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BGC Argo quality control manual for particles backscattering

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BGC Argo quality control manual for particles backscattering

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History

Date (dd/mmm/yyyy)	Comment
04/04/2019	Version 0.9, preliminary version (not official) but assigned to a DOI
01/09/2023	First official version

Reference Documents

Reference N°	Title	Link
#RD1	Argo Quality Control Manual for CTD and Trajectory Data	http://dx.doi.org/10.13155/33951
#RD2	Argo Quality Control Manual for Biogeochemical Data	http://dx.doi.org/10.13155/40879
#RD3	Argo user manual	http://dx.doi.org/10.13155/29825
#RD4	Processing Bio-Argo particle backscattering at the DAC level	http://dx.doi.org/10.13155/39459

Preamble

During the ADMT16, it has been decided to split the Argo quality control manual in two manuals:

- the Argo quality control manual for CTD and trajectory data (JULD, LATITUDE, LONGITUDE, PRES, TEMP, PSAL, TEMP, CNDC, #RD1) and,
- the Argo quality control manual for biogeochemical data (#RD2).

As there are many different groups of experts in charge of the assessment of different biogeochemical data set, the Argo quality control manual for biogeochemical data should be considered as the cover document of all biogeochemical data quality control manuals, while this document is dedicated to the description of the specific tests for the quality control of the particles backscattering and the related intermediate parameters.

> Users should be aware that although biogeochemical data are now freely available at the Argo Global Data Assembly Centres (GDACs) along with their CTD data, the accuracy of these biogeochemical data at their raw state is not suitable for direct usage in scientific applications. Users are warned that the raw biogeochemical data should be treated with care, and that often, adjustments are needed before these data can be used for meaningful scientific applications.
>
> Any user of these biogeochemical data that would develop a specific and dedicated adjustment improving their accuracy is invited to contact the ADMT for potential inclusion of their method in a future edition of this document.

1. Introduction

The scattering coefficient (b) of a medium is the scattered fraction of incident light flux, divided by the infinitesimal thin layer of the medium through which light travels. It is usual, for bio-optical purposes, to decompose the scattering coefficient in two components depending on the direction of the scattered flux. The forward scattering coefficient (b_f), indicating the flux scattered from the beam in the forward direction, and the backscattering coefficient (b_b), related to light scattered from the beam in the backward direction. b_b is further divided into the contribution by seawater (b_{bsw}) and the contribution of particles (b_{bp}), assuming the contribution by dissolved materials to scattering to be negligible. b_{bp} is directly related to the concentration of particles, but also to their composition (i.e. organic vs inorganic) and size. Recently derived empirical relationships have been found, correlating b_{bp} to particulate organic carbon (POC) concentration and total suspended matter (Stramski et al., 2008, Neukermans et al., 2012, Cetinic et al., 2012) and b_{bp} to phytoplankton carbon (Martinez-Vicente et al, 2013, Graff et al., 2015).

This document is the Argo quality control manual for particles backscattering. It describes two levels of quality control:

- The first level is the real-time system that performs a set of agreed automatic checks.
    - Adjustment in real-time is performed and the real-time system can evaluate quality flags for adjusted fields
- The second level is the delayed-mode quality control system.

In core-Argo profile files, where <PARAM> = PRES, TEMP, PSAL (and sometimes CNDC), each <PARAM> has 5 qc and adjusted variables that are used to record real-time qc test results and delayed-mode adjustment information:

<PARAM>_QC, PROFILE_<PARAM>_QC, <PARAM>_ADJUSTED, <PARAM>_ADJUSTED_QC, and <PARAM>_ADJUSTED_ERROR.

In B-Argo profile files, <PARAM> can be classified into 3 groups:

(a). B-Argo <PARAM>: these are the ocean-state biogeochemical variables that will receive real-time qc tests, adjustment in real-time and delayed-mode adjustments. They are stored in both the B-Argo profile files and the GDAC synthetic files (https://doi.org/10.13155/55637).

(b). IB-Argo <PARAM>: these are the intermediate biogeochemical variables that are only stored in the B-Argo profile files. They will receive real-time qc tests and may receive adjustments.

(c). PRES: this is the stand-alone vertical index that links the core- and B-Argo profile files.

The following are some clarification on what qc and adjusted variables are included in the B-Argo profile files:

(a). B-Argo <PARAM>: all 5 qc and adjusted variables are mandatory for B-Argo PARAM in the B-Argo profile files.

(b). IB-Argo <PARAM>: <PARAM>_QC and PROFILE_<PARAM>_QC are mandatory for IB-Argo <PARAM>. <PARAM>_ADJUSTED, <PARAM>_ADJUSTED_QC and <PARAM>_ADJUSTED_ERROR are optional.

(c). PRES: the B-Argo profile files do not contain any qc or adjusted variables for PRES. They are in the core-Argo profile file.

