

Argo data management

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# Argo Quality Control Manual For Biogeochemical Data

Version 1.0

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**ARGO**

*part of the integrated global observation strategy*



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## **Argo Quality Control Manual For Biogeochemical Data**

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## History

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10/Nov/2015	Creation of the document by Virginie, Henry, Catherine, and Annie.
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## Reference Documents

Reference N°	Title	Link
#RD1	Argo Quality Control Manual for CTD and Trajectory Data	<a href="http://dx.doi.org/10.13155/33951">http://dx.doi.org/10.13155/33951</a>
#RD2	Argo Quality Control Manual for Biogeochemical Data	<a href="http://dx.doi.org/10.13155/40879">http://dx.doi.org/10.13155/40879</a>
#RD3	Argo user manual	<a href="http://dx.doi.org/10.13155/29825">http://dx.doi.org/10.13155/29825</a>
#RD4	Bio-Argo quality control manual for Chlorophyll-A concentration	<a href="http://dx.doi.org/10.13155/35385">http://dx.doi.org/10.13155/35385</a>
#RD5	Quality control for Bio-Argo particle backscattering	TBD
#RD6	Quality control manual for radiometry	TBD
#RD7	Quality control manual fo Nitrate concentration	TBD
#RD8	Quality control manual for CDOM	TBD

## 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 (this document, [#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 (this document) should be considered as the cover document of all biogeochemical data quality control manuals.

In this document, we present the generic tests applied to biogeochemical data and we provide links to documentations relative to each biogeochemical data reporting in detail all the quality control procedures (both generic and specific tests).

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 welcome to exchange with ADMT on the developed and applied method

# 1. Introduction

This document is the Argo quality control manual for biogeochemical data. 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.

Please note that at the present time, official quality control procedures don't exist for all biogeochemical parameters. This document will be updated as soon as other procedures are available.

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 biogeochemical 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 parameters and the following intermediate parameters:

- DOXY,
- TEMP\_DOXY,
- CHLA,
- BBP.

QC of other biogeochemical parameters and other intermediate parameters should be set to '0' (no QC was performed).

Each defined test has a unique number used to report the passed and failed tests list in the HISTORY\_QCTEST variable of the Argo format ([#RD3](#)).

The list of the already defined test is the following.

Test number	Test name	Type of parameter involved ('c', 'i', 'b')
1	Platform Identification	all
2	Impossible Date Test	all
3	Impossible Location Test	all
4	Position on Land Test	all
5	Impossible Speed Test	all
6	Global Range Test	all
7	Regional Range Test	'c' and 'i'
8	Pressure Increasing Test	'c'
9	Spike Test	all
10	Top and Bottom Spike Test : removed	n/a
11	Gradient Test	all
12	Digit Rollover Test	'c' and 'i'
13	Stuck Value Test	all
14	Density Inversion	'c'
15	Grey List	all
16	Gross salinity or temperature sensor drift	'c' and 'i'
17	Visual QC	all
18	Frozen profile	'c' and 'i'
19	Deepest pressure test	all
20	Questionable Argos position test	all
21	Near-surface unpumped CTD salinity test	'c'
22	Near-surface mixed air/water test	all
23	Real-time Quality Control Flag Scheme for float data deeper than 2000 dbar	all
24 to 56	Not used	
57	DOXY specific test	'b'
58	CDOM specific test	'b'
59	NITRATE specific test	'b'
60	PAR specific test	'b'
61	IRRADIANCE specific test	'b'
62	BBP specific tests	'b'
63	CHLA specific tests	'b'

## 2.2. Argo real-time quality control tests on 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.

#### 1. Platform identification

See Argo quality control manual ([#RD1](#)).

#### 2. Impossible date test

See Argo quality control manual ([#RD1](#)).

#### 3. Impossible location test

See Argo quality control manual ([#RD1](#)).

#### 4. Position on land test

See Argo quality control manual ([#RD1](#)).

#### 5. Impossible speed test

See Argo quality control manual ([#RD1](#)).

#### 6. Global range test

This test applies a gross filter on observed values for DOXY, TEMP\_DOXY, CHLA and BBP.

- DOXY in range  $[-5, 600]$  micromoles/kg
- TEMP\_DOXY in range  $[-2.5, 40.0]$  °C
- CHLA in range  $[-0.1, 50]$  mg/m<sup>3</sup> ([#RD4](#))
- BBP700 in range  $[-0.000025, 0.1]$  m<sup>-1</sup> ([#RD5](#))
- BBP532 in range  $[-0.000005, 0.1]$  m<sup>-1</sup> ([#RD5](#))

Action: Values that fail this test should be flagged with a QC = '4' for DOXY, TEMP\_DOXY and CHLA and with a QC = '3' for BBP700 and BBP532.

