

# Improvement of the assessment of Argo floats in the Southern Ocean including Weddell sea as part of the Argo Southern Ocean ARC

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v0.2	13 June 2022	Kamila Walicka	Executive summary and introduction; SO QC method, Review the floats
v0.3	20 September 2022	Kamila Walicka, Ingrid M. Angel-Benavides	Issues and Recommendations, CTD reference data for the SO
v0.4	30/09/2022	Kamila Walicka	Corrections to comments from the project partners
v1.0	17/10/2022	Kamila Walicka	Final version of deliverable



## **EXECUTIVE SUMMARY**

The objective of this task is to perform development works of the assessment of the temperature and salinity data in the Southern Ocean (SO). The first part of the task was focused on the validation of the homogeneity of the data set collected in this region, and the second part aimed to develop a method to routinely undertake a review of the core parameters collected by the Argo floats.

The CTD reference database used for Argo DMQC in the SO was improved during Euro-Argo-RISE by removing duplicated profiles and adding profiles from the PANGAEA dataset that were not previously present in the South Atlantic sector. Although recently collected profiles were made available, the number of profiles per cycle in the Weddell Gyre is low and there are large areas without any CTD reference data. A community effort will be necessary to further guarantee the flow of data (from repositories, and scientists) into the CTD reference database for Argo.

The quality assessment method in the SO uses the pre-classified core Argo float and climatological data belonging to similar water mass regimes using the Profile Characterisation Model (PCM). The SO assessment software has been developed based on the code created within the Euro-Argo RISE WP2.4 project at Ifremer/LOPS. The output of this software, which is the pre-classified reference data, is further used in the DMQC software - OWC analysis. This method allows the DMQC operator to avoid noise from other water masses leading to a more robust quality control analysis of salinity data in delayed mode. Besides having the full functionality of the code, the report also highlights the further need for its maintenance and also proposes future developments and wider implementation of the code.

The SO quality assessment method was tested on Argo floats which have been already analysed by DMQC operators from various DACs and submitted to GDAC. During testing the software we identified some inconsistencies in results often related to working with difficult floats, the use of different setups, versions of reference data or procedures used at the time the d-mode analysis was made. This project contributed to compiling the list of the typical problematic cases in the DMQC analysis which might be further addressed during the DMQC workshops to improve the best practices in assessing the quality analysis on the core Argo floats. In order to improve the DMQC operators experience and to ensure high-quality delivered data, there is a need to continue organising the DMQC workshops.

Moreover, the continuous development of the procedures and growing quality and availability of the reference database reveals a need to ensure further regular audits of already submitted floats in d-mode. The regular audits and support to DMQC operators of floats in the SO might be an activity led by the SOARC group. This would, however, require sufficient resources.



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# 1. Introduction

The Argo floats measurements at high latitudes in the Southern Ocean (SO) provide a unique and valuable source of data which allows researchers to monitor the long-term change within water masses and how it compares to the interannual variability. These data are crucial to estimating global climate change and better understanding the future important consequences of these changes (Johnson et al., 2021).

The SO is characterised by very strong ocean dynamics with a very wide spectrum of ocean regimes (Rintoul and Garabato 2013). Additionally, due to the presence of ice, the sampling of the temperature and salinity data in this region might be very challenging. The presence of the sea ice, represents a hazard to the integrity of the floats, prevents floats communication with satellites, and makes it difficult for conventional Argo floats to surface to transmit data. The newly developed ice-capable autonomous floats allow a number of profiles to be collected beneath the wintertime ice cover (Rise et al., 2018). However, the sea-ice cover is still a limitation for making ship-based operations.

As a result, the hydrographic data from the climatology and the Argo floats are relatively limited and sparse in the SO compared to many other ocean regions. For these reasons the quality control analysis of the core Argo float data in the SO is often very challenging for the delayed mode quality control operators and needs to be performed with very high care.

A regular check of the quality of Argo float data in delayed mode is necessary to ensure the consistency of analysed salinity data within the basin. Moreover, the DMQC analysis is often conducted by operators from various national data centres who have different experiences in analysis and oceanographic knowledge from specific regions. Another aspect is that the available reference datasets for DMQC analysis have evolved since the beginning of the Argo project, where a continuous increase in the amount of reference data gives a better opportunity in obtaining more robust results in verifying previous analyses.

The objective of this task is to assess the homogeneity of the data set collected in the SO and to develop a method to routinely undertake reviews of temperature and salinity reported by the Argo floats.

This report includes an assessment and improvement to the availability of the CTD reference data in the SO and a detailed description of the SO quality assessment. The SO quality assessment has been performed based on the DMQC analysis of the salinity data of Argo floats using the beforehand classified Argo float profiles and reference data profiles belonging to similar water mass regimes. An additional part of this document presents the review of the delayed mode (DM) floats in the SO using the quality assessment method and demonstrates some of the typical issues and discrepancies in the results compared to already analysed flotas in DM. The final part of the report includes the limitations and future recommendations related to the quality assessment in the SO.

### 1.1 Reference data in the Southern Ocean

Two common reference datasets are available for DMQC of Argo floats, formatted for its direct use with the OWC software: the Argo reference database and the CTD reference database, both updated at least once a year. The updates and changes are reported at the Argo Data Management Meetings



(ADMT). The Argo reference database is maintained by J. Gilson (Scripps Institution of Oceanography) and contains historical Argo profiles that after verification on DMQC have not required any salinity adjustments. The CTD reference database for Argo is maintained by the Coriolis/Ifremer team for operational oceanography. Every new release contains additional profiles that have been obtained from different sources. The origin of each profile is recorded in the variable QCLEVEL using a three-letter code. Usually, the profiles are obtained via downstream services: the updates of the Ocean Climate Laboratory/NODC to the World Ocean Database WOD (OCL), and data from the International Council for the Exploration of the Sea ICES (ICE), the CLIVAR and Carbon Hydrographic Data Office CCHDO (CCH) and their product GO-SHIP (GSH). More rarely, profiles are delivered directly by scientists/principal investigators from research cruises whose data is not public (SPI) or from CTD casts done during Argo float deployments (DPY). Also, visual quality control by period and platform are performed to ensure the good quality of the data.