In B-Argo profile files, biogeochemical parameters can receive adjustments at different times. Therefore the variable PARAMETER_DATA_MODE (N_PROF, N_PARAM) is added to B-Argo profile files to indicate the data mode of each <PARAM> in each N_PROF. The PARAMETER_DATA_MODE describes the data mode of the individual parameter :
R : real time data
A : real time data with adjusted values
D : delayed mode data

In B-Argo profile files, the variable PARAMETER_DATA_MODE associated with the variable PRES is always 'R', as adjusted values provided for PRES are only stored in the core profile file. Thus, to access the 'best' existing version of a parameter (<PARAM>) data, except PRES, the user should:

1. Retrieve the data mode of the <PARAM> parameter (from DATA_MODE(N_PROF) in a core-Argo profile file and from PARAMETER_DATA_MODE(N_PROF, N_PARAM) in a B-Argo profile file or a GDAC synthetic file),
2. Access the data:
    - If the data mode is 'R': In <PARAM>, <PARAM>_QC and PROFILE_<PARAM>_QC,
    - If the data mode is 'A' or 'D': In <PARAM>_ADJUSTED, <PARAM>_ADJUSTED_QC, PROFILE_<PARAM>_QC and <PARAM>_ADJUSTED_ERROR.

Note that the data mode of a IB-Argo parameter may depend on the DAC decision to include or exclude adjusted fields for IB-Argo parameters in the B-Argo profile file:

- If <PARAM>_ADJUSTED, <PARAM>_ADJUSTED_QC and <PARAM>_ADJUSTED_ERROR are present in the file, the data mode of the IB-Argo parameter can be 'R', 'A' or 'D',
- If not, the data mode of the IB-Argo parameter should always be 'R'.

2. Real-time quality control for BBP and associated intermediate parameters

2.1. Introduction

Because of the requirement for delivering data to users within 24-48 hours of the float reaching the surface, the quality control procedures on the real-time data are limited and automatic.

At the present time, real-time tests are defined for the following biogeochemical and intermediate parameters related to particles backscattering:

- BBP700

2.2. Argo real-time quality control tests for BBP vertical profiles

2.2.1. Common Argo real-time quality-control tests on vertical profiles

This section lists the real-time tests that are common between CTD data and biogeochemical data. The same real-time test numbers for CTD data are used here. See Argo quality control manual (#RD1, #RD2).

The following tests are directly relevant for BBP, See Argo Quality Control Manual for Biogeochemical Data (#RD2):

13. Stuck value test

15. Grey list

19. Deepest pressure test

2.2.2. Specific Argo real-time quality control tests on vertical profiles

This set of tests is documented in Dall'Olmo et al., 2023 and is available in a jupyter notebook https://github.com/euroargodev/BBP_RTQC.

If the following tests are passed, BBP700_QC = "1"

62. BBP700 specific Argo real-time quality control tests

In general, BGC-Argo floats sample at a variable vertical resolution that depends on the type of float, and the specified mission. Therefore to smooth BBP profiles, a median filter is used in some of the proposed tests with a window size (w =11) (the window size around the first 5 points and last 5 points (corresponding to maximum and minimum depths) will be shrunk to the available points).

Every time a "median filter" is mentioned in this document, we refer to this median filter with its output medfilt(BBP700).

2.2.2.1. Test 1 - Missing data test

This test detects and flags profiles that have a large fraction of missing data. Missing data could indicate shallow profiles (caused by a specific float mission and/or bathymetry) or incomplete profiles due to a malfunctioning sensor.

The upper 1000 dbar of the profile are divided into 10 pressure bins with the following lower boundaries (all in dbar):

50, 156, 261, 367, 472, 578, 683, 789, 894, 1000.

For example, the first bin covers the pressure range [0, 50) which is $0 \leq PRES < 50$, the second [50, 156), etc.

We define as a threshold the minimum number of data per bin MIN_N_PERBIN=1.

After counting how many data points are contained in each bin, we define the NUMBER_OF_BINS as the number of bins with a number of data greater or equal than MIN_N_PERBIN in each bin.