#### 7. Regional range test

This test applies to certain regions of the world where conditions can be further qualified. In this case, specific ranges for observations from the Mediterranean Sea and the Red Sea further restrict what are considered sensible values. The Red Sea is defined by the region 10N, 40E; 20N, 50E; 30N, 30E; 10N, 40E. The Mediterranean Sea is defined by the region 30N, 6W; 30N, 40E; 40N, 35E; 42N, 20E; 50N, 15E; 40N, 5W; 30N, 6W.

## Red Sea

- TEMP\_DOXY in range [21.7, 40.0] °C

## Mediterranean Sea

- TEMP\_DOXY in range [10.0, 40.0] °C

Action: If a value fails this test, it should be flagged as bad data (QC = '4').

## 9. Spike test

### Spike test for DOXY and TEMP\_DOXY

The difference between sequential measurements, where one measurement is significantly different from adjacent ones, is a spike in both size and gradient. This test does not consider differences in depth, but assumes a sampling that adequately reproduces changes in DOXY and TEMP\_DOXY with depth.

$$\text{Test value} = |V2 - (V3 + V1)/2| - |(V3 - V1)/2|$$

where V2 is the measurement being tested as a spike, and V1 and V3 are the values above and below.

For DOXY: The V2 value is flagged when

- the test value exceeds 50 micromol/kg for pressures less than 500 dbar, or
- the test value exceeds 25 micromol/kg for pressures greater than or equal to 500 dbar.

For TEMP\_DOXY: The V2 value is flagged when

- the test value exceeds 6 °C for pressures less than 500 dbar, or
- the test value exceeds 2 °C for pressures greater than or equal to 500 dbar.

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

### Spike test for CHLA

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 chlorophyll-A at a certain depth (V2) and a running median (5 values, V0, V1, V2, V3, V4) along the whole profile:

- $RES = V2 - \text{median}(V0, V1, V2, V3, V4)$

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  $i = 10\% * \text{number of samples in the profile}$ ). If the difference between the chlorophyll-A and the running median is smaller than  $2 * \text{percentile10}$ :

- $RES < 2 * \text{percentile10}(RES)$

then it is considered as a spike.

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

## Spike test for BBP

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:

- $RES = V2 - \text{median}(V0, V1, V2, V3, V4)$

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  $i = 10\% * \text{number of samples in the profile}$ ). If the difference between the BBP and the running median is smaller than  $2 * \text{percentile10}$ :

- $RES < 2 * \text{percentile10}(RES)$

then it is considered as a spike.

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

## 11. Gradient test

### Gradient test for DOXY and TEMP\_DOXY

This test is failed when the difference between vertically adjacent measurements is too steep. The test does not consider differences in depth, but assumes a sampling that adequately reproduces changes in DOXY and TEMP\_DOXY with depth.

Test value =  $| V2 - (V3 + V1)/2 |$

where V2 is the measurement being tested as a spike, and V1 and V3 are the values above and below.

For DOXY: the V2 value is flagged when

- the test value exceeds 50 micromol/kg for pressures less than 500 dbar, or
- the test value exceeds 25 micromol/kg for pressures greater than or equal to 500 dbar.

For TEMP\_DOXY: The V2 value is flagged when

- the test value exceeds 9 °C for pressures less than 500 dbar, or
- the test value exceeds 3 °C for pressures greater than or equal to 500 dbar.

Action: Values that fail this test should be flagged as bad data (QC = '4').

## 12. Digit rollover test

Only so many bits are allowed to store temperature values in a profiling float. This range is not always large enough to accommodate conditions that are encountered in the ocean. When the range is exceeded, stored values rollover to the lower end of the range. This rollover should be detected and compensated for when profiles are constructed from the data stream from the float.

This test is used to make sure the rollover is properly detected:

- TEMP\_DOXY difference between adjacent pressures  $> 10$  °C.

Action: When a rollover is detected, both values used to detect the jump in the data should be flagged with a QC = '4', other values of the profile with a QC = '3'.

### 13. Stuck value test

This test looks for all biogeochemical sensor outputs (i.e. 'i' and 'b' parameter measurements transmitted by the float) in a vertical profile being identical.

Action: Stuck values should be flagged as bad data (QC = '4').

### 15. Grey list

See Argo quality control manual ([#RD1](#)).

### 16. Gross temperature sensor drift

This test is implemented to detect a sudden and significant sensor drift. It calculates the average temperature from the deepest 100 dbar of a profile and the previous good profile. Only measurements with good QC are used.

Action: For TEMP\_DOXY, if the difference between the two average values is more than 1°C, then all TEMP\_DOXY values from the profile are flagged as probably bad data (QC = '3').

### 17. Visual QC

See Argo quality control manual ([#RD1](#)).

### 18. Frozen profile test

This test is used to detect a float that reproduces the same profile (with very small deviations) over and over again.

Typically the differences between two profiles are of the order of 0.01 °C for temperature.

