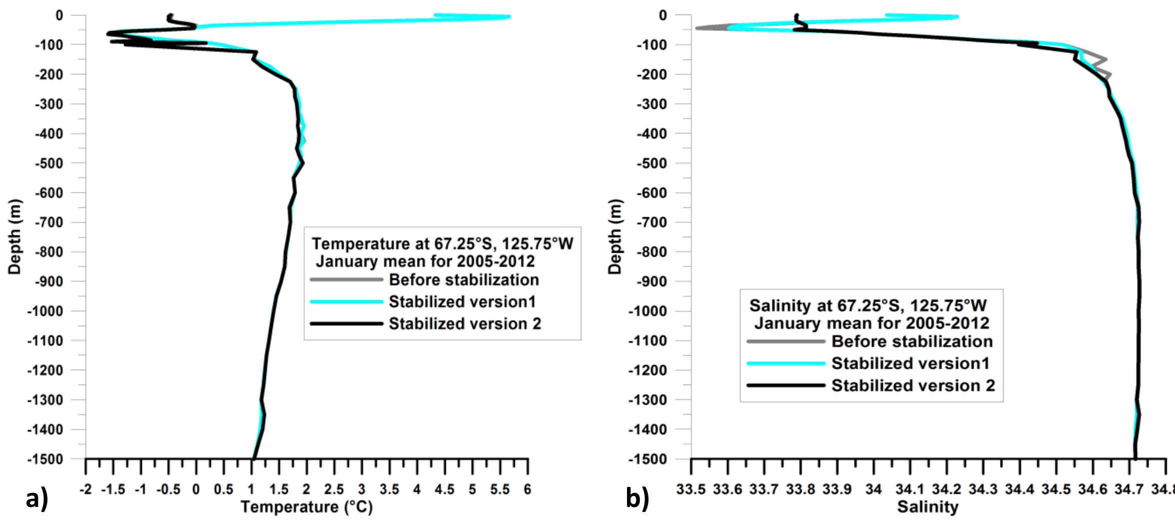


Figure 4: Vertical profiles at grid point 67.25°S, 125.75°W (location within warm feature in Figure 3a) for a) temperature and b) salinity. Stabilization in version 1 is set up to make the minimal adjustment to achieve stability, in this case resulting in anomalously high temperatures at the surface. Stabilization in version 2 adjusts only salinity.

How the mean values of temperature and salinity lead to large instabilities in the vertical water column has to do with the different distributions horizontally and vertically of temperature and salinity profiles and the non-linearity of the relationship between temperature and salinity with respects to density. These differences are exacerbated as the temperature and salinity are separately objectively analyzed. An extreme example occurs in the northern hemisphere high latitudes, in a polynya area east of Greenland. For the January mean in the time period 2005-2012, there are only two contributing oceanographic casts, an ice drifting buoy from 2006, and a profiling float from 2012 (Figure 5a,b, turquoise and grey lines, respectively). The ice drifter, as might be expected, has no measurements in the upper 20 m. with cold, fresh water directly below, with warming and saline gradients to 200m depth. The profiling float reaches the surface and has temperatures well above freezing near the surface, with relatively saline water. The profiling float cast extends to 1000m. When these two casts from very different oceanographic states are averaged, the mean profiles have only the warm, saline, profiling float data in the upper 20 m, followed by a combined (cooler, fresher) average down to 200m, the deepest extent of the ice drifter cast, and the profiling float cast only, again warm and saline, down to 1000 m. This creates a very large instability in the surface waters which is adjusted in this case by increasing the temperature in the upper 20 m from 1.1°C to > 2°C. There are few other data in this area for the objective analysis to modify the statistical mean.