- IF NUMBER_OF_BINS =1

  Action : BBP700_QC=4 for the whole profile

- IF NUMBER_OF_BINS >1 AND NUMBER_OF_BINS<10

  Action : BBP700_QC=3 for the whole profile

- IF No data at all
  Action : BBP700_QC=9 for the whole profile

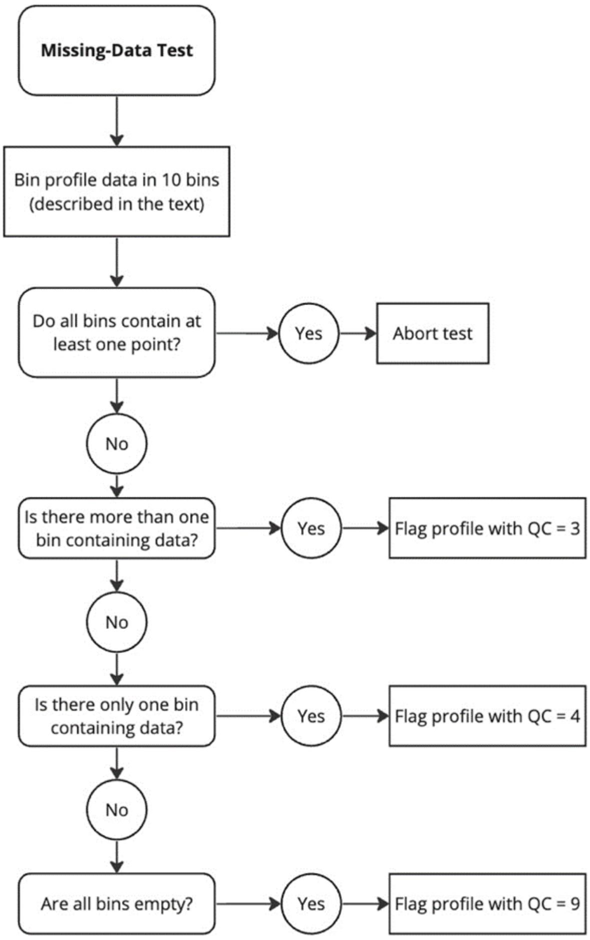

Figure 1: Flowchart of the missing-data test #1

2.2.2.2. Test 2 - High deep value test

This test is set to flag profiles with anomalously high BBP values at depth. High values at deeper depths could indicate a variety of problems, including biofouling, incorrect calibration coefficients, sensor malfunctioning. Note that high deep BBP values could also be valid data, for example in the case of sediment-resuspension events. High deep BBP values can result from a variety of reasons, including natural causes. In the latter case, the quality flag could be set to “good data” during DMQC.

We define

HIGH_DEEP_VALUE_THRESHOLD= 0.0005 m^{-1}

This value was selected as it is half of the value typical of surface BBP in the oligotrophic ocean (e.g., Dall’Olmo et al., 2012): median-filtered BBP data at depth are expected to be considerably lower than this threshold value (Poteau et al., 2017).

We also define

DEEP_VALUE_PRES_THRESHOLD = 700 dbar (the pressure below which the test is implemented)

N_of_ANOM_POINTS_THRESHOLD = 5 (the number of points below the threshold pressure value)

- **IF** there are at least N_of_ANOM_POINTS_THRESHOLD points below DEEP_VALUE_PRES_THRESHOLD, the test is applied to the median-filtered profile of BBP.
    - IF the median value of medfilt(BBP700) below DEEP_VALUE_PRES_THRESHOLD is greater than HIGH_DEEP_VALUE_THRESHOLD then the test fails and

    Action : BBP700_QC=3 for the whole profile.

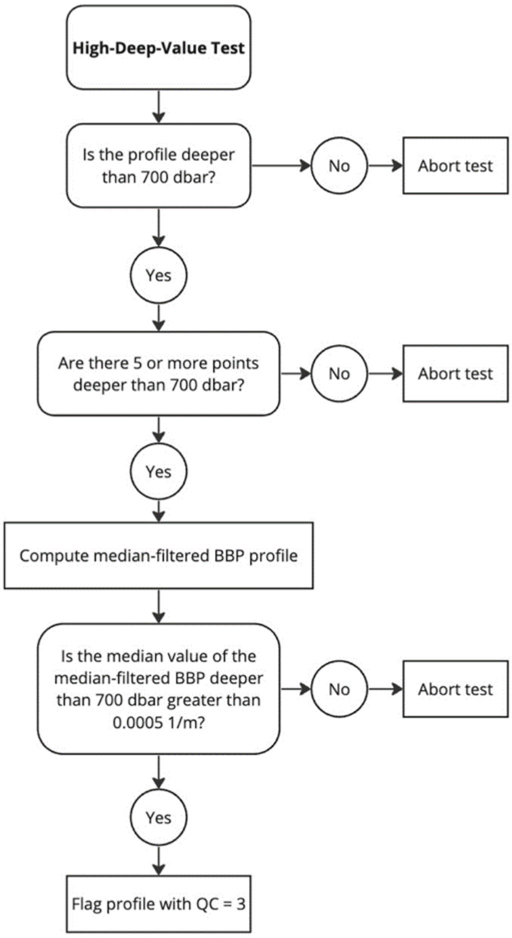

Figure 2: Flowchart of the high deep value test #2

2.2.2.3. Test 3 - Negative BBP test

This test flags data points or profiles with negative BBP values due to a variety of reasons including: sensor drift or malfunctioning, inaccurate calibration coefficients, or BBP sensor exposed to air.

Negative BBP values occurring only near the surface most likely represent data with a BBP sensor outside of the water: these are flagged with a 4. BBP sensors that generate negative BBP values deeper than 5 dbar are considered more at risk of malfunctioning. With just a few (10%) deep negative points at pressures greater than 5 dbar, the flag is set to 3 for the whole profile. If a larger proportion of negative values is found, the whole profile is flagged with a 4.

