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Argo Quality Control Manual for Dissolved Oxygen Concentration

Version 2.1

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ARGO

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Argo Quality Control Manual for Dissolved Oxygen Concentration, v2.1

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History

Date (dd/mmm/yyyy)	Comment
8/July/2016	Creation of the document by Virginie
Nov/2017	Update to include only DOXY-related information and to match structure of the other BGC-Argo QC manuals; Add details on how to adjust DOXY; Henry Bittig
Oct/2018 (v2.0)	Update with ADMT18 decisions on in-air MCs; interim adjustment notation added as well as details about recommended RT and DM adjustment process; added more info on further DM tasks; Henry Bittig
Feb/2021 (v2.1)	Set DOXY_QC=3 by default, set up new SCIENTIFIC_CALIB_XXX fields, propagation of TEMP_QC/PSAL_QC on DOXY_QC; Virginie Racapé, Catherine Schmechtig, Henry Bittig

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	Argo quality control document for Dissolved Oxygen concentration	http://dx.doi.org/10.13155/46542
#RD5	Processing Argo OXYGEN data at the DAC level	http://dx.doi.org/10.13155/39795

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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 dissolved oxygen concentration 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 welcome to exchange with ADMT on the developed and applied method

1 Introduction

This document is the Argo quality control manual for **dissolved oxygen** concentration. 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. **Real-time adjustments are a crucial step to allow scientific use of the data.**
- The second level is the delayed-mode quality control system.

1.1 Background

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

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 dissolved oxygen concentration:

- DOXY,
- TEMP_DOXY

2.1.1 Correspondance between core and DOXY parameter and QC flags

DOXY delayed-mode quality control and adjustment may occur before or after those of core Argo PTS variables. To have a common guide, the following specifications are made:

- In ‘R’ Mode, DOXY_ADJUSTED and DOXY_ADJUSTED_QC are FillValue.
- In ‘A’ Mode, DOXY_ADJUSTED(_QC) is computed from DOXY(_QC) (from raw P/T/S).
- In ‘D’ Mode: An optional step in DMQC after a float has died is to recalculate O2 using ADJUSTED PRES, TEMP, and PSAL to give DOXY_RECALCULATED (not stored in the Argo files!). DOXY_ADJUSTED can be computed from DOXY, or DOXY_RECALCULATED. Whatever step is used is recorded in the SCIENTIFIC_CALIB section. Whatever step is not used is accounted for in DOXY_ADJUSTED_ERROR.

In all three parameter data modes ‘R’, ‘A’, or ‘D’, DOXY is the raw value, computed from the raw PTS. DOXY_QC obeys the flag propagation policy from section §2.2.2 using the core QC flags.

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. See Argo quality control manual (#RD1, #RD2).

6. Global range test

This test applies a gross filter on observed values for DOXY and TEMP_DOXY.

- DOXY in range [−5, 600] micromoles/kg
- TEMP_DOXY in range [−2.5, 40.0] °C

Action: Values that fail this test should be flagged with a QC = ‘4’ for DOXY and TEMP_DOXY.

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

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.

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’).

11. Gradient test

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 test

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~~

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:

- delta_TEMP_DOXY = abs(TEMP_DOXY_prof - TEMP_DOXY_previous_prof)

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

- max(delta_TEMP_DOXY), min(delta_TEMP_DOXY), mean(delta_TEMP_DOXY)

D). To fail the test, require that:

- max(delta_TEMP_DOXY) < 0.3 °C
- min(delta_TEMP_DOXY) < 0.001°C
- mean(delta_TEMP_DOXY) < 0.02 °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

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

57. DOXY specific Argo real-time quality control tests

It was decided at the BGC Argo Data Management task team meeting on May 26, 2020 that real-time unadjusted DOXY data should receive a quality flag of '3'. This is because the majority of oxygen sensors deployed on BGC Argo profiling floats are Aanderaa optodes that suffer from predeployment storage drift that can reduce accuracy by up to 20 % or more (Bittig et al., 2019). As of July, 2020, the median value of optode sensitivity loss due to this issue (when compared to WOA percent saturation at the surface) is 7.6 % across the BGC Argo array. Because this is a known bias that affects the majority of oxygen sensors within the array, and because it is something that can be corrected (see Section 4 of this manual), DOXY_QC should be set to '3'. The following real-time test should be used in order to populate DOXY_QC:

```
If <PARAMETER> == DOXY
        DOXY_QC = 3
End
```

PRES, TEMP and PSAL are used to compute DOXY. Considering the impact of PRES and TEMP on DOXY calculation, when PRES_QC=4 and TEMP_QC=4, DOXY_QC should be set to 4

When PSAL_QC=4, DOXY_QC should be kept to 3 because in general PSAL is not bad enough to justify to put a QC=4 to DOXY.