As part of the Euro-Argo RISE project, several actions have led to the improvement of the CTD reference database. Careful identification and removal of duplicated profiles were performed on a global scale (WP2 and WP3 Task 3.2). Also, after an initial assessment shows that in the high latitudes, including the Southern Ocean, the profiles in this database are sparse and outdated, local updates were performed (WP2 and WP5). For this report, the efforts were focused on the Weddell Sea, a region of special interest to the Euro-Argo partners and will be described in Section 2.

## 1.2 Assessment of the method

The quality assessment of salinity data of Argo floats is performed for floats deployed in the SO region (south of 40° S). The SO quality assessment method has been designed based on our prior review of some other available methods used for the quality checks of Argo floats. These included a review of two software for the profile classifications and also the assessment of the DMQC-ed floats used by the Coriolis Argo Regional Centre in the North Atlantic. The first reviewed software, soarc floatchar allows the characterisation of the argo float profiles into ACC fonts and zones based on the temperature and salinity of water masses in the specific zones in the SO. The ranges of these properties were specified based on the literature review (Orsi et al., 1995; Sokolov and Rintoul, 2008, 2009a; Boehme et al., 2008). This software was developed in Matlab, by researchers from the University of Bristol, UK, however, allows only for classifying Argo profiles and is not customised and adapted to operate with the OWC software used for the DMQC analysis. The second software DMQC-PCM is based on a machine learning approach and uses the statistical classifier Profile Classification Model (PCM) operating in Python coding language. This software allows the classification of the Argo profile and climatological data (called further the reference data) used for validating Argo data. The PCM is a scientific analysis approach which allows the user to automatically assemble temperature and salinity profiles in clusters according to similarities in their vertical profile structure. It is based on the unsupervised and automatic classification of profiles with a Gaussian mixture model (Maze et al, 2017). This method allows, for instance, front detection, water mass identification, natural region contouring, and reference profile selection for validation (Maze et al, 2017). This code has been developed within the Euro-Argo RISE WP2.4 project at Ifremer/LOPS. A detailed description of the software can be found in <u>D2.4</u>. The code is already customised to operate with the Matlab version of the OWC software. After considering a variety of features of both software such as coding language, code performance, evaluation time, amount of developments and improvements needed, the DMQC-PCM software was chosen as the most proper software to use in the quality assessment of Argo floats in the SO.



The method of the quality assessment of the DMQC-ed floats in the Atlantic Argo Regional Centre (AARC) uses the OWC software. This quality assessment tests the salinity data corrections which already went through the delayed mode processing. For DMQC re-analysis analysis, the AARC uses the OWC software, where they calculate the time-varying correction of salinity based on a comparison with climatological data (Owens and Wong, 2009; Cabanes et al., 2016). More details about the AARC method can be found here <u>Consistency-checks-of-DM-salinity-corrections</u>. The OWC software is available in both Matlab (<u>matlab owc</u>) and Python (<u>argodmqc owc</u>) versions.

The review and testing of the currently available quality assessment methods mentioned earlier in this section allows us to design and develop a method which enables us to undertake a more routine review of the quality of core parameters of Argo floats. Our approach was to create the software which will include the combined DMQC-PCM and OWC software. We have found that this combination should most efficiently perform the quality assessment of Argo floats in the SO.



# 2. CTD reference dataset for the Southern Ocean DMQC

At the beginning of the project the status of the CTD reference database for Argo was checked (version 2019v01) using a Matlab tool developed for this purpose as part of both MOCCA and Euro-Argo RISE projects (<u>https://github.com/euroargodev/check\_CTD-RDB</u>). For this purpose, the SO definition used for the float assessment was slightly expanded to include all profiles south of 30°S, since the OWC procedure for quality control will likely use profiles north of 40°S for floats operating near this limit. The geographic distribution of the profiles is shown in Figure 2.1, where the year of acquisition is colour-coded. This map shows that:

- Most of the data is from the pre-argo era (dark blue points)
- There are large regions without any profiles, most notably in the Pacific Sector.
- The most recent data (dark yellow to yellow points) comes from cruise lines that are being revisited, and the spatial coverage seems to be deteriorating over the years.



**Figure 2.1** Position of the profiles in the Southern Ocean colour-coded by year in the CTD\_for\_DMQC\_2019v01.





Figure 2.2 Position of the profiles in the Weddell Gyre colour-coded by year in the CTD\_for\_DMQC\_2019v01.

The Weddell Gyre region was particularly outdated and scarcely populated (Figure 2.2). This concerns the work of BSH as responsible for the DMQC of German floats in the region. Particularly, NEMO floats (Argo float model manufactured by Optimare, now discontinued) deployed by the Alfred Wegener Institute (AWI) between 2011 and 2017, which were recently re-decoded, and adopted by BSH since they still need to undergo DMQC. This task needs to take into account the particularities of this float model (now discontinued) and ensure consistency in the DMQC decisions. When using the OWC DMQC method on these floats, the number of reference data available for each float is in general low (n <50), which combined with the aged profiles makes the DMQC results somewhat questionable. Therefore, a local update of the database (to 2021v01) was done using data from the PANGAEA data centre, which is not delivering it's data to the World Ocean Database managed by NCEI for IODE or other downstream services Argo use to update the CDT reference database(personal communication). This first exercise resulted in the addition of 332 profiles to the South Atlantic Sector of the SO (south of 30°S, 70° W to 30° E)), which was used internally for DMQC. A comparison between the OWC results of some floats before and after this update showed that the number of available reference data continued to be low with a slight increase of about 5 reference profiles per cycle and that there was no considerable impact on the DMQC decisions. This is exemplified using the AWI NEMO float WMO 7900464 (Figures 2.2 and 2.3) that operated between January 2017 and 2019 in the Weddell Gyre.

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**Figure 2.3** Profile positions of WMO 7900464 (left) and a number of reference selected data for each cycle using different CTD reference databases and OWC parameters (right).



**Figure 2.4** Changes in the number of reference profiles available per cycle (left) and the corresponding salinity corrections from OWC (legend as in Figure 2.3)

## 2.1. Removal of duplicated profiles

The CTD reference database was carefully checked for duplicates and near-duplicates, using Matlab scripts that are available on the GitHub repository <u>CTD-RDB\_for2021v01 release</u>. This update was released for the CTD\_for\_DMQC\_2021v1 dataset. Table 2.1 summarises the results of this procedure in the Southern Ocean per subregions. Many profiles were duplicated and therefore there was a decrease in the number of profiles available in this release. Considering that this procedure removed



18,6% of the profiles (31693 of 169689) in the global ocean, the incidence of duplicates was larger for the Southern Ocean.