We define

NEGATIVE_PRES_THRESHOLD = 5 dbar

MAX_PERCENTAGE_OF_BAD_POINTS = 10

PERCENTAGE_OF_BAD_POINTS is defined as the percentage of levels below 5 dbar with negative BBP values data with respect to the number of BBP measurements below 5 dbar

- **IF** PRES < NEGATIVE_PRES_THRESHOLD **AND** BBP700 < 0

  Action : BBP700_QC=4

- **IF** PRES ≥ NEGATIVE_PRES_THRESHOLD
  - **IF** ((PERCENTAGE_OF_BAD_POINTS > 0) **AND** (PERCENTAGE_OF_BAD_POINTS < MAX_PERCENTAGE_OF_BAD_POINTS))

    Action: BBP700_QC = 3 for the whole profile

- **IF** PRES ≥ NEGATIVE_PRES_THRESHOLD
  - **IF** PERCENTAGE_OF_BAD_POINTS ≥ MAX_PERCENTAGE_OF_BAD_POINTS

    Action : BBP700_QC = 4 for the whole profile

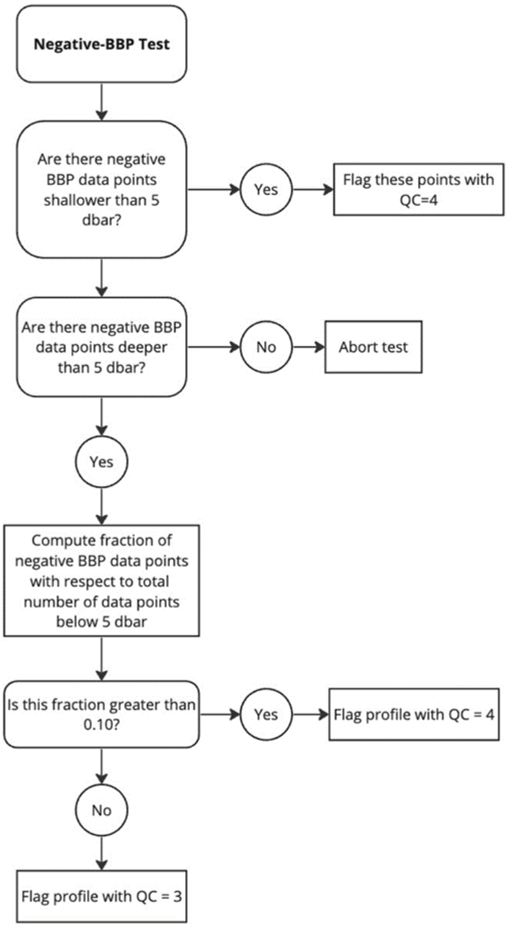

Figure 3: Flowchart of the negative value test #3

2.2.2.4. Test 4 - Noisy profile test

This test is set to flag profiles that are affected by noisy data. This noise could indicate sensor malfunctioning, spikes caused by organisms attracted to the light emitted by the BBP sensor (Haëntjens et al., 2020), or other anomalous conditions.

We define

RES = | medfilt(BBP700) - BBP700 | (note the absolute value)

NOISY_PRES_THRESHOLD = 100 dbar

RES_THRESHOLD = 0.0005 m^{-1}

MAX_PERCENTAGE_OF_OUTLIER = 10

PERCENTAGE_OF_OUTLIER is defined as the percentage of BBP measurements below NOISY_PRES_THRESHOLD with RES > RES_THRESHOLD .

The absolute residuals between the median-filtered BBP and the raw BBP values are computed below a pressure threshold NOISY_PRES_THRESHOLD = 100 dbar (this is to avoid surface data, where spikes are more common and generate false positives). These threshold values were selected after visual inspection of profiles from a subset (~60) of floats.

- IF PERCENTAGE_OF_OULIER ≥ MAX_PERCENTAGE_OF_OUTLIER
  Action: BBP700_QC = 3 for the whole profile