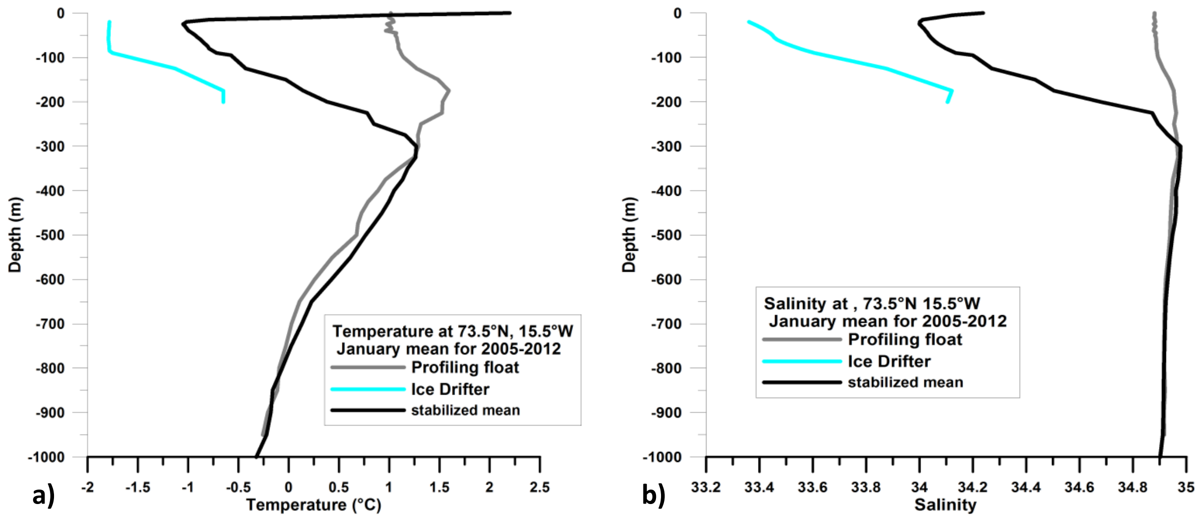


Figure 5: Vertical profiles of January a) mean temperature and b) mean salinity in time period 2005-2012 at the one-degree grid box centered at 73.5°N, 15.5°W (black line) and both oceanographic casts which were taken in the grid box for the period. Turquoise is an ice-drifting buoy cast, grey is a profiling float.

Freezing point check: The relationship of temperature and salinity climatological mean values is already exploited in the stabilization procedure. Now we also use this relationship to restrict final values of temperature at high latitudes. Before stabilization, temperature is adjusted to the value at freezing point for the corresponding climatological mean salinity value if the temperature is originally lower than freezing point. This check is performed a second time after initial stabilization and stabilization is performed again if temperature is altered. The check is not performed a third time.

Reason: Due to the dearth of data in high latitudes, especially in hemispheric winter, the objective analysis procedure used to calculate WOA13 can give unrealistically low temperature values. The lowest allowable temperature value in the analysis procedure is -2.10°C. This value necessitates a salinity value of 38.1 (at the surface), often an unrealistically high salinity value at high latitudes. There are more temperature data in many high latitude regions, historically, than salinity data, but the salinity data (before and after stabilization) can add important information to the calculated temperature value. This alteration in procedure does not cause much change in the climatological mean fields. There were < 1% one-degree grids over all depths which had temperature values below the calculated freezing point, and on average the amount below the freezing point was 0.12°C for 2005-2012 time period November climatological mean. After the freezing point check, there were virtually no temperature values below the calculated freezing point.

Additional/altered basin definitions: Very small changes in basin definitions were implemented for the area around the Panama coast and for a small coastal area of southwest Chile. The change around Panama consisted of shifting Pacific Ocean definition by 0.5° positional degrees to the south and west, while in the southwest of Chile, a new basin 'Chiloe' was added for the area between the island of Chiloe and the coast of mainland Chile. There is small difference between temperature near Chiloe between WOA13 v1 (Figure 6a, new Chiloe basin represented by off-white box) and WOA13v2 (Figure 6b). The difference in salinity between WOA13 v1 (Figure 6c) and WOA13 v2 (Figure 6d) is represented by fewer contours west of Chiloe representing a diminished offshore gradient.

Reason: Two grids for the quarter-degree analyzed fields were defined as Pacific despite being north of Panama on the Atlantic side. This led to a small discontinuity between these two grids and the surrounding area. West of Chile, new data east of the island of Chiloe with very low salinities were causing unrealistic values west of the island of Chiloe in the open Pacific in a data sparse area. Not allowing mixing between the new Chiloe basin and the open Pacific removed this problem.

Removed mixing barrier around tip of South America: The basin mask in WOA13 defines specific large oceanic regions (e.g. Pacific Ocean, Atlantic Ocean, Indian Ocean) as well as smaller regions (e.g. Mediterranean Sea, Persian Gulf). The WOA13 mixing mask assigns a value between -2 and 2 to each grid-box around the globe. When analyzing a grid-box, information from surrounding grid-boxes will only be used if they are in the same basin, or in different basins where the sum mixing number of the analyzed grid-box and the grid-box in question add up to a value > 0. This prevents analysis using oceanic regions which do not directly influence a given grid-box, such as Pacific water south of Panama for analysis of a grid-box north of Panama, in the Caribbean. The mixing numbers directly west and east of the southern tip of South America were reset to allow information to be used for analyses of grid-boxes on either side of the continent.