Southern Ocean regions	Number of profiles 2020v01	Number of profiles 2021v01	Number of profiles excluded	% Excluded
South Atlantic	3624	2786	838	23,1%
South Pacific	4232	2660	1572	37,1%
Indian	4994	3368	1626	32,6%
Weddell Gyre	2846	2009	837	29,4%
East Antarctic Coast	1898	1246	652	34,4%
Ross Gyre	2853	2043	810	28,4%

**Table 2.1**. Summary of changes in the CTD reference database after removing duplicated profiles.

Checking for duplicates in the database is necessary to avoid data redundancies, which lead to an artificially high number of profiles available for DMQC and therefore improves the selection of the reference profiles. Moreover, having a robust and automatic duplicate check procedure in place makes maintaining the database up-to-date way easier, since one can collect profiles from all possible sources without manually checking if the data is already available.

## 2.2. Update with PANGAEA data

Data from PANGAEA is not delivered directly to downstream services like WOD (personal communication) and therefore these profiles are not fed automatically into the CTD database for Argo DMQC. PANGAEA was searched for profiles acquired by the German Research Vessel and Icebreaker Polarstern in the Southern Hemisphere from 2009 onwards (Access: 21.06.2021). The data is provided in \*.tab format files. A total of 23 files were downloaded corresponding to cruises: ANT-XXVI, ANT-XXVII, ANT-XXVIII, ANT-XXIX, PS82, PS89, PS95, PS96, PS111, PS117, and PS118; as well as data from an experiment conducted in the Atka Bay. Data from PS113 (2018) is under moratorium while data from PS112 is password-protected raw CTD data. BSH has established communication with the Alfred Wegner Institute (AWI) in order to pursue easy and more timely access to all PANGAEA data for Argo DMQC. From the 1346 profiles in those files, 632 profiles in the South Atlantic Sector of the Southern Ocean (70°W - 30°E, south of 30°S) fulfilled the criteria of having a maximum recorded pressure deeper than 900 db and were selected for the update (Figure 2.5). Initially, these profiles were added to the 2021v01 and used for the DMQC tests in the Weddell Sea described above, but since the release of 2021v02 became available since then, the procedure was repeated and the results are shown here. The profiles were assigned the code 'PAN' to indicate that they were obtained from PANGAEA.

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During the merging procedure, it was identified that 130 of the profiles were already in the database. Of those, 49 were exact metadata duplicates (latitude, longitude and date) which were obtained by CCHDO (45) or OCL (4); 82 were content duplicates, which were mostly from GO-SHIP Deep Argo (66), and some from CCH (14) and OCL (2).

Additional 46 PANGAEA profiles were excluded since they did not pass the "monotonically increasing pressure" test. This is an automatic procedure that was implemented to identify profiles containing more than one CTD cast that was present in the Nordic Seas. In those cases, the pressure increases

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monotonically until the end of the first cast and then decreases when the next CTD cast starts (see Angel-Benavides et al. 2020 Fig. 9). Closer inspection of the PANGAEA profiles that failed this test showed that most of the non-monotonically increasing pressure occurs in small sections likely because the CTD was stopped mid-depth. Such profiles need to be corrected before delivering the update to the Coriolis Team for future release.

Finally, a total of 478 PAN profiles were kept. Their temporal distribution is shown in Figure 2.6. Figure 2.7 shows the year of the latest profiles in each 5° x 5° bin before and after the update. The objective of adding more recent data (brighter yellow bins) in the Weddell Gyre region was achieved, and boxes in the south are newly populated (before in white). However, Figure 2.8 shows that the issue of large areas without reference data remains since most of the data comes from monitoring cruises that repeat the same lines.



Figure 2.6 Temporal distribution of the Polarstern profiles new to the database.



**Figure 2.7** Year of the latest profile per 5° x 5° bin in the CTD\_for\_DMQC\_2021v2 before (left panel) and after (right panel) the addition of Polarstern data.





**Figure 2.8** Position of the profiles in the South Atlantic Sector of the Southern Ocean colour-coded by year after the addition of Polarstern data to CTD\_for\_DMQC\_2021v2

For the next release of the CTD reference database is necessary:

- To remove 170 near duplicate profiles already present in CTD\_for\_DMQC\_2021v2 (South Atlantic sector only). All of them were added recently (GSD: GO-SHIP Deep Argo) but were already in the database. GSD profiles will be kept (following the ADMT22 reference database report). It is still necessary to ensure the proper workflow of all involved in the updates to guarantee that the duplicate check, for which scripts are publicly available, is the last step of the database update
- Perform a quality check of the PANGAEA profiles excluded for having non-monotonically increasing pressure to select the profiles (and samples) that should be added to the database.
- Visual checks for each WMO box before the release. This is a common practice to ensure that the data does not contain outliers.
- Establish a continuous exchange with PANGAEA to obtain the data from their cruises more rapidly until they serve the downstream services regularly. A meeting with the data manager of PANGAEA will be performed in November 2022.



# 3. The quality assessment method in the Southern Ocean

## 3.1 Software

The SO quality assessment software is designed based on the currently available version of DMQC-PCM and the OWC software. In this task, we performed a series of developments to combine and improve functionality and automatisation of the process. The key changes to the software are as floors.

The currently available codes in the DMQC-PCM software include two separate Jupyter notebooks. The first one is the BIC (Bayesian Information Criteria) used to help the user to estimate the best number of classes for a training dataset to model. The output could be further used in the second Jupyter notebook including the DMQC-PCM codes. In this study, we have integrated both software into a merged SO quality assessment code which can be evaluated in the local Python software using only one code. We also refactored both codes to reduce repetition in calculations and in loading data. Moreover, we also implement the functionality to run this software for multiple floats. This reduces the time of calculations and allows for the processing of more floats.

Another implemented improvements and developments were to create one master code including all necessary codes to perform a quality assessment. This include (1) retrieving data from the local repository or GDAC (using <u>argopy</u> package), (2) code for automatically generating the source files of Argo float profiles (using <u>argopy</u> package), (3) previously combined by us code with BIC function and DMQC-PCM software, (5) run OWC software.

Before our efforts, the DMQC-PCM software(written in Python) output was working with the Matlab version of the OWC software. In this study, we have expanded this and now the DMQC-PCM software output is well integrated with the Python version of the OWC software. This development improves the functionality of the entire workflow of the quality assessment and allows for the elimination of licence issues related to the use of Matlab software.