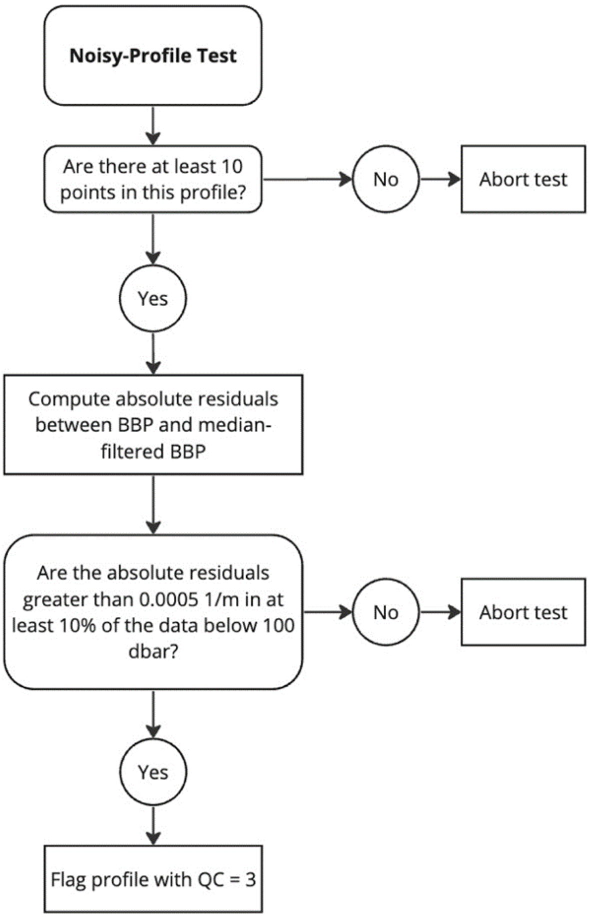

Figure 4: Flowchart of the noisy profile test #4

2.2.2.5. Test 5 - Parking hook test

When the float is drifting with the currents while at its parking pressure (typically 1000 dbar), particles may be depositing on the float and BBP sensor. These accumulated particles are likely released back into the water when the float descends to its maximum pressure (typically 2000 dbar), before starting the ascending profile during which data are collected. However, if the float does not descend to 2000 dbar (or to a depth deeper than the parking depth) before starting the BBP measurements, but immediately starts ascending towards the surface and measuring, then the accumulated particles might be measured by the BBP sensor as they are released back into the water. This is the likely cause of an increase in BBP at the start of the profile, when the parking pressure is close to the maximum pressure. The objective of this test is to flag these anomalous BBP points.

Note that this test should be applied to ascending profiles only.

We define

DELTA_PRES0 =100 dbar

DELTA_PRES1 = 50 dbar

DELTA_PRES2= 20 dbar

DEV = 0.0002 m^{-1}

First, we verify that the nearest BBP measurement above max(PRES) is ≤ DELTA_PRES2 dbar away: if it is not, the test cannot be applied to this profile. This is to ensure that the baseline (computed below) is not too far away from the maximum pressure of the profile and thus that it is representative of the values of BBP at max(PRES). If the BBP measurement above max(PRES) is ≤ DELTA_PRES2 dbar away, we check that the profile starts from the parking pressure (PARK_PRES could be extracted from the mission configuration valid for the float cycle under exam, alternatively the PARK_PRES can be retrieved from the PRES of the last measurement acquired in the drift phase) by testing that the absolute difference between the max(PRES) and PARK_PRES is smaller than DELTA_PRES0. If the ascending profile does not start from the parking pressure, the test is aborted.

If the profile starts from the parking pressure, a first pressure range is defined over which the baseline for the test is calculated:

max(PRES) - DELTA_PRES2 > PRES ≥ max(PRES) - DELTA_PRES1.

This baseline is computed over this first pressure range as

baseline = median(BBP) + DEV

- IF BBP[PRES ≥ max(PRES) - DELTA_PRES1] > baseline

  Action : BBP700_QC = 4

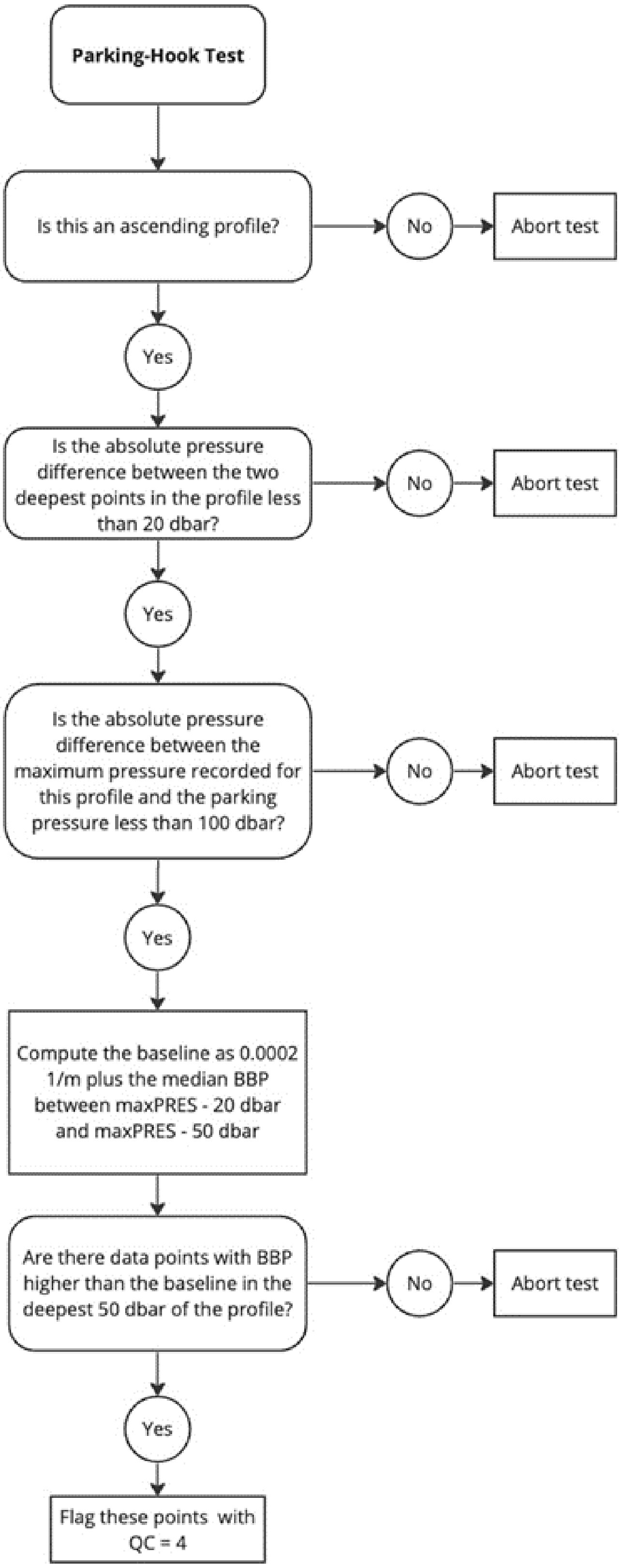

Figure 5: Flowchart of the parking hook test #5

2.2.3. Scientific calibration information for each profile

If PARAMETER_DATA_MODE is 'R', there is no reason to fill the scientific calibration information, thus:

For PARAMs (B-Argo PARAMs and IB-Argo PARAMs) in 'R'-mode	
SCIENTIFIC_CALIB_COMMENT	FillValue
SCIENTIFIC_CALIB_EQUATION	FillValue
SCIENTIFIC_CALIB_COEFFICIENT	FillValue
SCIENTIFIC_CALIB_DATE	FillValue

A specific comment should however be set for PRES parameter

For PRES	
SCIENTIFIC_CALIB_COMMENT	'Adjusted values are provided in the core profile file'
SCIENTIFIC_CALIB_EQUATION	FillValue
SCIENTIFIC_CALIB_COEFFICIENT	FillValue
SCIENTIFIC_CALIB_DATE	FillValue

(see in Chapter 3 and Chapter 4 how to fill scientific calibration information when PARAMETER_DATA_MODE is 'A' or 'D' respectively).

2.3. Argo real-time quality control tests for BBP data in trajectory files

The following tests are applied in real-time to BBP data stored in the trajectory files.

Some trajectory file data are duplicates of vertical profile data (for example dated levels of PROVOR/ARVOR profiles are present in the profile file (without their times) and duplicated in the trajectory file (with their associated times)). These data should be duplicated with their associated QC values, which were set during the real-time quality control tests performed on the vertical profiles.

This is used to flag negative BBP values near the surface that most likely represent data with a BBP sensor outside of the water.

IF PRES < 5 dbar **AND** BBP700 < 0

Action : BBP700_QC=4

2.4. Argo real-time quality control tests for BBP on near-surface data

No tests are defined yet on near-surface data for BBP.

2.5. Argo real-time quality control tests for deep-float data

No tests are defined yet on deep data for BBP.

2.6. Quality control flag application policy

The QC flag value assigned by a test cannot override a higher value from a previous test. Example: a QC flag ‘4’ (bad data) set by Test 15 (grey list) cannot be decreased to QC flag ‘3’ (bad data that are potentially correctable) set by Test 2 – High deep value test.

When a biogeochemical parameter is calculated from other intermediate (IB-Argo) parameter, its associated QC is initialized to the worse QC value of the input data.

For example, BBP700 (B-Argo parameter) is calculated from BACKSCATTERING_BBP700 (IB-Argo parameter), then if BACKSCATTERING_BBP700_QC = ’4’ after the stuck value test, the corresponding BBP700_QC is initialized to ‘4’.

3. Real-Time quality control for BBP data adjusted in Real-Time

Presently, the need to adjust and how to adjust BBP in real time is still ongoing work. BBP700 is pushed in BBP700_ADJUSTED in order to encourage users to use “ADJUSTED” fields as the "best available" Argo data.

For IB-Argo PARAMs in ‘A’-mode	
SCIENTIFIC_CALIB_COMMENT	FillValue
SCIENTIFIC_CALIB_EQUATION	FillValue
SCIENTIFIC_CALIB_COEFFICIENT	FillValue

SCIENTIFIC_CALIB_DATE	FillValue

A specific comment should however be set for PRES parameter

For B-Argo PARAMS in 'A'-mode	
SCIENTIFIC_CALIB_COMMENT	"BBP700_ADJUSTED is being filled with BBP700 directly in real time. Adjustment method may be enhanced in the future. RTQC_APPLIED 11111 RTQC_FAILED 00001"*
SCIENTIFIC_CALIB_EQUATION	BBP700_ADJUSTED = BBP700
SCIENTIFIC_CALIB_COEFFICIENT	FillValue
SCIENTIFIC_CALIB_DATE	YYYYMMDDHHMISS

* The RTQC_APPLIED and RTQC_FAILED strings were added temporarily in the SCIENTIFIC_CALIB_COMMENT in order to report in detail the status of the different tests. The strings (_APPLIED, _FAILED) report, from left to right, for each test, "0" ("no"), or "1" ("yes"). The example presented here reports that all tests were applied and the parking hook test failed.

Test 1 - Missing data test
Test 2 - High deep value test
Test 3 - Negative BBP test
Test 4 - Noisy profile test
Test 5 - Parking hook test

There is ongoing discussion and work to write specifications in the HISTORY section to report this information. Once it is finished, this section will be updated accordingly.

4. Delayed mode quality control for BBP data

4.1. Editing raw qc and adjusted qc flags in delayed-mode

Delayed-mode operators should examine profile data for pointwise errors such as spikes and jumps, and edit and check the qc flags in <PARAM>_QC and <PARAM>_ADJUSTED_QC (when the adjustment is performed in Real Time). Here, <PARAM> refers to the biogeochemical parameters that have been through the delayed-mode process.