Reason: While ocean waters do mix through the Drake Passage and the Magellan Straits, there were so few data along the south west coast of Chile that shelf water east of Argentina were heavily influencing the analysis of the west coast values, leading to unrealistic features. Now, with the addition of many data along the southwest Chilean coast this was no longer a problem. But because the mixing was turned off west and east of the tip of South America, including north and south of the defined Atlantic and Southern Ocean interface (50°S) adjacent waters were not used to analyze grid boxes near this interface. The lack of allowed mixing across this interface coupled with the added data caused a small (0.4°C) temperature discontinuity across the interface (Figure 6a) at 50°S west of South America in WOA13 v1, most visible between 90°W and 75°W, which has been removed in WOA13 v2 (Figure 6b) . There is also a salinity discontinuity near the South American coast (Figure 6c) which has been removed in WOA13 v2. Allowing the mixing at the southern tip of South America removed the discontinuities.

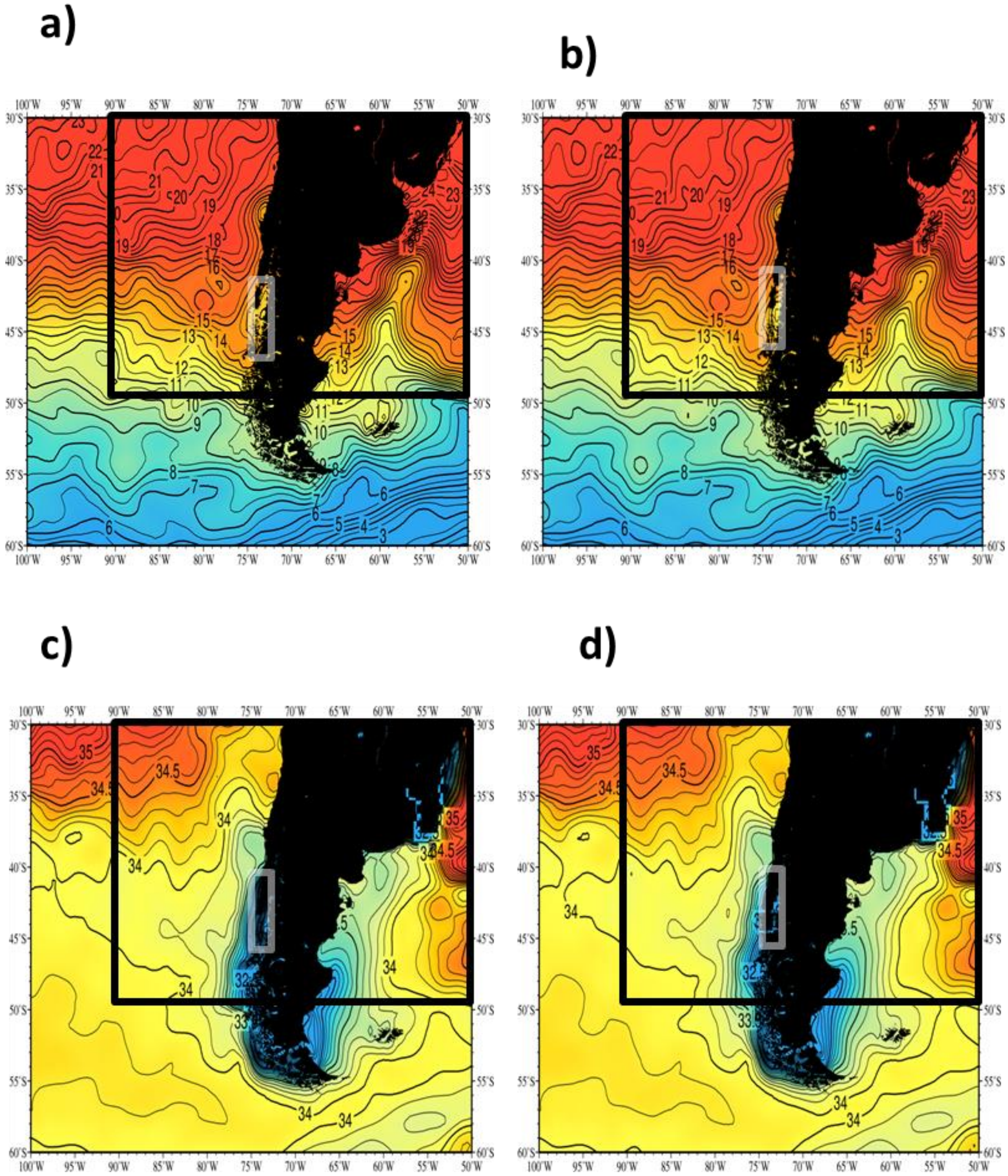


Figure 6. a) WOA13v1 temperature, b) WOA13v2 temperature, c) WOA13v1 salinity, d) WOA13v2 salinity for 2005-2012 Austral Summer. Inserted black box is mixing barrier which was present in WOA13v1, removed in WOA13v2. Inserted small white box is Chiloe basin, not present in WOA13 v1, present in WOA13 v2. Contour interval for temperature is 0.25°C. Contour interval for salinity is 0.1 on the Practical Salinity Scale 1978.