The SO quality assessment software is stored in the GitHub repository as an additional branch to the currently available DMQC-PCM repository (<u>SO\_assesment</u>). This branch of the repository includes the two versions of the SO assessment software which have been produced in the Euro-Argo RISE WP5 5.3 task:

- DMQC-PCM-main which includes the DMQC-PCM and OWC Matlab software
- DMQC-PCM-Python which includes the DMQC-PCM and OWC Python software

This allows the users to select the most optimal version for their needs.

## 3.2 The SO assessment workflow

The general workflow of the SO quality assessment method is presented in figure 3.1. In the first step, the software uses the *argopy* package to retrieve the Argo float temperature and salinity profiles from the local repository (it can be also set up to pull data directly from GDAC). Then, these data are used to generate the source data file including appended Argo float profiles. The source data files are used as the input to both the DMQC-PCM classification software and further to the DMQC OWC



software. Both software uses as input files the configuration file and the reference data (from both CTD and/or Argo climatology data). The configuration file used in the method includes all necessary directories and setups. The reference data are used for comparison with the Argo float profiles. The DMQC PCM firstly runs the BIC function to estimate the number of classes for a training dataset to the PCM model. Then the output from the BIC is automatically implemented in the DMQC PCM code. This code generates the classification figures, the trained model and the text file containing the classification labels corresponding to each Argo float profile. The classification labels file is then read by the DMQC OWC software, which produces the suggested salinity correction outputs and associated diagnostic plots. In this step, the DMQC operator can assess if the Argo float is affected by any salinity drift or offset and decide to apply appropriate adjustments.

The performance assessment and implementation plan for the DMQC-PCM software has been already provided in the Euro-Argo RISE deliverable report D2.4. It has been shown that the DMQC-PCM software is able to improve the detection of salinity drift and temperature or salinity outliers. Moreover, when combined with the standard salinity calibration method, DMQC-PCM software is able to reduce the error on the correction while preserving confidence in this correction amplitude.

The example output from the SO quality assessment for float 1901495 can be found in Attachment A.



Figure 3.1: Workflow of the SO quality assessment method.

## 3.3. Implementation and usage of the SO quality assessment software

In BODC, the SO quality assessment of salinity data of Argo floats is performed for floats deployed south of 40  $^{\circ}$  S). The quality assessment method is used to verify the quality of Argo floats which have been already analysed by DMQC operators in delayed mode, from various DACs and submitted to GDAC. The list of floats already present at GDAC in d-mode is generated using the following code:

### > master\_argo\_index\_reader.py

The code reads the *ar\_index\_global\_prof.txt* file with a list of all available Argo floats from the location from a local BODC copy of Argo profiles from GDAC. This local copy is automatically synchronised with the GDAC Ifremer every week. The output file is the excel *SO\_argo\_floats.xlsx* file including the following information: DAC, float WMO number, mode, profile number, profile date, latitude and longitude. Based on the snapshot made in January 2022, the total number of all DM Argo



floats requiring the SO quality assessment was 2025. For easier management of floats in analysis, all of these floats have been grouped by the deployment sector to the South Atlantic (70° W to 30° E), the Indian Ocean (30° E to 120° E) and the South Pacific Ocean (120° E to 70° W), respectively.

Since the SO quality assessment software is designed for both Matlab and Python users of OWC software, hence the procedures for running the software are slightly different. The code used and their description are as follows.

## DMQC-PCM-main

(1) Setup configuration files

• pcm-config.txt

This file is used by the DMQC-PCM Python software and includes the directories to the local archive including the weekly updated NetCDF data from GDAC. Moreover, it also includes the following constants: the maximal interpolation depth from which reference data (MAX\_DEPTH = 1000), correlation distance (CORR\_DISTANCE = 50), number of runs in BIC for each class (NUMBER\_RUNS = 10) and maximal number of classes to explore (NK = 10).

• ow\_config\_linux\_ctd\_argo.txt

This file includes the configurations used in OWC Matlab software for the Argo floats analysis. To best represent the dynamic condition in this region and for further comparison of output with the DM data the constant values of the objective mapping parameters have been used (Table 3.1). In Task 5.3, the floats which are going through the SO quality assessment analysis are firstly run using the first "SO1" configurations. The other sets of configurations are used if the specific float requires more iterations. Moreover, this file also includes the option for including the class labels from the PCM analysis (USE\_PCM=1).

(2) Select floats for analysis and run the codes in software

The list of WMO numbers of floats which are intended to go through the SO quality assessment needs to be inserted in the following codes. After these edits, the following codes need to be run:

#### • so\_dmqc\_master.py

This Python code (1) retrieves data from the local repository or GDAC (using argopy package), (2) automatically generates the source code for OWC analysis (using argopy package), (3) runs the BIC function which is estimating the most suitable number of classes for a training dataset to model, (4) runs the DMQC-PCM software and generate the output plots, model and class labels.

#### • ow\_calibration\_pcm.m

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This Matlab code runs the OWC software including the class labels from the PCM and generates the diagnostic plots.

**Table 3.1:** Configuration setup for the objective mapping parameters.

OWC CONFIGURATION	SO1	SO2	SO3
CONFIG_MAX_CASTS	310	310	310
MAP_USE_PV	1	1	1
MAP_USE_SAF	1	1	1
MAPSCALE_LONGITUDE_LARGE	4	4	4
MAPSCALE_LONGITUDE_SMALL	2.5	2.5	2.5
MAPSCALE_LATITUDE_LARGE	3	3	3
MAPSCALE_LATITUDE_SMALL	1.5	1.5	1.5
MAPSCALE_PHI_LARGE	0.1	0.1	0.1
MAPSCALE_PHI_SMALL	0.02	0.02	0.02
MAPSCALE_AGE	5	5	5
MAPSCALE_AGE_LARGE	20	20	20
MAP_P_EXCLUDE	100	100	100
MAP_P_DELTA	150	150	150
Reference database	CTD +Argo	CTD +Argo	CTD +Argo
Set_calseries			
Constant on chosen levels	None	>1000	<1000
Max breaks	1	1	1

## DMQC-PCM-Python

#### (1) Setup configuration files

All necessary directories, constant values for PCM, and objective mapping parameters which are needed to run both PCM and OWC software can be set in one initial file below. The configurations used are the same as in the DMQC-PCM-main software.

