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BGC Argo quality control manual for particles backscattering

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Table of contents

History

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13/March/2017	Creation of the document by Catherine Schmechtig
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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. 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 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 can also be 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-files and the GDAC merged files.

(b). I-Argo <PARAM>: these are the intermediate biogeochemical variables that are only stored in the b-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-files.

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

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

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

(c). PRES: the b-files do not contain any qc or adjusted variables for PRES. They are in the core-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
D : delayed mode data
A : real time data with adjusted values

In b-Argo profile files, the variable PARAMETER_DATA_MODE associated to 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 c-file and from PARAMETER_DATA_MODE(N_PROF, N_PARAM) in a b-file or a m-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 I-Argo parameter may depend on the DAC decision to include or not adjusted fields for I-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 I-Argo parameter can be 'R', 'A' or 'D',
- If not, the data mode of the I-Argo parameter should always be 'R'.

2. Real-time quality control for particles backscattering data 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,
- BBP532.

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 linked to BBP, See Argo Quality Control Manual for Biogeochemical Data (#RD2).

6. Global range test

This test applies a gross filter on observed values for BBP.

- BBP700 in range [−0.000025, 0.1] m^{-1}
- BBP532 in range [−0.000005, 0.1] m^{-1}

Action: Values that fail this test should be flagged with a QC = '3' for BBP700 and BBP532.

9. Spike test

Difference between sequential measurements, where one measurement is quite different than adjacent ones, is considered as a spike. With respect to biogeochemistry, most of the time, spikes contain information, mainly in case of positive spikes. This is the reason why we set up a test to discriminate negative spikes.

We calculate the difference between the BBP at a certain depth (V2) and a running median (5 values, V0, V1, V2, V3, V4) along the whole profile:

- RES = V2 - median(V0,V1,V2,V3,V4)

Then we calculate the percentile10 of this difference for the entire profile. (To get the percentile10, sort RES in ascending order, then find the value of RES at the index i where i = 10% * number of samples in the profile). If the difference between the BBP and the running median is smaller than 2*percentile10:

- RES < 2*percentile10(RES)

then it is considered as a spike.

Action: Values considered as a spike should be flagged as bad data (QC = '4').

13. Stuck value test

15. Grey list

17. Visual QC

19. Deepest pressure test

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

2.2.2.1. Bad offset test

First we apply a 5-point median filter to profile to smooth the signal. If the minimum of this smooth profile is smaller than the range minimum, we estimate a threshold under which values are probably bad (biased by > 5% due to bad dark offset)

For BBP700

BBP700_smooth = median_filter(5, BBP700) (Equation 1)

IF min(BBP700_smooth) < -0.000025 m^{-1} (Test 1) then

QC_THRESHOLD_700 = -20*min(BBP700_smooth) (Equation 2)

IF BBP700 < QC_THRESHOLD_700 then BBP700_QC=3 (Test 2)

IF BBP700 ≥ QC_THRESHOLD_700 then BBP700_QC=2 (Test 3)

For BBP532

BBP532_smooth = median_filter(5, BBP532) (Equation 1b)

IF min(BBP532_smooth) < -0.000005 m^{-1} (Test 1b) then

QC_THRESHOLD_532 = -20*min(BBP532_smooth) (Equation 2b)

IF BBP532 < QC_THRESHOLD_532 then BBP532_QC=3 (Test 2b)

IF BBP532 ≥ QC_THRESHOLD_532 then BBP532_QC=2 (Test 3b)

2.2.3. Test application order on vertical profiles

The Argo real time QC tests on vertical profiles are applied in the order described in the following table.

Order	Test number	Test name
1	19	Deepest pressure test
2	1	Platform Identification test

3	2	Impossible Date test
4	3	Impossible Location test
5	4	Position on Land test
6	5	Impossible Speed test
7	6	Global Range test
8	7	Regional Range test
9	9	Spike test
10	11	Gradient test
11	12	Digit Rollover test
12	13	Stuck Value test
13	15	Grey List test
14	16	Gross temperature sensor drift
15	18	Frozen profile
16	62	Biogeochemical parameter specific tests
17	17	Visual QC

2.2.4. 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 I-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 on trajectories

The following tests are applied in real-time on trajectory data.

Some trajectory data are duplicates of vertical profile ones (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.

2.3.1. Common Argo real-time quality control tests on trajectories

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

The following common tests on trajectories are directly linked to particles backscattering, See Argo Quality Control Manual for Biogeochemical Data (#RD2).

6. Global range test

2.3.2. Specific Argo real-time quality control tests on trajectories

No specific tests are defined for trajectories

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 11 (gradient test) cannot be decreased to QC flag ‘3’ (bad data that are potentially correctable) set by Test 15 (grey list).

A value with QC flag ‘4’ (bad data) or ‘3’ (bad data that are potentially correctable) is ignored by the quality control tests.

When a biogeochemical parameter is calculated from other intermediate (‘i’ parameter), biogeochemical (‘b’ parameter) or core (“c” parameter) data, we should define how the input QC is reflected on the final QC. TBD

BBP is calculated from TEMP and PSAL:

BBP=2*pi*chi*((BETA_BACKSCATTERING-DARK_BACKSCATTERING)*SCALE_BACKSCATTERING-BETASW)

where BETASW is the contribution by the pure seawater computed as a function of TEMP and PSAL.

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

There's no need for adjustment in RT for BBP

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

If a data centre chooses to include these 3 adjusted variables for I-Argo <PARAM> in the B-profile file, then these 3 adjusted variables must be filled when the I-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- profile file does not carry any qc or adjusted variables. It is used as a stand-alone vertical index that links the core- and b- 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 I-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 I-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 I-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- 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- and b- 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- 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- 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 M- profile file receive delayed-mode adjusted values, the file name changes from MR<WMO_ID>_xxx.nc to MD<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.

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_BBPxxx

If the ADJUSTED fields of the intermediate parameters are available in the Argo netcdf b-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-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.

4.3.5. References for BBP

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