A). Derive TEMP\_DOXY profiles by averaging the original profiles to get mean values for each profile in 50 dbar slabs (TEMP\_DOXY\_prof, TEMP\_DOXY\_previous\_prof). This is necessary because the floats do not sample at the same level for each profile.

B). Obtain absolute values of the difference between the averaged temperature profiles as follows:

- $\text{delta\_TEMP\_DOXY} = \text{abs}(\text{TEMP\_DOXY\_prof} - \text{TEMP\_DOXY\_previous\_prof})$

C). Find the maximum, minimum and mean of the absolute values of the averaged differences between profiles for temperature:

- $\text{max}(\text{delta\_TEMP\_DOXY}), \text{min}(\text{delta\_TEMP\_DOXY}), \text{mean}(\text{delta\_TEMP\_DOXY})$

D). To fail the test, require that:

- $\text{max}(\text{delta\_TEMP\_DOXY}) < 0.3 \text{ } ^\circ\text{C}$
- $\text{min}(\text{delta\_TEMP\_DOXY}) < 0.001 \text{ } ^\circ\text{C}$
- $\text{mean}(\text{delta\_TEMP\_DOXY}) < 0.02 \text{ } ^\circ\text{C}$

Action: If a profile fails this test, all measurements from the profile are flagged as bad data (QC = '4'). If a float fails this test on 5 consecutive cycles, it is inserted in the grey list.

### **19. Deepest pressure test**

This test requires that the profile has pressures that are not higher than *CONFIG\_ProfilePressure\_dbar* plus 10%.

*CONFIG\_ProfilePressure\_dbar* configuration value comes from the meta-data file of the float.

Action: If there is a region of incorrect pressures, all pressures and corresponding 'i' and 'b' parameter measurements should be flagged as bad data (QC = '4').

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

### 2.2.2.1. For DOXY

No specific tests are defined yet for DOXY parameter.

### 2.2.2.2. For CHLA

#### **63. CHLA specific Argo real-time quality control tests**

CHLA specific tests are described in “Bio-Argo quality control manual for Chlorophyll-A concentration” ([#RD4](#)).

They all should be reported with the same test #63.

### 2.2.2.3. For BBP

#### **62. BBP specific Argo real-time quality control tests**

BBP specific tests are described in “Quality control for Bio-Argo particle backscattering” ([#RD5](#))

They all should be reported with the same test #62.

### 2.2.2.4. For IRRADIANCE

#### **61. IRRADIANCE specific Argo real-time quality control tests**

IRRADIANCE specific tests are described in “Quality control manual for radiometry” ([#RD6](#))

They all should be reported with the same test #61.

### 2.2.2.5. For PAR

#### **60. PAR specific Argo real-time quality control tests**

PAR specific tests are described in “Quality control manual for radiometry” ([#RD6](#))

They all should be reported with the same test #60.

### 2.2.2.6. For NITRATE

#### **59. NITRATE specific Argo real-time quality control tests**

NITRATE specific tests are described in “Quality control manual for Nitrate concentration” ([#RD7](#))

They all should be reported with the same test #59.

### 2.2.2.7. For CDOM

#### **58. CDOM specific Argo real-time quality control tests**

CDOM specific tests are described in “Quality control manual for CDOM” ([#RD8](#))

They all should be reported with the same test #58.

## 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	“appropriate test number”	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:

<b>For PARAMs (B-Argo PARAMs and I-Argo PARAMs) in ‘R’-mode</b>	
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

<b>For PRES</b>	
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 0 how to fill scientific calibration information when PARAMETER\_DATA\_MODE is ‘A’ or ‘D’ respectively).

## 2.3. Argo real-time quality control tests 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

#### 1. Platform identification

See Argo quality control manual ([#RD1](#)).

#### 2. Impossible date test

See Argo quality control manual ([#RD1](#)).

#### 3. Impossible location test

See Argo quality control manual ([#RD1](#)).

#### 4. Position on land test

See Argo quality control manual ([#RD1](#)).

#### 5. Impossible speed test

See Argo quality control manual ([#RD1](#)).

#### 6. Global range test

This test applies a gross filter on observed values for DOXY, TEMP\_DOXY, CHLA and BBP.

- DOXY in range  $[-5, 600]$  micromoles/kg
- TEMP\_DOXY in range  $[-2.5, 40.0]$  °C
- CHLA in range  $[-0.1, 50]$  mg/m<sup>3</sup> ([#RD4](#))
- BBP700 in range  $[-0.000025, 0.1]$  m<sup>-1</sup> ([#RD5](#))
- BBP532 in range  $[-0.000005, 0.1]$  m<sup>-1</sup> ([#RD5](#))

Note that, as statistical values can also be stored in the trajectory file, the global range test should not be performed for all measurement codes. In particular relative measurement code “MC minus 6” is used to store standard deviation values and should then be excluded from this test.