Modified standard deviation check near Gulf Stream – One of the main quality checks for data which are the input for the WOA is the standard deviation check. This check flags data which are 3, 4, or 5 standard deviations from the calculated means (depending on proximity to coast and/or ocean bottom) based on five-degree latitude/longitude box statistics. This check flags data which are either of poor quality or anomalous – outside of norms for the area. This is a valuable check, but it is predicated on a Gaussian distribution of values within the five-degree box. For one particular five-degree box mainly to the north of the Gulf Stream, 65°W to 60°W, 40°N to 45°N, the south-eastern section was switched to use the five-degree statistics from the adjacent five-degree box at 60°W to 55°W, 40°N to 45°N.

Reason: Because the original five-degree statistics are overwhelmingly from the area to the north and west of the Gulf Stream, cooler and fresher relative to the Gulf Stream, the mean and standard deviation were skewed toward this area and essentially flagged most data in the southeast section of the box, which touches the Gulf Stream, as anomalous (Figure 7a). The black triangle in Figure 7a is the area which was switched to use the five-degree statistics in the adjacent box (directly to the east). The box directly to the east has a more even distribution of data from north of the Gulf Stream and from the Gulf Stream itself, and hence a wider standard deviation about the mean. The modified standard deviation check results in more data preserved in the southeast corner of the original five-degree box (Figure 7b), and hence a more representative objectively analyzed mean field.