- pcm\_ow\_config.ini
- (2) Select floats for analysis and run the codes in software

The list of WMO numbers of floats which are intended to go through the SO quality assessment needs to be specified in the following code below. This code is also used to run the entire software.

• so\_dmqc\_master.py

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In addition to the code from the DMQC-PCM-main, this code is also performing the automatic OWC Python calculations.

# 4. Review of the delayed mode floats from the Southern Ocean

## 4.1 Testing the SO quality assessment method

The functionality of the SO quality assessment method was tested by comparing the results from our method with d-mode data already submitted to GDAC. The tested floats were mostly coming from the Atlantic sector, with a small subsample of floats from the Pacific Ocean. The analysed floats came from a wide range of DMQC operators and DACs.

Our comparison analysis between the output from the traditional OWC and the SO quality assessment tool in the majority of cases were showing very similar results. The key improvement that this method brough was a significant reduction of the variability in the reference data used for analysis and also a reduction of the error bars of suggested corrections by the software. The improvements have been specifically found in areas in the SO where floats were passing through different water mass regimes, and where their natural variability is very high, such as in the Argentine Basin, or the areas of the Agulhas retroflexion current. These results are very comparable to those obtained in Deliverable D2.4. Overall, the SO quality assessment method allows the DMQC operators to improve their confidence in decision-making during performing the DMQC analysis. This will lead to more robust estimations of corrections which need to be applied to the salinity data of Argo profiles and thereby higher-quality science-ready data.

During testing, we found some instances where the suggested salinity corrections from the SO assessment method were substantially different from those already present in d-mode data. The analysis has been conducted both using the traditional OWC software and using the SO quality assessment tool, respectively. In both cases, results agreed that the corrections applied by DMQC operators to some of the d-mode floats need to be changed and floats re-submitted. Please note that the identified differences could have different reasons. These may come from

- a different (older version of the OWC software or version of the Matlab) software used at the time when the d-mode analysis was made. The SO assessment method often reduces the variability of the reference data and an error cast to the suggested corrections, which in many cases is a very critical decision making process of DMQC analysis. In cases where the variability of analysed data is very large or suggested corrections from traditional OWC are not reasonable the operators are more keen to not apply corrections which might be not realistic.
- limited guidelines at the time when DMQC analysis were made the guidelines for performing the DMQC analysis and decision making process have strongly developed from the beginning of the project, where some thresholds, flags or error estimates procedures differ to the most recently published in the Argo quality control manual for CTD and

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trajectory data (<u>Wong et al., 2022</u>). This may explain the decision made by operators for floats analysed at the early stages of the Argo project.

- different versions of the reference databases used at the time of making DMQC analysis,
- different configuration setups used by the DMQC operators and those used in this assessment,
- and finally different experiences of each DMQC operator in the decision-making process.

The workflow of our re-analysis in testing the SO quality quality assessment of floats in d-mode was as follows. The first step was to retrieve the d-mode data from GDAC and generate the output from the SO assessment method. The comparison was performed by calculating the differences between the suggested salinity corrections output from the SO quality assessment method (from the cal\_series.m file) and the d-mode adjusted Argo salinity float data. The output plot visualising the difference is presented in figure 3.2. Floats with a salinity correction difference exceeding +/- 0.01 were selected for more detailed checks. This includes multiple DMQC OWC iterations including different settings e.g. split time series, select pressure or theta levels, comparing data with CTD casts collected at the nearest time and space from the float deployment. Any indication of the significant discrepancy between the analysed data was described in the generated report. We have started to generate the reports to each problematic float and our results and send them to the DMQC operators responsible for this float with a request for further review.

The comparison codes used in testing are as follow

#### • For DMQC-PCM-main version

Compassion is performed using the dac\_comparison.m code included in the software directory. The output of this code is the list of floats which went through the comparison with DM data with an associated comment informing if the float has been adjusted correctly or requires further review and generates the comparison plot (Figure 3.2).

• For DMQC-PCM-Python version

Compassion is performed using the master\_dac\_comp.py code included in the software directory.

Overall, we reanalysed 368 floats using the SO quality assessment method. These include 332 floats from the Atlantic sector (14 from Italy; 31 from EU [MOCCA, MERSEA]; 33 from the Netherlands; 110 from France; 12 from AWI; 20 from BSH; 20 from BODC; 41 from SIO; 18 from KIOST; 15 from Argentinian floats, DMQC-ed by AOML; 18 from JAMSTEC) and 36 floats from the Pacific Ocean (floats from PMEL).





**Figure 3.2:** Comparison of the salinity data between the SO assessment method and salinity data in D-mode files. Top panel: Time series of absolute raw unadjusted salinity data (blue) along with adjusted salinity in d-mode available at GDAC (red) and adjusted salinity data suggested by the SO DMQC assessment method (green). Please note that if the blue line is not visible, that means that the DMQC operator did not apply any changes to the original Argo data. Middle panel: Time series of absolute differences between raw unadjusted salinity and adjusted salinity in d-mode already at GDAC (red) along with time series of differences between raw unadjusted and adjusted salinity suggested by the SO DMQC assessment method (green). Bottom panel: Time series of absolute differences between adjusted salinity from d-mode (magenta). The displayed differences are the absolute values.

# 4.2 Review and list the typical issues with the DMQC analysis in the Atlantic sector of the Southern Ocean

This section highlights the discrepancies in some of the DMQC analysis of Argo floats identified in reviewing the d-mode salinity data using the SO quality assessment method. From about 368 reviewed floats, we have found 31 questionable decisions of salinity data in d-mode. This gives



around 8.4 % of currently re-analysed floats which needs to be additionally checked by DMQC to agree with our findings. We have started to compile the reports with our findings which we are sending to the organisation or DMQC operator responsible for the float. Some of the DMQC operator's feedback can be found in Attachment B.

These findings might be very beneficial to identify potential gaps in the DMQC training of the DMQC operators and highlight the aspects which need to be more deeply explained in dedicated DMQC workshops for core Argo parameters.

The most common identified uncertainties are as follows:

### • Difficulties in identifying the beginning of salty drift. We have identified drifting floats where the salinity corrections are applied from the profile

exceeding 0.01, instead from the profile when drift actually began. As a result, the adjusted salinity data shows an artificial jump in corrected salinity data.