Action: Values that fail this test should be flagged with a QC = '4' for DOXY, TEMP\_DOXY and CHLA and with a QC = '3' for BBP700 and BBP532.

## 7. Regional range test

This test applies to certain regions of the world where conditions can be further qualified. In this case, specific ranges for observations from the Mediterranean Sea and the Red Sea further restrict what are considered sensible values. The Red Sea is defined by the region 10N, 40E; 20N, 50E; 30N, 30E; 10N, 40E. The Mediterranean Sea is defined by the region 30N, 6W; 30N, 40E; 40N, 35E; 42N, 20E; 50N, 15E; 40N, 5W; 30N, 6W.

Red Sea

- TEMP\_DOXY in range [21.7, 40.0] °C

Mediterranean Sea

- TEMP\_DOXY in range [10.0, 40.0] °C

Note that, as statistical values can also be stored in the trajectory file, the regional range test should not be performed for all measurement codes. In particular relative measurement code "MC minus 6" is used to store standard deviation values and should then be excluded from this test.

Action: If a value fails this test, it should be flagged as bad data (QC = '4').

## 20. Questionable Argos position test

See Argos quality control manual ([#RD1](#)).

### 2.3.2. Specific Argos real-time quality control tests on trajectories

#### 2.3.2.1. For DOXY

## 57. DOXY specific Argos real-time quality control tests

In some cases, float equipped with an oxygen sensor acquired data while at the sea surface. Those data are stored in the trajectory file using the PPOX\_DOXY variable and with the measurement codes MC=1100 and associated relative measurement codes (i.e. 1099 to store a single measurement, 1090 to store a serie of measurement, etc ...).

When those measurements are done in the air with Aanderaa optode, they are used to correct bias and drift if necessary. Those data are usable.

When the oxygen sensor is a Seabird SB63, the surface measurements are not acquired in the air but in the water remaining in the CTD sensor (whose pumped was switched off typically at 5 dbar during the ascent). Those data acquired while the float is at the sea surface are not usable.

Action: All oxygen measurements sampled in the air with a Seabird SB63 should be flagged as bad data (QC = '4'); (i.e. If (PARAMETER\_SENSOR = OPTODE\_DOXY) and (SENSOR\_MODEL = SBE63\_OPTODE) and (MC = 1100 or any relative measurement) then PPOX\_DOXY\_QC = '4').

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

The near-surface data described in this section are specialised data that are collected with vertical sampling methods different from the primary CTD profiles. These specialised near-surface data can be selected with a criterium specific to each parameter. They are stored as additional profiles ( $N\_PROF > 1$ ) and are identifiable by **VERTICAL\_SAMPLING\_SCHEME = “Near-surface sampling”**.

### 2.4.1. Common Argo real-time quality control tests on near-surface data

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.

#### 1. Platform identification

See Argo quality control manual ([#RD1](#)).

#### 2. Impossible date test

See Argo quality control manual ([#RD1](#)).

#### 3. Impossible location test

See Argo quality control manual ([#RD1](#)).

#### 4. Position on land test

See Argo quality control manual ([#RD1](#)).

#### 5. Impossible speed test

See Argo quality control manual ([#RD1](#)).

#### 6. Global range test

See 2.2.1.

#### 7. Regional range test

See 2.2.1.

#### 9. Spike test

##### **Spike test for DOXY and TEMP\_DOXY**

See 2.2.1.

##### **Spike test for CHLA**

See 2.2.1.

## 11. Gradient test

### Gradient test for DOXY and TEMP\_DOXY

See 2.2.1.

## 12. Digit rollover test

See 2.2.1.

## 15. Grey list

See Argo quality control manual ([#RD1](#)).

## 17. Visual QC

See Argo quality control manual ([#RD1](#)).

## 19. Deepest pressure test

See 2.2.1.

## 21. Near-surface unpumped DOXY test

Unpumped DOXY data from SBE63 oxygen sensor are of dubious quality because the flow rate and the water masses in front of the sensing foil are wrong when the pump is switched off. This test specifies that unpumped (or partially pumped) oxygen data returned by an SBE63 sensor should be flagged as “probably bad data” in real time.

Action: Unpumped (or partially pumped) oxygen data returned by an SBE63 sensor are flagged as “probably bad data” in real time. That is, DOXY\_QC = ‘3’.

### (a). PROVOR/ARVOR (bin averaged data)

Data returned by some PROVOR/ARVOR floats are bin averaged and are not separated into pumped and unpumped types. This separation is done during data processing at the DACs by checking when the CTD pump is switched off.

Please refer to the document “Argo DAC profile cookbook” on how to identify unpumped or Partially-pumped near-surface data from PROVOR/ARVOR floats.

*(b) To be specified for other float types if relevant*

## 22. Near-surface mixed air/water test

### Near-surface mixed air/water test for DOXY and TEMP\_DOXY

Most near-surface profiles extend all the way to the sea surface. Therefore the shallowest part of a near-surface profile will contain some mixed air/water measurements. This test identifies broadly the pressures at which this shallowest part of a near-surface profile takes place, and specifies that data in that pressure range are “probably bad data”.