Action:

If TEMP_QC=4 or PRES_QC=4, then DOXY_QC=4

If PSAL_QC=4, then DOXY_QC=3

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. See Argo quality control manual (#RD1, #RD2) for tests not listed in §2.2.1.

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:

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

(see in Chapter §3.4 and Chapter §4.4 how to fill scientific calibration information when PARAMETER_DATA_MODE is 'A' or 'D' respectively).

2.3 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"**.

Near-surface DOXY data are only stored in an additional profile (N_PROF > 1) if they are concurrent with other data that require such a separation, like pumped / unpumped PSAL. If they are sampled independently, DOXY data are not split into profile and near-surface at Pcutoff, but stored in a single N_PROF (Decision of ADMT18).

2.3.1 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. See Argo quality control manual (#RD1, #RD2)

If no details are given for a test, they follow the specifications of §2.2.1.

6. Global range test

7. Regional range test

9. Spike test

11. Gradient test

12. Digit rollover test

~~**17. Visual QC**~~

19. Deepest pressure test

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

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 <= 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 <= 0.5 dbar should be flagged as “probably bad data”. That is, TEMP_DOXY_QC = ‘3’.

(c). NOVA

TBD

(d). APEX

TBD

(e). NAVIS

TBD

2.3.2 Specific Argo real-time quality control tests on near-surface data

See §2.2.2 for details.

2.3.3 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 DOXY 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~~

2.4 Argo real-time quality control tests on deep float data

No specific tests are defined yet on deep float data.

2.5 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.

2.5.1 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)

If no details are given for a test, they follow the specifications of §2.2.1.

6. Global range test

7. Regional range test

2.5.2 Specific Argo real-time quality control tests on trajectories

57. DOXY specific Argo real-time quality control tests

See §2.2.2 for DOXY specific QC test details on vertical profiles, which apply for trajectory data as well.

Moreover, 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 base measurement codes MC and associated relative measurement codes as follows:

- X – 10 = in-water samples, part of end of profile, shallower than nominal 10 dbar
- X + 10 = in-water samples, part of surface sequence
  (guidance for real-time: before air-bladder inflation / before max. buoyancy)
- X + 11 = in-air samples, part of surface sequence
  (guidance for real-time: after air-bladder inflation / after max. buoyancy)
- X – 1 = individual surface observations

Data to include should all be in PPOX_DOXY. Users should be warned that the distinction between X–10, X+10, X+11 is known definitively for some floats (e.g. some newer Apf9i APEX with Optode), but is only a best guess estimate for other floats (e.g. PROVORs). The X + 10 / X + 11 codes apply only for X = 100 (DST), 600 (AET), 700 (TST) and 800 (TET), i.e., when the float is at the surface.

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 = any relative measurement X+10, X+11) then PPOX_DOXY_QC = '4').

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 DOXY_QC flag ‘4’ (bad data), or with a DOXY_ADJUSTED_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 for data adjusted in Real-Time

3.1 Compulsory variables to be filled for data adjusted in Real-Time

When a B-Argo <PARAM> receives an adjustment in real-time, the following 4 mandatory _QC and ADJUSTED variables must be filled in the BR profile file:

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

It is highly recommended to fill the following ADJUSTED variable, too:

- <PARAM>_ADJUSTED_ERROR

As a consequence of real-time adjustment, the real-time quality control tests defined in the previous section are performed on the ADJUSTED parameters similarly to the raw parameters. PROFILE_<PARAM>_QC should be re-computed when <PARAM>_ADJUSTED_QC becomes available.

In addition, the SCIENTIFIC_CALIB section must be filled with adequate information on the real-time adjustment (see §3.4).

3.2 Data Adjustment Process

3.2.1 Based on previous delayed-mode adjustments

This is the recommended way for real-time adjustment. If no previous DM adjustment is available, however, a basic real-time adjustment procedure is described in §3.2.2.