Examples where <PARAM>_QC, <PARAM>_ADJUSTED_QC should be edited in delayed-mode include:

- <PARAM>_QC/<PARAM>_ADJUSTED_QC should be changed to '4' for bad and uncorrectable data that are not detected by the real-time tests; and

- <PARAM>_QC/<PARAM>_ADJUSTED_QC should be changed to '1' or '2' for good data that are wrongly identified as probably bad by the real-time tests.

4.2. Compulsory variables to be filled in a BD profile file

This section lists the compulsory variables that must be filled in an Argo netCDF B-Argo profile file that has been through the delayed-mode process.

4.2.1. QC and ADJUSTED variables

Each B-Argo <PARAM> has 5 mandatory qc and adjusted variables in the B-Argo profile file:

- <PARAM>_QC
- PROFILE_<PARAM>_QC
- <PARAM>_ADJUSTED
- <PARAM>_ADJUSTED_QC
- <PARAM>_ADJUSTED_ERROR

When a B-Argo <PARAM> has been through the delayed-mode process, the above 5 mandatory qc and adjusted variables must be filled in the BD profile file. PROFILE_<PARAM>_QC should be re-computed when <PARAM>_ADJUSTED_QC becomes available.

For IB-Argo <PARAM>, <PARAM>_QC and PROFILE_<PARAM>_QC are mandatory, but the 3 adjusted variables are optional in the B-Argo profile file: <PARAM>_ADJUSTED, <PARAM>_ADJUSTED_QC, <PARAM>_ADJUSTED_ERROR.

If a data centre chooses to include these 3 adjusted variables for IB-Argo <PARAM> in the B-Argo profile file, then these 3 adjusted variables must be filled when the IB-Argo <PARAM> has been through the delayed-mode process, and PROFILE_<PARAM>_QC should be re-computed with <PARAM>_ADJUSTED_QC.

Note that PRES in the B-Argo profile file does not carry any qc or adjusted variables. It is used as a stand-alone vertical index that links the core-Argo and B-Argo profile files. Users who want delayed-mode adjusted pressure values (PRES_ADJUSTED) should obtain them from the core- files.

4.2.2. Scientific calibration information for each profile

It is compulsory to fill the scientific calibration section of a BD- profile file.

PARAMETER should contain every parameter recorded in STATION_PARAMETER (including PRES), even though not all STATION_PARAMETER have delayed-mode qc.

When a biogeochemical parameter ('b' parameter) has been through a delayed-mode procedure its PARAMETER_DATA_MODE is set to 'D'. The PARAMETER_DATA_MODE of all intermediate parameters ('i' parameters) associated to this adjusted biogeochemical parameter are also set to 'D' when they have an _ADJUSTED field (but let to 'R' if not).

If PARAMETER_DATA_MODE is 'D', none of the scientific calibration information should be set to FillValue and every information should be filled.

Here are the indications on how to fill the scientific calibration section of a BD profile file.

For IB-Argo PARAMs with no corresponding _ADJUSTED field and for which the associated B-Argo PARAMs have been through delayed-mode qc	
SCIENTIFIC_CALIB_COMMENT	'not applicable'
SCIENTIFIC_CALIB_EQUATION	'not applicable'
SCIENTIFIC_CALIB_COEFFICIENT	'not applicable'
SCIENTIFIC_CALIB_DATE	YYYYMMDDHHMISS(*)

For IB-Argo PARAMs with corresponding _ADJUSTED fields and for which the associated B-Argo PARAMs have been through delayed-mode qc	
SCIENTIFIC_CALIB_COMMENT	Content depends on <PARAM> (See Section 4.3.4 for intermediate parameters associated to BBP)
SCIENTIFIC_CALIB_EQUATION	Content depends on <PARAM> (See Section 4.3.4 for intermediate parameters associated to BBP)
SCIENTIFIC_CALIB_COEFFICIENT	Content depends on <PARAM> (See Section 4.3.4 for intermediate parameters associated to BBP)
SCIENTIFIC_CALIB_DATE	YYYYMMDDHHMISS(*)

For PARAMs that have been through delayed-mode qc	
SCIENTIFIC_CALIB_COMMENT	Content depends on <PARAM> (See Section 4.3 for BBP)
SCIENTIFIC_CALIB_EQUATION	Content depends on <PARAM> (See Section 4.3 for BBP)
SCIENTIFIC_CALIB_COEFFICIENT	Content depends on <PARAM> (See Section 4.3 for BBP)
SCIENTIFIC_CALIB_DATE	YYYYMMDDHHMISS(*)

(*): for a given calibration, the SCIENTIFIC_CALIB_DATE of an adjusted B-Argo parameter and of its associated IB-Argo parameters should be identical.

The three fields SCIENTIFIC_CALIB_COMMENT, _EQUATION, and _COEFFICIENT have netCDF dimensions (N_PROF, N_CALIB, N_PARAM, STRING256). This means that for each N_CALIB, each field is a 256-length character string. If character strings longer than 256-length are needed, the procedure should be separated and stored as multiple N_CALIB.