Example floats: 3900646, 3901961,

**Figure 4.1:** Example float: 3900646. The operator applied the correction to the float from profile around 200 where the vertically averaged salinity exceeded 0.01. Moreover, the applied correction is very erratic. Our analysis shows that this float is significantly drifting from much earlier from the beginning of the float life.





**Figure 4.2:** Example float: 3901961. The DMQC operator applied correction from around profile 55. Our analysis suggests that salinity data should be adjusted from around profile 30 when the drift began.

#### • Applying too large salinity correction to float

The salinity corrections applied to the data substantially exceed those corrections suggested by the SO assessment method or OWC analysis run separately. This might be associated with a relatively lower amount of reference data available in the SO at the time when the float was analysed, which might bias the estimated salinity correction.



Example float: 5900454, 3900069

**Figure 4.3:** Example float 5900454. The salinity applied correction by the operator strongly overcorrects the float.



#### • Applying too small salinity correction to float

We found that for some cases the correction applied by the operators is relatively lower compared to results from our re-analysis.



#### Example float: 3900994

**Figure 4.4:** Example float: 3900994. The correction applied by the operator suggests a relatively lower adjustment than those suggested by our analysis. Even by considering whether the float is drifting or only offsetting the applied correction is still relatively lower than the SO assessment result.

• No salinity corrections were applied to the float when corrections were needed

Some of the floats have no salinity corrections applied while the salinity offset or drift was identified. This might be associated with the automatic acceptance of the default values of QC=1 and error = 0.01. Another suspected reason might be a lack of enough confidence or understanding of how to assess the error value to the float.

Example floats: 3900661, 3901927, 6901979, 3900991, 3901000, 1900338, 6902638, 6901690, 6902779, 1900335, 6901501,1901221.

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**Figure 4.5:** Example float: 3900661. No OWC corrections were applied by the operator to the salinity data. Our analysis suggests that the float is affected by fresh drift from around profile 160.

• A need to clarify procedures for salinity corrections for data about 0.05 difference with the climatology data

In the analysed data we have found that there is little agreement in procedures for correcting the salinity data exceeding 0.05 of differences compared to the climatology. For some cases, large OWC corrections have been applied (6901713). In other cases no correction has been applied- might be due to accepting the automatic default values of QC=1 and error = 0.01 (3901000, 3900999, 1900337, 6901650).



**Figure 4.6:** Example float: 6901713. The DMQC operator did apply corrections to this float which exceeds 0.05. Our analysis shows that float is affected by an abrupt salty drift reaching up to 0.13 which should be flagged as QC=4.





**Figure 4.7:** Example float: 3901000. The DMQC operator didn't apply any corrections to this float. Our analysis is suggesting that float is affected by a salty offset of 0.06.



**Figure 4.8:** Example float: 6901650. The DMQC operator didn't apply any corrections to this float. Our results show that the differences between the float and climatology exceed 0.1, and the salinity data should be flagged with QC=4.

• Overcorrecting the salinity data by using too many breaking points suggested by the OWC software or added by operator

We have identified that some operators apply the salinity corrections with too many breaking points which are automatically suggested by the OWC software. This can cause overcorrection of the float as in the example below.





Examples: 6903217, 6903258, 6900750, 5902065

**Figure 4.9:** Example float: 6903217. The corrections applied by the operator overcorrected the float which is reducing its natural variability of the time series. Our analysis is suggesting that float is affected by a fresh offset of around 0.012.



**Figure 4.10:** Example float: 6900750. The operator applied salinity drift corrections of around 0.02 for the first 37 profiles, and below 0.01 to the end of the float life. Our analysis suggests that rather no corrections were needed to this float.

• *applying offsets close to 0.01 of salinity difference between float and climatology data* The general procedure agreed by the Argo DMQC community is to not apply corrections



where the difference between salinity of float and climatology is below 0.01 because this threshold is also a boundary for the manufacturer error. However, in cases where the offset is very distinctive in comparison with climatology or the comparison with the ship-based CTD data, then DMQC operators are applying corrections below 0.01.

We identified that in some cases where the offset or drift is very close or just exceeds 0.01, operators are not confident to correct the float from the SO. This caution is justified by reflected limited temporal and spatial coverage or the reference data and potential bias caused by using old climatology.



Examples: 1900338, 6901641, 1900471,

**Figure 4.11:** Example float: 1900338. No OWC corrections were applied by the operator to the salinity data. Our analysis suggests that float is affected by fresh offset developing further to drift. Operator's feedback: "I probably would have corrected for this fresh offset, but not sure if the fresh drift at the end is real (comes mostly from a shift in the reference data)"

#### • Need for more consistency in applying flags to the salinity data

We have found that there is low consistency in the approach of applying flags to salinity data exceeding 0.05 difference with climatology. For some floats we found that operators applied QC= 3, while for other QC=4. This might be related to the fact that flagging procedures and guidelines from the early stages of the Argo project might not be as detailed as agreed on or described compared to more recent recommendations.

Examples: 1900422, 5900723

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**Figure 4.12:** Example float: 1900422. No OWC corrections were applied by the operator to the salinity data, the applied flag QC=3 (probably bad data). The float shows fresh salinity drift with a difference with climatology reaching up to 1.3 PSU. The current recommendations are to consider applying QC=4 (bad data) for salinity differences exceeding 0.05 PSU.

The review of the subsample of floats from the SO shows that the major issue in the DMQC analysis leading to the discrepancies was **no salinity corrections applied to the data by operators, where the corrections were needed**. This could be associated with the case where the results obtained by operators using relatively older reference data versions did not show enough evidence to justify that the correction was needed, due to, for instance, large variability or poor reference data representation. Another assumed reason can be not enough experience of new DMQC operators in the decision making process. Finally, some cases of floats might suggest that the corrections were not applied due to human error or operator's internal software to apply correction failure, when the default corrections ('no correction', QC=1, error = 0.01) were accidentally applied.

The results from the review are pointing our also some other issues such as difficulties in identifying the beginning of faulty drift, applying too large or too small salinity correction, overcorrecting the float due to the use of setting up too many breaking points in the time series during the estimates of the salinity corrections by OWC software. However, these are only found in a few very sporadic cases.

Another matter causing some discrepancies might be caused by changes in the recommendations in guidelines in setting errors and flagging data which have been developed and improved for the beginning of the Argo project.

From the initial feedback from the DMQC operators (Attachment B) in majority of cases operators agree with our results and intend to correct and re-submit their floats.