Action: Data from the shallowest part of a near-surface profile, which may contain mixed air/water measurements, are flagged as “probably bad data” (QC = ‘3’) in real-time.

(a). PROVOR/ARVOR (bin-averaged data)

For PROVOR/ARVOR floats that return bin-averaged data, if the first bin closest to the sea surface has PRES  $\leq$  1 dbar, then the temperature value from that first bin is suspected to contain averages of mixed air/water measurements and should be flagged as “probably bad data”. That is, TEMP\_DOXY\_QC = ‘3’.

(b). PROVOR/ARVOR (spot-sampled data)

For PROVOR/ARVOR floats that return spot-sampled data, temperature observed at PRES  $\leq$  0.5 dbar should be flagged as “probably bad data”. That is, TEMP\_DOXY\_QC = ‘3’.

(c). NOVA

TBD

(d). APEX

TBD

#### 2.4.2. Specific Argo real-time quality control tests on near-surface data

No specific tests are defined yet on near-surface data.

#### 2.4.3. Test application order on near-surface profiles

The Argo real time QC tests on near-surface 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	21	Near-surface unpumped CTD salinity test
8	22	Near-surface mixed air/water test
9	6	Global Range test
10	7	Regional Range test
11	9	Spike test
12	11	Gradient test
13	12	Digit Rollover test
14	15	Grey List test
15	17	Visual QC

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

Some profiling floats equipped with an oxygen sensor have the capability to sample deeper than the original Argo profiling pressure target of 2000 dbar. However the accuracy of the raw data from these deep Argo floats below 2000 dbar is not yet well understood. Pilot studies of deep Argo data indicated possible pressure dependent salinity and oxygen bias, and the performance of the pressure sensor below 2000 dbar has not been validated by manufacturers. Therefore an interim real-time quality control flag scheme is implemented to warn users that the raw data from deep Argo floats below 2000 dbar may not be suitable for research applications requiring high data accuracy.

### Test 23. Interim rtqc flag scheme for float data deeper than 2000 dbar

This test specifies that for float data deeper than 2000 dbar:

- real-time QC flag = '2' for temperature (TEMP\_DOXY);
- real-time QC flag = '3' for oxygen (DOXY) and associated intermediate parameters (XXX\_DOXY).

Action:

For profiles from deep Argo floats that extend deeper than 2000 dbar, real-time qc, tests defined previously should be applied to the full-depth profiles. Float data deeper than 2000 dbar that have passed all previous real-time qc tests should be flagged in the following way TEMP\_DOXY\_QC = '2', DOXY\_QC = '3'.

## 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) or biogeochemical ('b' parameter) data, its associated QC is initialized to the worse QC value of the input data.

For example, CHLA ('b' parameter) is calculated from FLUORESCENCE\_CHLA ('i' parameter), then if FLUORESCENCE\_CHLA\_QC = '4' after the stuck value test, the corresponding CHLA\_QC is initialized to '4'.

### 3. Real-Time quality control of biogeochemical data adjusted in Real-Time

#### 3.1. Argo real-time quality control tests on vertical profiles

Some biogeochemical data receive an adjustment in real time. As a consequence, the real-time quality control tests defined in the previous section are performed on the ADJUSTED parameters similarly to the raw parameters. For example, NITRATE and NITRATE\_ADJUSTED are provided in real time as well as CHLA and CHLA\_ADJUSTED. The corresponding QC fields, NITRATE\_ADJUSTED\_QC and CHLA\_ADJUSTED\_QC, are assessed automatically.

Some real-time adjustment methods are accompanied by error estimates and therefore B-Argo PARAMs \_ADJUSTED\_ERROR fields could also be filled.

#### 3.2. Scientific calibration information for each profile

When a biogeochemical parameter ('b' parameter) has been through an adjustment procedure, its PARAMETER\_DATA\_MODE is set to 'A' which means "adjusted in real-time". The PARAMETER\_DATA\_MODE of all intermediate parameters ('i' parameters) associated to this adjusted biogeochemical parameter are also set to 'A' when they have an \_ADJUSTED field (but let to 'R' if not).

If PARAMETER\_DATA\_MODE is 'A', none of the scientific calibration information should be set to FillValue and every information should be filled.

As mentioned in §1, for I-Argo <PARAM>, while <PARAM>\_QC and PROFILE\_<PARAM>\_QC are mandatory, <PARAM>\_ADJUSTED, <PARAM>\_ADJUSTED\_QC and <PARAM>\_ADJUSTED\_ERROR are optional (DAC decision).