For dissolved oxygen, Bittig et al. (2018) recommend to adjust OPTODE_DOXY data on partial pressure, i.e., <PARAM> should be PPOX_DOXY in mbar (see #RD5 for unit conversions).

The sequence of delayed-mode adjustments follow the common SCIENTIFIC_CALIB_EQUATION of §4.4.4 that summarizes the typical information required for the oxygen correction.

PPOX_DOXY_ADJUSTED =

(SLOPE · (1 + DRIFT/100 · (profile_date_juld – launch_date_juld)/365)
+ INCLINE_T · TEMP) · (PPOX_DOXY + OFFSET)

Based on the drift character of oxygen optodes (Bittig et al, 2018), offsets are often negligible for well-calibrated optodes. Temperature corrections (INCLINE_T) are often equal to zero for newer, well calibrated optodes on most recent BGC-Argo floats (see §4.4.4). In most cases, optode oxygen is thus adjusted primarily by the gain (including time trends in the gain).

For example:

SCIENTIFIC_CALIB_COEFFICIENT(DOXY):

OFFSET=0; SLOPE=1.0373; DRIFT=0.510; INCLINE_T=0;
launch_date_juld=20161017070000

As the real time adjustement is performed to remove the bias affecting the majority of oxygen sensors (see §2.2.2), DOXY_ADJUSTED_QC should be set to '1'.

Note that adjustments in real time will essentially be past the last correction obtained from delayed-mode, i.e., an extrapolation. To account for the extrapolation beyond delayed-mode adjustments, the PPOX_ADJUSTED_ERROR is augmented by a conservative sensor drift estimate of 1 mbar $year^{-1}$ (Bittig et al., 2018) (see §3.3.1).

3.2.2 Based on WOA surface O2sat if no previous delayed-mode adjustment is available

The prime purpose of this basic real-time adjustment is to remove a systematic low bias that exists for O2 optodes (Takeshita et al., 2013, Bittig et al., 2018) if no delayed-mode adjustments are available.

Preference should be given to more sophisticated adjustments / delayed-mode adjustments (e.g., involving optode in-air measurements) and their propagation in real-time (see §3.2.1).

The proposed, basic real-time adjustment is only applicable to O2 optodes (Aanderaa 3830 or 4330, Seabird SBE63, ARO(D)-FT). It consists of a gain-only adjustment without additional offsets / temperature corrections where the gain is derived from comparison to an O2sat surface climatology.

If oxygen is adjusted just by a gain G – **and only for gain-only adjustments** – the value of G is numerically the same when applied on PPOX_DOXY, O2sat, or DOXY, i.e.,

PPOX_DOXY_ADJUSTED = G · PPOX_DOXY   is equivalent to

O2sat_ADJUSTED = G · O2sat   is equivalent to

DOXY_ADJUSTED = G · DOXY

as the conversion factors (SCOR WG 142 recommendations on O_2 quantity conversions, #RD5) cancel each other on both sides.

G is derived as the median ratio between shallowest profile DOXYs of the float converted to O2sat (SCOR WG 142 recommendations on O_2 quantity conversions, #RD5) or PPOX and surface $O2sat_{clim}$ or $PPOX_{clim}$ of the World Ocean Atlas (WOA18) (or another climatology) interpolated to the profile positions for the first 10 profiles or 3 months of float life (whatever is shorter). $PPOX_{clim}$ from $O2sat_{clim}$ and from TEMP and PSAL float data at the atmospheric pressure of 1 atm.

$$G = \text{median}(g_i) = \text{median}\left(O2sat_{clim,i} / O2sat_{float,i} \right)$$

$$\text{with} \quad i=\text{cycle}(1) \ldots \text{cycle}(\min(10, T_i - T_1 >= 3 \text{ months}))$$

Cycles where the float is under ice are excluded from the median.

Data files for $O2sat_{clim}$ (nominal O2 saturation at 1013 mbar atmospheric pressure) for WOA18 (objectively analyzed mean; annual climatology) are available at:

https://www.nodc.noaa.gov/OC5/woa18/woa18data.html

DOXY is then adjusted in real-time according to

PPOX_DOXY_ADJUSTED = G · PPOX_DOXY,

DOXY_ADJUSTED = f(PPOX_DOXY_ADJUSTED).

The median gain factor G is stored in the SCIENTIFIC_CALIB_COEFFICIENT of the given cycle with the common SCIENTIFIC_CALIB_EQUATION. See next section for how to fill the DOXY_ADJUSTED_ERROR field accordingly.