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## 5. Conclusions

## 5.1 Limited reference data in the Southern Ocean

Due to the few research cruises in the region and the data moratoriums the reference data in the SO are very limited. For the Atlantic region of the SO, PANGAEA is an important source of data that should be regularly checked for updates. However, each Argo national programme needs to search in their national repositories for CTD reference data and make sure that all available data is included in the DMQC reference database. The underlying assumption is that obtaining data to be available in the password-protected DMQC reference database is easier at a national level, especially in the cases where the data is non-public.

The recommendation here is to make efforts to engage with the SO observational community to expand the CTD reference database with new data in a timely manner. Perform a CTD cast at deployment whenever possible to assist the DMQC analysis.

The key role for partners in Euro-Argo RISE is to ensure that there is a clear flow of climatology data supplied to the ship CTD reference for Argo database managed by Coriolis team at Ifremer.

# 5.2 Development and maintenance of the quality assessment method in the Southern Ocean beyond the Euro-Argo RISE project

The SO quality assessment code is a fully operational tool which can be accessed by GitHub (<u>SO\_assesment</u>). The next development plan with regard to this code is to first integrate this software with the currently available repository of the main DMQC-PCM branch, which is based on the SO assessment tool. Further aspiration to this software is a publication of the code as additional functionality to the OWC software in Matlab and Python toolboxes. This allows the code to be visible to the international Argo community and become an open-source tool to ensure its further maintenance and development.

The successful implementation of this new sophisticated method based on the machine learning method in the quality assessment of core Argo floats in the Southern Ocean might also find their implementation in other Argo missions. We believe that further development of this method might strongly improve and simplify the quality control of other parameters from both the BGC and Deep Argo floats. This work will be presented at the next Argo Datamanagement meeting in Miami in December 2022 for endorsement by the international community.

With the accessibility and improved automatisation of developed software, the SO quality assessment code can be also implemented by the DMQC operators to support their daily analysis of core Argo floats. This will allow the DMQC operators to gain more confidence in reviewing and improving the decision-making process on their floats resulting in more robust DMQC analysis and higher quality of analysed data ready for the science use.

In order to ensure future maintenance and sustainability of the SO quality assessment tool Euro-Argo RISE partners will need to secure a sufficient source of funding to support this activity.

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# 5.3 Ensure further regular audit of delayed mode floats from the entire Southern Ocean

The need for a wider international audit and improving the quality of d-mode Argo floats have been already highlighted and started to be implemented by the DMQC core Argo-focused group. This is motivated by the fact that a higher percentage of SBE CTDs are now experiencing sensor drifts, which may not be easily identifiable by only examining individual time series. Moreover, the amount of high-quality reference data used for the comparison with Argo floats has significantly increased compared to the times when the initial DMQC analysis was made. Together with growing reference data also the guidelines and recommendations also developed and changed helping DMQC operators to make more robust decisions over time.

In this deliverable report, our analysis of the DM core Argo floats was performed mostly on Argo floats deployed in the Atlantic sector of the SO. Additionally, the reviews have also been performed on several floats from the Pacific Ocean. The key motivation here was to focus on reviewing the Argo floats coming on the European fleet, but also extend the checks to the international Argo fleet. Due to a number of various cases of questionable DMQC analysis identified in this study, where some of which were not captured by the international audit of the DMQC focus group, **it is strongly recommended to continue the regular quality assessment checks of salinity data from Argo floats covering all other sections of the SO**. This activity is extremely valuable and crucial to ensure the highest quality of the currently available Argo reference database used for the DMQC analysis of Argo floats and also for the Argo data users.

The DMQC assessments and floats review require well-qualified and experienced DMQC operators and PIs working in the specific regions of the SO. We are suggesting that this activity could be undertaken and monitored by the SOARC group. However, the key limitation is insufficient and limited funding to the SOARC group members to carry out these quality assessment checks. For instance, BODC as a previous leader of the SOARC group and pioneer in developing the SO quality assessment tool is currently unable to undertake this responsibility due to limited resources.

It is important within Euro-Argo RISE to study with the Euro-Argo ERIC governance what would be needed to ensure sustainable support to coordinate enhancements and maintenance of the SOARC activities to provide high-quality data at GDAC for scientific use.

## 5.4 Limited opportunities to disseminate lessons learnt

As was highlighted before, well-qualified DMQC operators (aware of the most recent sensor failure patterns, consciousness about the availability of the reference data and knowledge about very dynamic physical ocean behaviours in the SO) are crucial for making the most appropriate decisions to core data in delayed mode. To improve the decision-making process in d-mode one of the key recommendations is to improve the overall consistency of the Argo DMQC procedures and operator skills development through regular workshops.

To address this need NOC in collaboration with other European and international partners intended to organise the 2nd European Argo/7th International Argo Delayed-mode QC Workshop for CTD data, initially scheduled for 12-15 May 2020 in Liverpool, UK. This workshop aimed to include the DMQC analysis for both core (2000 m) and deep (4000 m - 6000 m) Argo floats, with the latter being a focus

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of the Euro-Argo RISE project WP3 on developing deep DMQC methods. However, due to continuation of the COVID-19 situation forced a further postponement. The meeting was planned to be rescheduled, but the recent COVID-19 situation did not allow for any tentative date.

The additional solution to the workshop in person became a series of *Argo DMQC Discussion* online meetings initiated and led by the Australian Argo team at CSIRO (<u>ArgoDM-Disc</u>). The Euro-Argo Rise partners have been very active contributors to these meetings. These virtual discussions helped to promote collaboration between DMQC operators and interested members of the Argo community. This forum gives an opportunity for newer operators to improve their skills and get advice on the concerning and difficult floats, promote a sense of community, and contribute to the adaptation of more consistent DMQC practices.

These virtual discussions are a valuable addition to support the DMQC operators, however, will not replace a need for very valuable workshops in person. This reveals a need for support for national programs enhancing training and collaboration opportunities. All Euro-Argo RISE partners should contribute to organised workshops, with the aim of contributing experience to date, and implementing decisions in the European Argo data system.





# **Attachment A**

# Example of the output from the SO assessment method

## **DMQC-PCM** output plots

These plots will allow to determine if classes show a spatial or temporal coherence needed to differentiate the reference profiles.



**Figure A.1:** Float 7900533. Left panel: Bayesian Information Criteria with 8 optimized number of classes used in the model. Middle panel: Pie chart of the number of classes and associated percent of profiles. Right panel: Table with a number of profiles associated with each class.