For a single calibration that needs multiple N_CALIB:

- the SCIENTIFIC_CALIB_DATE should be identical for all N_CALIB,
- once the different fields are correctly filled, the remaining empty fields (unused) should be filled as follows:
  - ✓ SCIENTIFIC_CALIB_COMMENT: ‘No additional comment’,
  - ✓ SCIENTIFIC_CALIB_EQUATION: ‘No additional equation’,
  - ✓ SCIENTIFIC_CALIB_COEFFICIENT:’No additional coefficient’.

4.2.3. Other variables in a BD profile file

Here are other variables in a B-Argo profile file that need to be updated after delayed-mode qc.

- The variable DATA_STATE_INDICATOR should record '2C' or '2C+'.

- The variable DATE_UPDATE should record the date of last update of the netCDF file, in the format YYYYMMDDHHMISS.

- In both the core-Argo and B-Argo profile files, the variable DATA_MODE(N_PROF) is not related to a specific parameter. The value of DATA_MODE(N_PROF) is set to ‘D’ when adjusted values for one or more <PARAM> in each N_PROF become available. In B-Argo profile files, there are additional biogeochemical parameters which can receive delayed-mode adjustments at different times. Therefore the variable PARAMETER_DATA_MODE(N_PROF, N_PARAM) is added to B-Argo profile files to indicate the data mode of each <PARAM> in each N_PROF.

  The adjusted section (<PARAM>_ADJUSTED, <PARAM>_ADJUSTED_QC and <PARAM>_ADJUSTED_ERROR) for each <PARAM> in each N_PROF should then be filled independently according to its PARAMETER_DATA_MODE.

  For example, in a B-Argo profile file with DOXY and NITRATE, it is possible that

  PARAMETER_DATA_MODE = ’D’ for DOXY, and

  PARAMETER_DATA_MODE = ’R’ for NITRATE.

  In this case:

  -the adjusted section for DOXY should be filled with their adjusted values;

  -the adjusted section for NITRATE should be filled with FillValues.

- A history record should be appended to the HISTORY section of the netCDF file to indicate that the netCDF file has been through the delayed-mode process. Please refer to the Argo User's Manual (§5 "Using the History section of the Argo netCDF Structure") on usage of the History section.

4.2.4. Profile files naming convention

When one or more <PARAM> in a single-cycle core-Argo profile file receive delayed-mode adjusted values, the file name changes from R<WMO_ID>_xxx.nc to D<WMO_ID>_xxx.nc.

When one or more <PARAM> in a single-cycle B-Argo profile file receive delayed-mode adjusted values, the file name changes from BR<WMO_ID>_xxx.nc to BD<WMO_ID>_xxx.nc.

When one or more <PARAM> in a single-cycle S-Argo profile file receive delayed-mode adjusted values, the file name changes from SR<WMO_ID>_xxx.nc to SD<WMO_ID>_xxx.nc.

4.3. Suggestions for BBP

This section contains some suggestions on how to fill the scientific calibration fields for BBP after the completion of delayed-mode qc.

4.3.1. BBP that are bad and cannot be corrected

When BBP for the whole profile are bad and cannot be corrected, for example here for BBP700:

BBP700_ADJUSTED = FillValue

BBP700_ADJUSTED_ERROR = FillValue

BBP700_ADJUSTED_QC = ‘4’.

SCIENTIFIC_CALIB_EQUATION	‘none’
SCIENTIFIC_CALIB_COEFFICIENT	‘none’
SCIENTIFIC_CALIB_COMMENT	‘Bad data; not adjustable’

4.3.2. BBP that are good and do not need correction

When BBP for the whole profile are good and do not need to be corrected,

BBP700_ADJUSTED = BBP700

BBP700_ADJUSTED_ERROR = to be provided by the PI. (TBD)

BBP700_ADJUSTED_QC = ‘1’.

SCIENTIFIC_CALIB_EQUATION	‘none’
SCIENTIFIC_CALIB_COEFFICIENT	‘none’
SCIENTIFIC_CALIB_COMMENT	‘No adjustment was necessary’

4.3.3. BBP that are good but need a correction

To be defined

4.3.4. Intermediate parameters xxx_BBP700

If the ADJUSTED fields of the intermediate parameters are available in the Argo netcdf B-Argo profile files, they should also be filled during the delayed-mode process. Their PARAMETER_DATA_MODE should be set to 'D'.

4.3.4.1. No delayed-mode procedure applied to the intermediate parameters

If no delayed-mode procedure is applied to the intermediate parameters in the netcdf B-Argo profile files, then:

<PARAM>_ADJUSTED = <PARAM>

<PARAM>_ADJUSTED_ERROR = FillValue

<PARAM>_ADJUSTED_QC = <PARAM>_QC

SCIENTIFIC_CALIB_EQUATION	<PARAM>_ADJUSTED = <PARAM>
SCIENTIFIC_CALIB_COEFFICIENT	'none'
SCIENTIFIC_CALIB_COMMENT	'No adjustment procedure applied; The adjusted data are simply a copy of the raw data'

4.3.4.2. A delayed-mode procedure is applied to the intermediate parameters

To be defined when relevant.

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