If a delayed-mode adjustment is not available after 1 year, we recommend to recompute the median gain factor G from comparison with WOA data over a 1 year time window and to reprocess the existing cycles.

3.3 Adjusted error for data adjusted in Real-Time (Recommendations)

3.3.1 Based on previous delayed-mode adjustments

If DOXY_ADJUSTED is based on a previous DM QC adjustment, the last accuracy estimate, e_{last}, of this adjustment is used for DOXY_ADJUSTED_ERROR. It is increased by a conservative drift estimate of 1 mbar per year that is added to the uncertainty. Note that the accuracy estimate for DOXY is made on partial pressure, PPOX_DOXY, which is then converted to DOXY in umol kg^{-1}, using the SCOR WG 142 recommendations on O_2 quantity conversions (see #RD5), i.e.,

$$\text{PPOX\_DOXY\_ADJUSTED\_ERROR} = e_{last} + 1 \text{ mbar year}^{-1} \cdot (T - T_{last}),$$

$$\text{DOXY\_ADJUSTED\_ERROR} = f(\text{PPOX\_DOXY\_ADJUSTED\_ERROR}),$$

where T is the profile time, T_{last} the time of the last profile with an DM QC adjustment, and e_{last} the accuracy error estimate of this last profile (as partial pressure; based on DM QC).

For example:

Delayed-mode adjustments have been performed by use of a climatology: Section §4.4.4.2 suggests a DOXY_ADJUSTED_ERROR “equiv. 4–6 mbar (or specified by PI)” for corrections based on a climatology. In this example, we use the middle, 5 mbar.

To account for the uncertainty of the underlying optode O2-T-calibration and the validity of the drift behaviour characterization, the error estimate from the reference (here: the climatology, 5 mbar) is increased according to the underlying calibration (see section §4.2.3, or Bittig et al., 2018). In this example, we have an Aanderaa 4330 optode with SVU multipoint calibration, i.e., +2 mbar for multi-point calibrated optodes (see §4.2.3).

The DOXY_ADJUSTED_ERROR for real time adjusted data would thus be:

`DOXY_ADJUSTED_ERROR`	`7 mbar + 1 mbar * (JULD - JULD_last_DMQC)/365`

The DOXY_ADJUSTED_ERROR in units of O2 partial pressure PPOX_DOXY (mbar) are then converted to units of DOXY (micromoles per kg) with help of SCOR WG 142 recommendations on O_2 quantity conversions (#RD5).

3.3.2 Based on WOA surface O2sat if no previous delayed-mode adjustment is available

If DOXY_ADJUSTED is not based on a previous DM QC adjustment but on a surface climatologicaly, the accuracy estimate PPOX_DOXY_ADJUSTED_ERROR of this adjustment is set to the larger value of either the PARAMETER_ACCURACY of the given calibration / O2 cookbook case (see #RD5) or 10 mbar, which is slightly more conservative than in Takeshita et al. (2013). This accounts for the different dynamics between a smoothed climatology and in-situ data, and the difference between a 1-point (here) and 2-point correction (Takeshita et al., 2013). Moving forward in time, the increase in error estimate due to in situ drift of 1 mbar per year is added to the uncertainty.

For example:

No delayed-mode adjustments are available and real time adjustments are based on WOA surface O2sat. The float has an Aanderaa 4330 optode with SVU multipoint calibration, for which the O2 cookbook (#RD5) gives a PARAMETER_ACCURACY of 10 umol/kg (cookbook CASE_202_20x_305). Thus, the base adjusted error in this case is equiv. 10 mbar. The DOXY_ADJUSTED_ERROR for real time adjusted data would thus be:

DOXY_ADJUSTED_ERROR	10 mbar + 1 mbar * (JULD – JULD_last_DMQC)/365

3.4 Scientific calibration information for each profile

It is compulsory to fill the scientific calibration section of a BR-profile file for a parameter with real-time adjustments.

When a biogeochemical parameter (‘b’ parameter) has been through a real-time adjustment, its PARAMETER_DATA_MODE is set to ‘A’. 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.

For a given calibration, the SCIENTIFIC_CALIB_DATE of an adjusted B-Argo parameter and of its associated I-Argo parameters should be identical. It should match the date of the last DM QC adjustment.