<b>For I-Argo PARAMs with no corresponding _ADJUSTED field and for which the associated B-Argo PARAMs have been through adjustment in real-time</b>	
SCIENTIFIC_CALIB_COMMENT	'not applicable'
SCIENTIFIC_CALIB_EQUATION	'not applicable'
SCIENTIFIC_CALIB_COEFFICIENT	'not applicable'
SCIENTIFIC_CALIB_DATE	YYYYMMDDHHMISS <sup>(*)</sup>

<b>For I-Argo PARAMs with corresponding _ADJUSTED fields and for which the associated B-Argo PARAMs have been through adjustment in real-time</b>	
SCIENTIFIC_CALIB_COMMENT	Content depends on <PARAM>. See #RD4 for CHLA, #RD7 for NITRATE, #RD8 for CDOM.
SCIENTIFIC_CALIB_EQUATION	Content depends on <PARAM>. See



	# <a href="#">RD4</a> for CHLA, # <a href="#">RD7</a> for NITRATE, # <a href="#">RD8</a> for CDOM.
SCIENTIFIC_CALIB_COEFFICIENT	Content depends on <PARAM>. See # <a href="#">RD4</a> for CHLA, # <a href="#">RD7</a> for NITRATE, # <a href="#">RD8</a> for CDOM.
SCIENTIFIC_CALIB_DATE	YYYYMMDDHHMISS <sup>(*)</sup>

**For B-Argo PARAMs that have been through adjustment in Real-Time**

SCIENTIFIC_CALIB_COMMENT	Content depends on <PARAM>. See # <a href="#">RD4</a> for CHLA, # <a href="#">RD7</a> for NITRATE, # <a href="#">RD8</a> for CDOM.
SCIENTIFIC_CALIB_EQUATION	Content depends on <PARAM>. See # <a href="#">RD4</a> for CHLA, # <a href="#">RD7</a> for NITRATE, # <a href="#">RD8</a> for CDOM.
SCIENTIFIC_CALIB_COEFFICIENT	Content depends on <PARAM>. See # <a href="#">RD4</a> for CHLA, # <a href="#">RD7</a> for NITRATE, # <a href="#">RD8</a> for CDOM.
SCIENTIFIC_CALIB_DATE	YYYYMMDDHHMISS <sup>(*)</sup>

(\*): 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. Delayed mode quality control of biogeochemical 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.

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

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

<b>For PARAMs that have been through delayed-mode qc</b>	
SCIENTIFIC_CALIB_COMMENT	Content depends on <PARAM> (See Section 4.3 for DOXY)
SCIENTIFIC_CALIB_EQUATION	Content depends on <PARAM> (See Section 4.3 for DOXY)
SCIENTIFIC_CALIB_COEFFICIENT	Content depends on <PARAM> (See Section 4.3 for DOXY)
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 dissolved oxygen DOXY

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

#### 4.3.1. DOXY that are bad and cannot be corrected

When DOXY for the whole profile are bad and cannot be corrected,

DOXY\_ADJUSTED = FillValue

DOXY\_ADJUSTED\_ERROR = FillValue

DOXY\_ADJUSTED\_QC = '4'.

SCIENTIFIC CALIB EQUATION	'none'
SCIENTIFIC CALIB COEFFICIENT	'none'
SCIENTIFIC CALIB COMMENT	'Bad data; not adjustable'

#### 4.3.2. DOXY that are good and do not need correction

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

DOXY\_ADJUSTED = DOXY

DOXY\_ADJUSTED\_ERROR = to be provided by the PI.

DOXY\_ADJUSTED\_QC = '1'.

SCIENTIFIC CALIB EQUATION	'none'
SCIENTIFIC CALIB COEFFICIENT	'none'
SCIENTIFIC CALIB COMMENT	'No adjustment was necessary'

#### 4.3.3. DOXY that needs to be recomputed from raw data

The salinity compensation coefficients  $B_0$  to  $B_3$  and  $C_0$  provided by Aanderaa differ from those recommended by the SCOR WG (SCOR Working Group 142 on "Quality Control Procedures for Oxygen and Other Biogeochemical Sensors on Floats and Gliders"). The SCOR Working Group 142 coefficients are strongly recommended for the computation of salinity compensation (Thierry et al, 2016).

Consequently, when MOLAR\_DOXY is computed on board the float with a reference salinity (Sref) different from 0, the salinity compensation should be re-calculated by

1. removing the optode-internal Sref compensation using the Aanderaa Salinity Compensation coefficients and converting it to S=0 (i.e., a "MOLAR\_DOXY"), and then
2. apply the salinity compensation with the correct PSAL and the SCOR WG 142 recommended coefficients.