**Figure A.2:** Float 7900533. Time series of the float trajectory with the associated class to each float profile.

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**Figure A.3:** Float 7900533. Time series with the calculated robustness of each profile. Unlikely (0 - 33 %), as likely as not (33 % - 66 %), likely (66 % - 90 %), very likely (90 % - 99 %), Virtually certain (99 % - 100 %).



**Figure A.4:** Float 7900533. Classification of the spatial distribution of float using CTD and Argo reference database plotted against the float trajectory (black circles).



**Figure A.5:** Float 7900533. The percentage of the temporal representation of profiles in each class by month (left panel) and by season (right panel).





Different vertical structures from figures A.6 for salinity and A.7 for temperature data are the foundation of the PCM, the "distance" of a profile to each of the typical vertical structures controls the classification outcome. The median profiles represent the best idea of the typical profile of a class and the other quantiles, the possible spread of profiles within a class. It is with the spread which can be determined if a class has captured a homogeneous water mass (small spread) or a layer with gradients (large spread, like a thermocline for instance) (Classif ArgoReferenceDatabase).



**Figure A.6:** Float 7900533. The graphic representation of quantile profiles of the vertical structure of salinity data from each class.



Vertical structure of classes for: 7900533

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**Figure A.7:** Float 7900533. The graphic representation of quantile profiles of the vertical structure of temperature data from each class.



**Figure A.8:** Float 7900533. Vertical structure of salinity (left panel) and temperature (right panel) data of quantiles plotted together representing the differences between classes.

# OWC output plots with pre-classified reference data used produced by OWC python software



Figure A.9: Float 7900533. The trajectory of the float with CTD and Argo reference data.





Figure A.10: Float 7900533. Uncalibrated float data and mapped salinity.



**Figure A.11:** Float 7900533. Top left: Temperature and salinity variance on theta levels. Top right: T/S distribution plot plotted with the theta levels. Vertical distribution of temperature (left bottom) and salinity(right bottom) data plotted with the theta levels.





Figure A.12: Float 7900533. Time series of the salinity data at the specific theta level.



Figure A.13: Float 7900533. Potential conductivity (top) and vertically averaged salinity (bottom) with errors.





Figure A.14: Float 7900533. Uncalibrated salinity anomaly on theta levels.



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# **Attachment B**

# Feedback from the DMQC operators

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This section aimed to list some initial feedback from the DMQC operators regarding the results from their re-analysis and decision about the correction of salinity data.

Institution	wмо	Feedback from DMQC operators	
lfremer	6901713	I could not tell which one of the corrections is better. (DMQC operator refers to the differences between OWC-PCM and classical OWC) This float is probably an ASD, I would have flag PSAL to 4 anyway	
	6901650	Similar results between OWC-PCM and classical OWC (big fresh offset and fresh drift), so "No correction" is a DM operator decision. I probably would have corrected for this fresh offset, but not sure if the fresh drift at the end is real.	
	5902065	I could not tell which one of the corrections is better, the difference is quite small.	
	3901927	Similar results between OWC-PCM and classical OWC if levels chosen >1000db (fresh offset). "No correction" is a DM operator decision. I probably would have corrected for this fresh offset.	
	3901000	Similar results between OWC-PCM and classical OWC (salty offset $\sim$ 0.06). "No correction" is a DM operator decision. I probably would have corrected for this salty offset.	
	3900999	Similar results between OWC-PCM and classical OWC (salty offset ~ 0.05). "No correction" is a DM operator decision. I probably would have corrected for this salty offset.	
	3900994	I could not tell which one of the corrections is better. It is clear there is a big salty offset from the beginning (~0.055)	
	3900991	Similar results between OWC-PCM and classical OWC (fresh offset ~0.03). "No correction" is a DM operator decision. I probably would have corrected for this fresh offset.	
	1900338	Similar results between OWC-PCM and classical OWC if levels chosen >1000db (fresh offset ~0.01 and fresh drift after cycle 40 ). I probably would have corrected for this fresh offset, but not sure if the fresh drift at the end is real (comes mostly from a shift in the reference data)	

 Table B.1: Feedback from the DMQC operators to the floats from the re-analysis.

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	1900337	Similar results between OWC-PCM and classical OWC (fresh offset ~0.05). Don't know where the small varying corrections applied by the DM operator come from?
BSH	6901979	For this float I did finally submit d-files with corrections in May 2022. Maybe it is a matter of timing when new D-files files were submitted and when files for this analysis were downloaded. The lack of trust in the fitted corrections was a reason why no corrections were earlier applied. This float had extremely high variability in its deep values causing huge fluctuations and there getting a 'good' fit needed a longer time series to be established. Maybe we should also suggest if that is the case to increase errors to highlight this to the users.
	6902638	Corrections would just have exceeded 0.01 I decided not to correct. And additionally on isothermals mapped values agree with climatologies within error bars. Maybe we need clearer rules on what to do when the suggested corrections are close to that 0.01, the threshold which is a bit arbitrary anyway.
	6900750	I agree the float needs no correction and particularly none as strange as shown here. The log files from 2015 do not really indicate what happened. Maybe something unexpected happened when the decisions were transferred to the netcdf files. But I will submit new d-files asap
	6902559	Is similar to 6902559, but in my run of owc gave a fresh offset just at the threshold of 0.01. Your repeated owc analysis included in the request in review is using very shallow reference levels from 400-800 m, while I used levels below 1500. I would think the shallower water mass used are prone to long-term trends and the more stable deep waters are therefor a better choice
BODC	3900069	I agree the corrections applied by the DMQC operator were too large and should be removed. It was probably due to the use of only very old profiles with CTD data data.
	1901221	The float was processed by not very experienced operators who were not sure about his decision. As a result instead of offset, the operator applied a larger error (0.02) to the salinity data. I agree float require applying offset to profiles 240-318 of 0.02.
OGS	6903217	For float 6903217 and 6903258 the salinity difference between the two
	6903258	with the output of your assessment. I think this could depend on the version of the reference dataset used.
	6901961	For float 6901961, the second run confirms what was done in the first run for the first 30 profiles and the salinity difference between our



	analysis and yours reaches a maximal value of about 0.0035. Then, in the second part of the float lifetime we are in line with your results. Hence, regarding the first 30 profiles, I would say that the difference is not significant since it is very small and close to the sensor accuracy.
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