3.4.1 Based on previous delayed-mode adjustments

For DOXY in ‘A’-mode	
SCIENTIFIC_CALIB_COMMENT	DOXY_ADJUSTED is estimated from the last valid cycle with DM adjustment; DOXY_ADJUSTED_ERROR recomputed from a PPOX_DOXY_ERROR = [xx] mbar increasing with 1 mbar per year
SCIENTIFIC_CALIB_EQUATION	PPOX=f(DOXY); PPOX_DOXY_ADJUSTED=(SLOPE*(1+DRIFT/100*(profile_date_juld-launch_date_juld)/365)+INCLINE_T*TEMP)*(PPOX_DOXY+OFFSET); DOXY_ADJUSTED=f(PPOX_DOXY_ADJUSTED)
SCIENTIFIC_CALIB_COEFFICIENT	*OFFSET=a; SLOPE=b; DRIFT=c; INCLINE_T=d; launch_date_juld=yyyymmddHHMMSS*
SCIENTIFIC_CALIB_DATE	*YYYYMMDDHHMISS*

3.4.2 Based on WOA surface O2sat if no previous delayed-mode adjustment is available

For DOXY in 'A'-mode	
SCIENTIFIC_CALIB_COMMENT	DOXY_ADJUSTED is estimated from an adjustment of in water PSAT or PPOX float data at surface by comparison to WOA PSAT climatology or WOA PPOX in using PSAT_WOA and TEMP and PSAL_float at 1 atm; DOXY_ADJUSTED_ERROR recomputed from a PPOX_DOXY_ERROR = [xx] mbar increasing by 1 mbar per year
SCIENTIFIC_CALIB_EQUATION	PPOX=f(DOXY); PPOX_DOXY_ADJUSTED=(SLOPE*(1+DRIFT/100*(profile_date_juld-launch_date_juld)/365)+INCLINE_T*TEMP)*(PPOX_DOXY+OFFSET); DOXY_ADJUSTED=f(PPOX_DOXY_ADJUSTED)
SCIENTIFIC_CALIB_COEFFICIENT	*OFFSET=a; SLOPE=b; DRIFT=c; INCLINE_T=d; launch_date_juld=yyyymmddHHMMSS*
SCIENTIFIC_CALIB_DATE	*YYYYMMDDHHMISS*

4 Quality control for data adjusted in Delayed-Mode

4.1 Compulsory variables to be filled in a delayed-mode 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.

4.1.1 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.

4.1.2 Scientific calibration information for each profile

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

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.

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 Data adjustment process

The below comments on the data adjustment process focus on Aanderaa and Sea-Bird SBE63 optodes. Information for SBE43 sensors and the JAC optode will be added when available.

4.2.1 Drift behaviour characterization

Takeshita et al. (2013) present results from 130 floats with Aanderaa optodes deployed on floats, that show a significant bias with respect to their laboratory / factory calibration when compared to a climatology (mean bias of –5.0 % O2 saturation at 100 % O2 saturation). Bittig et al. (2018) re-confirm earlier results that the bias is mainly caused by a reduction on O2 sensitivity, i.e., proportional to O2. The decrease in O2 sensitivity can be on the order of several % per year (Bittig et al., 2018), where "newly produced" sensing foils tend to drift faster than "older" sensing foils: D'Asaro and McNeil (2013) report an exponential decrease in drift rate at 100 % O2 saturation with a time constant about 2 years, which is confirmed by Bittig et al. (2018).

Various ways to correct O2 sensitivity drift have been proposed in the literature (e.g., Aanderaa documentation; Takeshita et al., 2013; Bittig et al., 2018): a phase (slope and/or offset) adjustment, a DOXY adjustment (slope and/or offset), a PPOX_DOXY adjustment (slope and/or offset), …

From repeated multi-point calibrations, Bittig et al. 2018 demonstrate that a drift correction on phase is not adequate but creates non-linear artifacts. A phase (slope) correction should be avoided. Given the principle and construction of oxygen optodes (equilibrium between sensing foil and seawater pO_2), Bittig et al. (2018) propose to correct the O2 sensitivity drift on PPOX_DOXY. This is also recommended for the Argo adjustment process. For more details, please consult the studies themselves.

Based on the drift character of oxygen optodes (Bittig et al, 2018), offsets will be typically (close to) zero. Oxygen is mainly adjusted by the gain (including time trends in the gain).