See Thierry et al, 2016 for details on the calculation.

$$\text{DOXY\_ADJUSTED} = \text{DOXY} * \text{Scorr1} * \text{Scorr2}$$

With:

$$\text{Scorr1} = \exp[(-\text{Sref}) \times (\text{OldB0} + \text{OldB1} \times \text{TS} + \text{OldB2} \times \text{TS}^2 + \text{OldB3} \times \text{TS}^3) + \text{OldC0} \times (-\text{Sref}^2)];$$

$$\text{Scorr2} = \exp[(\text{PSAL}) \times (\text{NewB0} + \text{NewB1} \times \text{TS} + \text{NewB2} \times \text{TS}^2 + \text{NewB3} \times \text{TS}^3) + \text{NewC0} \times (\text{PSAL}^2)];$$

DOXY\_ADJUSTED\_ERROR = to be provided by the PI depending on the rest of the adjustment procedure

$$\text{DOXY\_ADJUSTED\_QC} = '1'.$$

SCIENTIFIC_CALIB_EQUATION	DOXY_ADJUSTED = DOXY*Scorr1*Scorr2; Scorr1 = exp[(- Sref)×(OldB0 + OldB1×TS + OldB2×TS^2 + OldB3×TS^3) + OldC0×(- Sref^2)]; Scorr2 = exp[(PSAL)×(NewB0 + NewB1×TS + NewB2×TS^2 + NewB3×TS^3) + NewC0×( PSAL^2)];
SCIENTIFIC_CALIB_COEFFICIENT	Sref=Sref; OldB <sub>0</sub> = -6.24097e-3, OldB <sub>1</sub> = -6.93498e-3, OldB <sub>2</sub> = -6.90358e-3, OldB <sub>3</sub> = -4.29155e-3, OldC <sub>0</sub> = -3.11680e-7; NewB <sub>0</sub> = -6.24523e-3, NewB <sub>1</sub> = -7.37614e-3, NewB <sub>2</sub> = -1.03410e-3, NewB <sub>3</sub> = -8.17083e-3, NewC <sub>0</sub> = -4.88682e-7
SCIENTIFIC_CALIB_COMMENT	'Recomputation of the salinity compensation term according to SCOR WG 142 recommendations'

#### 4.3.4. DOXY that have calibration drift and can be corrected

Oxygen corrections are still an evolving field: The examples below should therefore only be considered as phrasing suggestions for – as of now – established methods. PI's are free to use other methods as long as they provide adequate documentation / references

To correct DOXY, there is an approx. two dimensional field of common practices:

- A–C: depending on what oxygen quantity is used in the correction (oxygen concentration, saturation, or partial pressure) (referred to [PART 1] hereafter)
- 1–4: depending on what reference is used in the correction (climatology, reference profile, predeployment in-air measurements or continuous in-air measurements) (referred to [PART 2] hereafter)

#### 4.3.4.1. PART 1: methods according to oxygen quantity used in the correction

##### A. Correction using oxygen concentration

DOXY\_ADJUSTED corrected as a linear function of DOXY as in Takeshita et al. (2013).

DOXY_ADJUSTED_ERROR	specified by PI
SCIENTIFIC_CALIB_EQUATION	$DOXY\_ADJUSTED=A*DOXY+B$
SCIENTIFIC_CALIB_COEFFICIENT	$A=a; B=b$
SCIENTIFIC_CALIB_COMMENT	Oxygen concentration corrected as a linear function of DOXY [PART2]

##### B. Correction using oxygen saturation

DOXY\_ADJUSTED corrected via the correction of the percent saturation PSAT as in Takeshita et al. (2013).

DOXY_ADJUSTED_ERROR	specified by PI
SCIENTIFIC_CALIB_EQUATION	$PSAT=f(DOXY);$ $PSAT\_ADJUSTED=A*PSAT+B;$ $DOXY\_ADJUSTED=f(PSAT\_ADJUSTED)$
SCIENTIFIC_CALIB_COEFFICIENT	$A=a; B=b$
SCIENTIFIC_CALIB_COMMENT	Percent saturation corrected as a linear function of PSAT [PART2]; PSAT converted from DOXY and DOXY_ADJUSTED converted from PSAT_ADJUSTED

##### C. Correction using oxygen partial pressure

DOXY\_ADJUSTED corrected via the correction of the partial pressure PPOX as in Bittig and Körtzinger (2015).

DOXY_ADJUSTED_ERROR	specified by PI
SCIENTIFIC_CALIB_EQUATION	$PPOX=f(DOXY);$ $PPOX\_ADJUSTED=A*PPOX+B;$ $DOXY\_ADJUSTED=f(PPOX\_ADJUSTED)$
SCIENTIFIC_CALIB_COEFFICIENT	$A=a; B=b$
SCIENTIFIC_CALIB_COMMENT	Partial pressure corrected as a linear function of PPOX [PART2]; PPOX converted from DOXY and DOXY_ADJUSTED converted from PPOX_ADJUSTED

#### 4.3.4.2. PART 2: methods according to reference used in the correction



## 1. Correction based on a climatology

DOXY\_ADJUSTED corrected based on the climatology *CLIM\_NAME* as in Takeshita et al. (2013). The climatology *CLIM\_NAME* used for the adjustment must be specified. It can be WOA13 or CARS09 for instance.