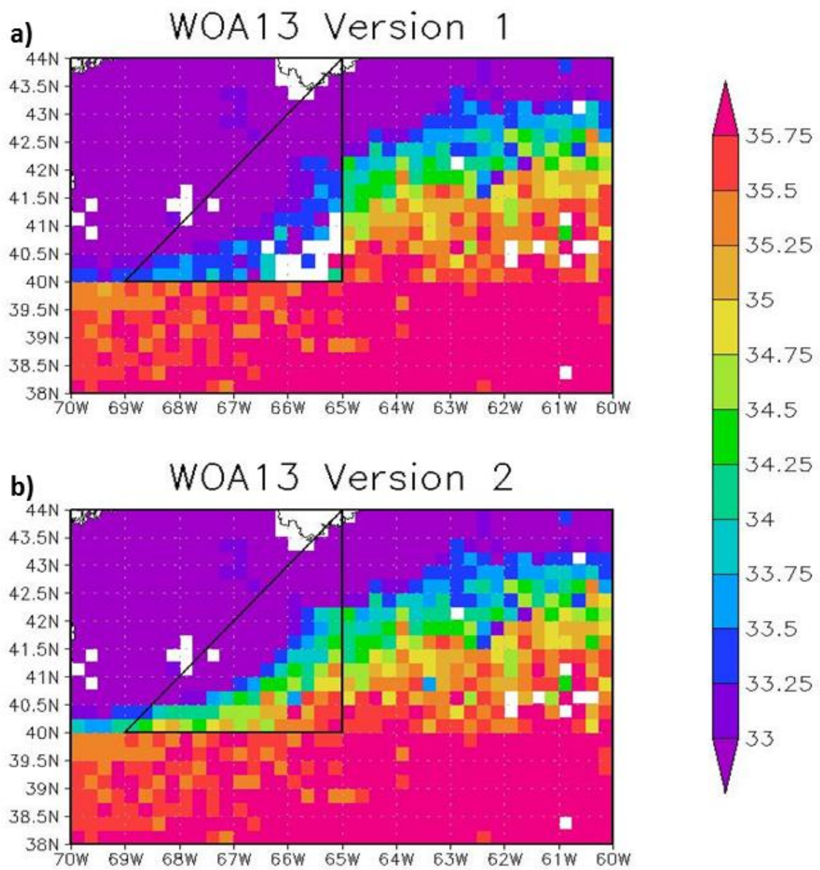


Figure 7 1955-2012 one-degree statistical mean salinity (annual) at 55 m depth for a) WOA13v1 and b) WOA13v2. Black triangle delineates area which uses five-degree statistics from adjacent five-degree box (directly to the east).

Seasonal fields below 1500 m depth: In WOA13v1 all seasonal temperature and salinity values below 1500m were identical to the annual values. In WOA13v2, the seasonal values for temperature and salinity are representative only of data exclusively for that season.

Reason: The seasonal cycle for temperature and salinity below 1500 m depth over most of the ocean is small. Small measurement, calibration, or data handling errors at these deeper levels can lead to regional seasonal differences which are more closely associated with data distributions and measurement and calculation uncertainties than with a true seasonal signal. However, the aggregation of historical and recent data in the World Ocean Database 2013 and increased quality control has lowered the uncertainties in deeper measurements and grid box means. The need to reduce uncertainties in global ocean heat and salt content calculations is the impetus to include any possible seasonal cycle in the climatological mean fields of temperature and salinity. Here the annual cycle is represented by the temperature in the season with maximum mean minus the temperature in the season with minimum mean for each one-degree grid box. For perspective the annual amplitude of temperature at the surface is shown in Figure 8a and the annual amplitude of temperature at 1000 m depth is shown in Figure 8b. In the 1600 m depth level, immediately below the maximum depth level for WOA13 monthly climatologies (1500 m), the annual cycle is < 0.2°C over most of the ocean, with a few areas > 0.3°C, notably just outside of the Red Sea outflow area.