4.2.2 Adjustment using profile data

Profile reference data from a climatology has been used by Takeshita et al. (2013) or Johnson et al. (2015) as comparison. Discrete water sample or CTD-O2 profile data has been used as reference, e.g., in the studies of Bittig and Körtzinger (2015) or Bushinsky et al. (2016). Note that the source or kind of reference data is independent on the way O2 is adjusted mathematically.

Profile reference data can have the advantage to cover a wide O2 range as well as T range, though conditions will depend on the water structure of the given reference profile. As drawback, spatial or temporal mismatches with respect to float profile observations can hinder their utility for O2 adjustmemt.

The uncertainty of the adjustment depends on the accuracy of the reference data (e.g., climatology vs. calibrated CTD-O2 profile) as well as on the proximity of reference and float with respect to the dynamics of the region.

4.2.3 Adjustment using repeated optode in-air data

Repeated in-air observations by floats provide a stable reference to oxygen optode observations that can be used both for O2 sensitivity correction as well as in-situ drift/stability assessment. They are recommended for all Argo O2 observations by the SCOR WG 142 on "Quality Control Procedures for Oxygen and Other Biogeochemical Sensors on Floats and Gliders" (SCOR WG 142, 2015).

In-air observations, however, provide data at one cluster only, i.e., near 100 % O2 saturation. The O2 adjustment should therefore focus on a 1-degree of freedom, slope-only adjustment of PPOX_DOXY.

Bittig and Körtzinger (2015) derive the O2 slope by including a correction for a so called 'carry-over' effect, to account for the observation that optode in-air data do not represent pure air but show a bias by in-water O2 saturation excess/deficiency. Johnson et al. (2015) confirm the 'carry-over' effect for optodes close (~20 cm) to the water surface. They derive the O2 slope from the simple average of all surface observations, without consideration of a 'carry-over' bias, arguing that the bias tends to be small for many cases. Bushinsky et al. (2016) employ special floats with optodes farther above the water surface (~61 cm), where they observe only a negligible 'carry-over' effect. From their data, they observe a daytime dependence of the O2 slope that suggests to give preference to nighttime measurements.

For Argo using in-air data, we recommend to include the 'carry-over' correction if possible, i.e., if enough surfacings (>20) are available. It both removes an identified bias (which is most relevant for cases with strong super-/undersaturation and/or carry-overs) and reduces uncertainty on the O2 slope factor. The equation for linear regression is as follows (see, e.g., Bittig et al., 2018):

$$m \times pO2^{optode}_{surface\ in-air} - pO2^{reference}_{in-air} = c \times \left(m \times pO2^{optode}_{surface\ in-water} - pO2^{reference}_{in-air}\right)$$

where

m is the O2 slope factor: m = pO$_2$_adjusted / pO$_2$,

$pO2^{optode}_{surface\ in-air}$ is the oxygen partial pressure observed by the optode in-air (i.e., close to the water surface), e.g., MC = X+11 or MC = X–1,

$pO2^{reference}_{in-air}$ is the reference oxygen partial pressure in-air, e.g., from re-analysis data,

$pO2^{optode}_{surface\ in-water}$is the oxygen partial pressure observed by the optode at the water surface (in-water), e.g., MC = X+10 or profile MC = X–10, and

c is the slope of the 'carry-over' effect, i.e., the water-fraction of the observed optode in-air data.

Above equation can be used for linear regression to obtain m and c from data of the partial pressures (from several cycles together). From the regression, the 95 % confidence interval (CI) of the O2 slope factor m can be used to indicate the uncertainty of the in-air observations. We recommend to use

eO(in-air) = 95 % CI of m x 205 mbar

as estimate of the error/uncertainty for the in-air adjustment, where 205 mbar corresponds to a typical air pO2.

The average O2 slope factor (Johnson et al., 2015) is simply calculated as mean of all slope factors

$$m_i = pO2^{optode}_{surface\ in-air,i} \,/\, pO2^{reference}_{in-air,i}$$

of all available surfacings i. As estimate of the uncertainty of this average gain, we recommend to use

eO(in-air) = 2 x std(m_i) x 205 mbar

where 2 times the standard deviation of all individual m_i's correspond to the 95 % confidence of the O2 slope factor.