DOXY_ADJUSTED_ERROR	2-3% (or specified by PI)
SCIENTIFIC_CALIB_COMMENT [PART 2]	[PART 1] by comparison to a climatology (WOA13) as in Takeshita et al. (2013); [PART 1]

## 2. Correction based on a reference profile

(a). DOXY\_ADJUSTED corrected based on a reference profile and profile matching on isobaric surfaces as in Takeshita et al. (2013).

DOXY_ADJUSTED_ERROR	2-3% (or specified by PI)
SCIENTIFIC_CALIB_COMMENT [PART 2]	[PART 1] by comparison to a single reference profile (isobaric match as in Takeshita et al. (2013)) on cycle 0; [PART 1]

The cycle number 0 indicates a deployment reference profile. For match-ups with later float profile, the cycle number needs to be adjusted accordingly.

(b). DOXY\_ADJUSTED corrected based on a reference profile and profile matching on isopycnal surfaces as in Takeshita et al. (2013).

DOXY_ADJUSTED_ERROR	2-3% (or specified by PI)
SCIENTIFIC_CALIB_COMMENT [PART 2]	[PART 1] by comparison to a single reference profile (isopycnal match as in Takeshita et al. (2013)) on cycle 0; [PART 1]

The cycle number 0 indicates a deployment reference profile. For match-ups with later float profile, the cycle number needs to be adjusted accordingly.

(c). DOXY\_ADJUSTED corrected based on a reference profile and profile matching on a mixed isobaric/isopycnal surface as in Bittig and Körtzinger (2015).

DOXY_ADJUSTED_ERROR	2-3% (or specified by PI)
SCIENTIFIC_CALIB_COMMENT [PART 2]	[PART 1] by comparison to a single reference profile (mixed isobaric/isopycnal match as in Bittig and Körtzinger (2015)) on cycle 0; [PART 1]

The cycle number 0 indicates a deployment reference profile. For match-ups with later float profile, the cycle number needs to be adjusted accordingly.

### 3. Correction based on a single in-air measurements

DOXY\_ADJUSTED correction based on a single in-air measurement, e.g., on-ship before deployment.

DOXY_ADJUSTED_ERROR	2% (or specified by PI)
SCIENTIFIC_CALIB_COMMENT [PART 2]	[PART 1] using a single in-air measurements before cycle 0; [PART 1]

### 4. Correction based on continuous in-air measurements

DOXY\_ADJUSTED correction based on surface in-air measurements as in Bittig and Körtzinger (2015) or Johnson et al. (2015) or Bushinsky et al. (2016).

DOXY_ADJUSTED_ERROR	1% (or specified by PI)
SCIENTIFIC_CALIB_COMMENT [PART 2]	[PART 1] using continuous in-air measurements as in [REF]; [PART 1]

### Examples

Two examples of completely filled fields using one of the options A–C and one of the options 1–3 are shown here. The lists A–C and 1–3 do not claim completeness and can be expanded by the respective PI.

#### **- A & 2 isobaric: Correction using oxygen concentration based on a reference profile and an isobaric match**

DOXY_ADJUSTED_ERROR	3%
SCIENTIFIC_CALIB_EQUATION	DOXY_ADJUSTED=A*DOXY+B
SCIENTIFIC_CALIB_COEFFICIENT	A=a; B=b
SCIENTIFIC_CALIB_COMMENT	Oxygen concentration corrected as a linear function of DOXY by comparison to a single reference profile (isobaric match as in Takeshita et al (2013)) on cycle 0

#### **- C & 4: Correction using oxygen partial pressure based on continuous in-air measurements**

DOXY_ADJUSTED_ERROR	1%
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SCIENTIFIC_CALIB_EQUATION	PPOX=f(DOXY); PPOX_ADJUSTED=A*PPOX+B; DOXY_ADJUSTED=f(PPOX_ADJUSTED);
SCIENTIFIC_CALIB_COEFFICIENT	A=a; B=b
SCIENTIFIC_CALIB_COMMENT	Partial pressure corrected as a linear function of PPOX using continuous in-air measurements as in Bittig and Körtzinger (2015); PPOX converted from DOXY and DOXY_ADJUSTED converted from PPOX_ADJUSTED

#### 4.3.5. Intermediate parameters xxx\_DOXY

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'.

##### 4.3.5.1. 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'

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

To be defined when relevant.

#### 4.3.6. References for DOXY

Bittig, H. C. and A. Körtzinger (2015) Tackling Oxygen Optode Drift: Near-Surface and In-Air Oxygen Optode Measurements on a Float Provide an Accurate in Situ Reference. *J. Atmos. Oceanic Technol.*, 32, 1536–1543. <http://dx.doi.org/10.1175/JTECH-D-14-00162.1>

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