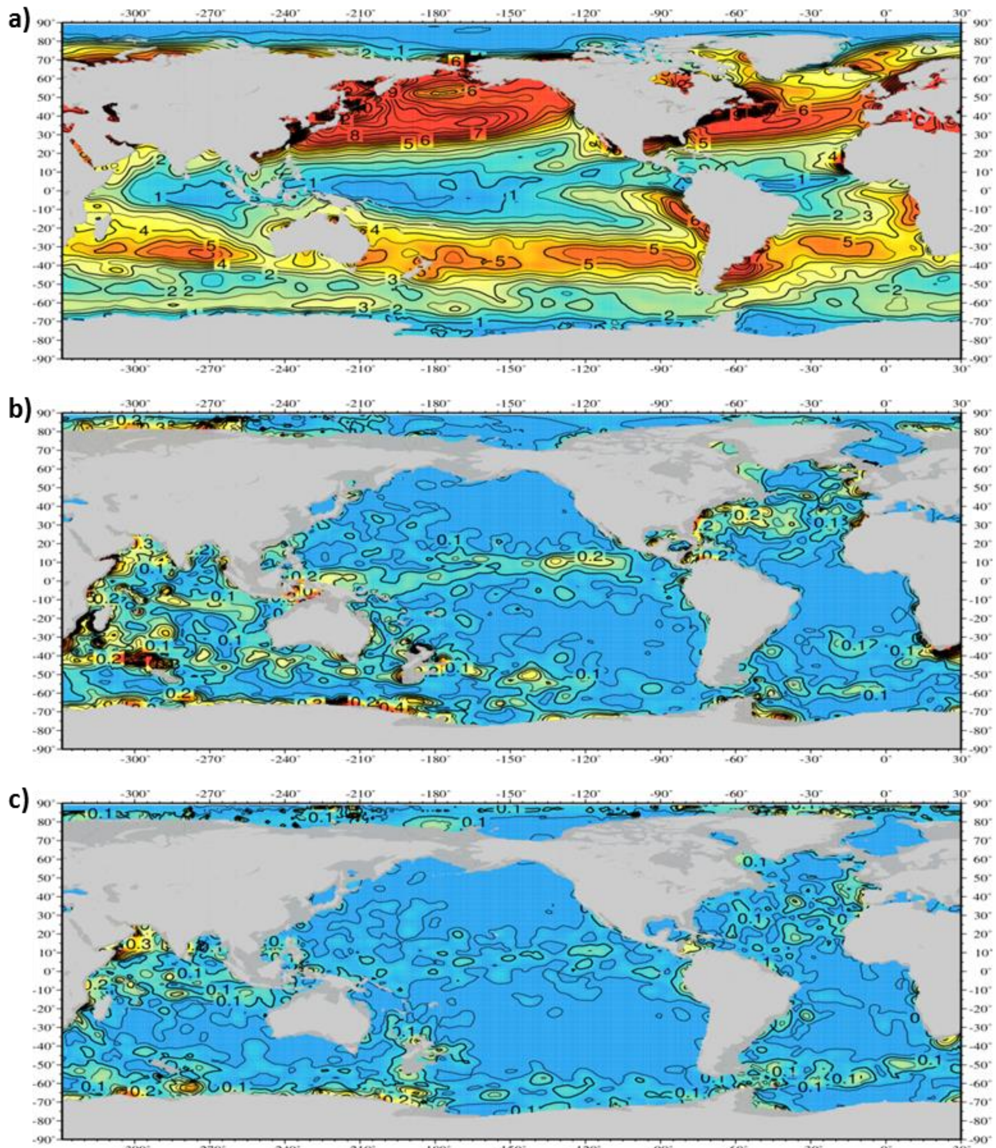


Figure 8: Amplitude of annual cycle of temperature (1955-2012 climatological mean) a) at the surface, contour interval 0.5°C, b) at 1000m depth, 0.1°C contour interval, c) at 1600m depth, 0.1°C contour interval.

Quality Flagging differences: Additional manual quality flagging was performed for WOA13v2.

Reason: Quality control decisions were based on the best available knowledge of regional and global oceanographic features. In some instances the decision to retain or flag data and exclude from use in climatological mean fields has been altered based on feedback from experts in a particular region which has led to reexamination of data. Methodology changes above have also had a small impact on the standard deviation quality control check. In the 2005-2012 climatological mean field for salinity at the surface, there are very few data between Panama and Colombia in the Pacific Ocean. This is an area of fresh river outflow, so low salinities are expected and represented in all decadal climatological means. However, the feature centered at 5°N, 89°W in WOA13v1 (Figure 9a) exhibits salinities lower than in any other decade and is the result of a single Argo float profile. This feature was reported by C. Maes, IFREMER, France (please see acknowledgements below for other reported features). Upon investigation, it was decided to remove the one Argo profiling float, as the salinities were not corroborated by any other data in the same decade and lower than any salinities in the area from profiles from other decades. It may be that the Argo float was accurately measuring the salinities, but without other measurements, it was deemed to be an anomaly and flagged. The resultant change represented in WOA13v2 (Figure 9b) greatly diminishes the low salinity feature found previously and brings salinities closer to values found for other decades. This is a subjective decision, one of many which are made by oceanographers with the help of the community of experts in different oceanographic regions.

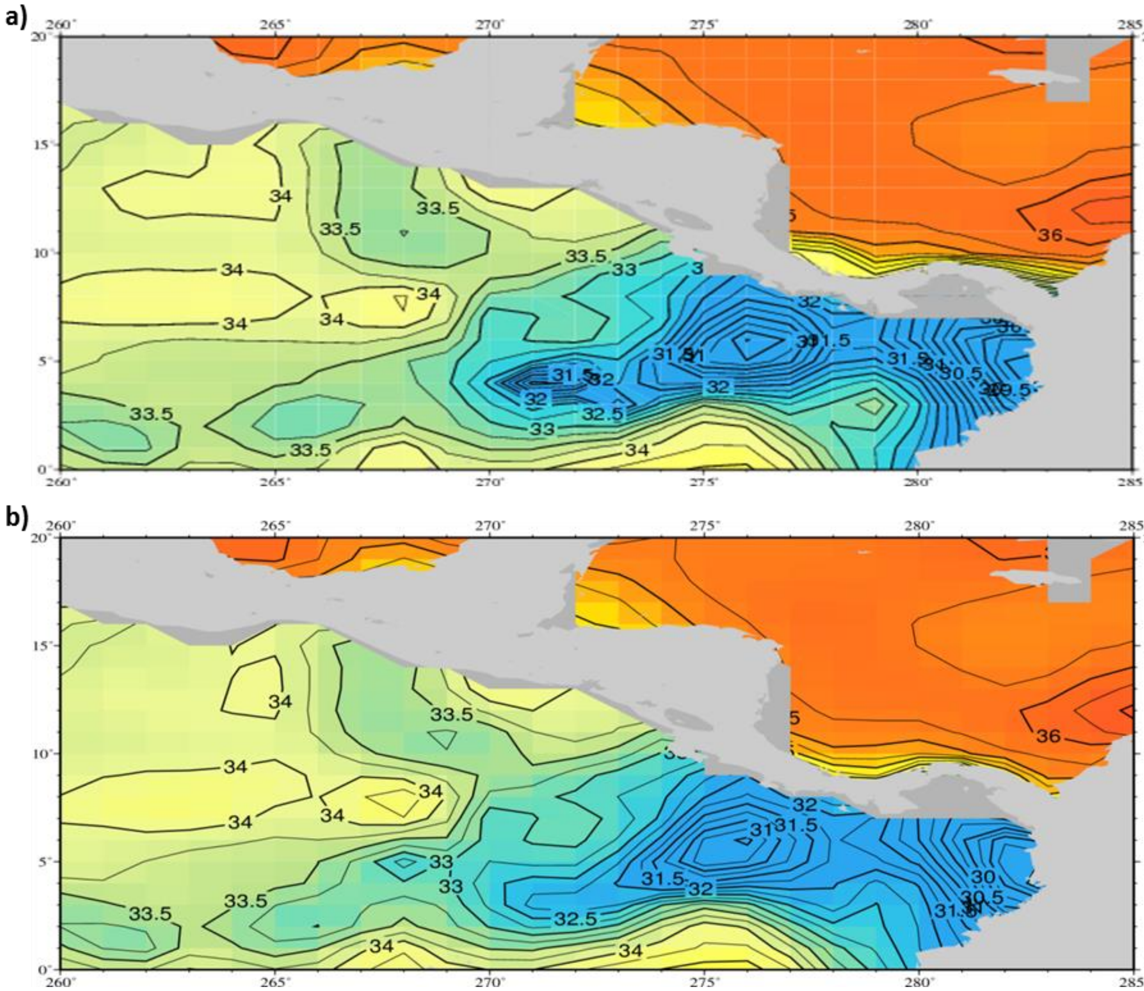


Figure 9. Quarter-degree mean February sea surface salinity for 2005-2012 for a) WOA13v1, b) WOA13v2.

Subjective flagging increased by roughly 1% in WOA13v2 (+416 temperature and +340 salinity profiles) This had a ripple effect on the standard deviation check, as the mean and standard deviation calculated at each successive iteration were tightened in areas where subjective flagging was added. In WOA13v1, 5.6% of all temperature profiles and 9.5% of all salinity profiles were completely flagged, mainly through the standard deviation check. There were a total of 11.1 million temperature profiles and 5.4 million salinity profiles. In version 2, 5.9% of temperature profiles and 9.8% of salinity profiles were completely flagged. In WOA13v1, 12.1% of all temperature profiles and 18.5% of all salinity profiles had at least one depth flagged. In WOA13v2 the percentages increased to 12.6% and 19.6% for temperature and salinity, respectively.

Acknowledgements: We would like to acknowledge the following researchers for bringing features in WOA13v1 to our attention which led to the procedure and quality control changes which have culminated in WOA13v2

- C. Maes, Institute de Recherch pour le Development/Laboratoire d'Etudes en Geophysique et Oceanographie Spatiales, (IRD/LEGOS), Toulouse, France – unusual freshening near-surface southwest of Panama, quarter-degree salinity 2005-2012, February
- J. Kjellsson, British Antarctic Survey, Cambridge, UK – Extremely low salinities in the Weddell Sea, quarter-degree salinity 1955-2012 decadal average, August.
- T. O'Brien, National Marine Fisheries Service/National Oceanographic and Oceanic Adminstration (NMFS/NOAA), Silver Spring, Maryland, USA - unnatural box corner gradient in statistical mean northwest of the Gulf Stream, quarter-degree salinity, 1955-2012 annual field.
- C. Regnier, Mercator-Ocean, Toulouse, France - unnatural straight line gradient at 50°S west of South America, quarter-degree temperature, 2005-2012 winter mean.