Error estimate at O2 concentrations away from 100 % saturation rely both on the in air accuracy (eO(in-air)) as well as on the O2-T-calibration and the validity of the drift behaviour characterization (§4.2.1). Bittig et al. 2018 suggest to increase eO(in-air) by ca. +2 mbar for multi-point calibrated optodes (e.g., typically 4330 optodes with Stern-Volmer calibration coefficients) and by ca. +4 mbar for optodes with foil batch calibration (e.g., 3830 and 4330 optodes with polynomial calibration coefficients), to account for the uncertainty introduced by the last two effects. We recommend to use this augmented uncertainty estimate for the accuracy or error estimate e_j in the delayed-mode adjustments calculations.

Repeated optode in-air observations allow the analysis of an in-situ O2 drift. Bittig et al. (2018) show that individual floats can drift significantly (order up to ±0.5 % per year). They also show that for a reliable drift estimate, the O2-T-calibration must be adequate (i.e., multi-point) or specifically include a temperature compensation (for batch foil calibrations). An in-situ O2 drift analysis and correction should be based on a sufficiently long float time series (min. 1 – 2 years).

4.2.4 Software tools to help with the adjustment process

- Locodox: Please get in contact with Virginie Thierry, LOPS, Ifremer, France. The source code is publicy at https://github.com/euroargodev/LOCODOX.git

- Sage-O2: Please get in contact with the SOCCOM data group at MBARI, USA (Tanya Maurer, Josh Plant, Ken Johnson). The source code is publicly at https://github.com/SOCCOM-BGCArgo/ARGO_PROCESSING.

- SAGE O2 adaptation in Python: Please get in contact with Chris Gordon, Fisheries and Oceans Canada. The source code is publicly available at https://github.com/ArgoCanada/bgcArgoDMQC.

4.3 Adjusted error estimate for data adjusted in delayed-mode

The drift character (see §4.2.1) suggests an uncertainty that scales with DOXY (O2 slope factor correction). However, repeated calibrations (e.g., Bittig et al. 2017) as well as field data (e.g., Nicholson et al. 2017) indicate a non-zero change at 0 O2. We therefore recommend to apply a constant uncertainty or error estimate eO (in mbar) for the entire O2 range.

This error estimate of the O2 adjustment (expressed as PPOX_DOXY_ADJUSTED_ERROR in mbar) is converted to DOXY_ADJUSTED_ERROR in umol/kg using the SCOR WG 142 recommendations on O2 quantity conversions (see #RD5).

In addition, Bittig et al. (2015) state an uncertainty of 0.3 % per 1000 dbar for the pressure compensation. This should be taken into account, e.g., for O2 adjustments based on surface (in-air) data or based on a deep O2 reference. From this reference pressure (e.g., 0 dbar or 1900 dbar), the DOXY_ADJUSTED_ERROR should be augmented by 0.3 % per 1000 dbar pressure difference from the reference pressure.

4.4 Scientific calibration information for each profile

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

4.4.1 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’

4.4.2 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’

4.4.3 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.

DOXY_ADJUSTED = DOXY*Scorr1*Scorr2

With:

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)];

DOXY_ADJUSTED_ERROR = to be provided by the PI depending on the rest of the adjustment procedure

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*; $OldB_0$ = -6.24097e-3, $OldB_1$ = -6.93498e-3, $OldB_2$ = -6.90358e-3, $OldB_3$ = -4.29155e-3, $OldC_0$ = -3.11680e-7; $NewB_0$ = -6.24523e-3, $NewB_1$ = -7.37614e-3, $NewB_2$ = -1.03410e-2, $NewB_3$ = -8.17083e-3, $NewC_0$ = -4.88682e-7
SCIENTIFIC_CALIB_COMMENT	‘Recomputation of the salinity compensation term according to SCOR WG 142 recommendations”

4.4.4 DOXY that have calibration drift and can be corrected

A common SCIENTIFIC_CALIB_EQUATION based on the oxygen partial pressure is proposed here to follow the sensing principle of optodes (Bittig et al. 2018). This common equation summarizes all potential information required for DOXY correction. This common equation is independent of the sensor and the adjustment method used [PART2]. This common equation is essential to retrieve and apply the last DM adjustment for the automatic correction of raw oxygen data in real time (§3.2.1 and 3.4.2).

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 and fill the common SCIENTIFIC_CALIB_EQUATION.

To correct DOXY, there is common practice to:

- use the partial pressure in the correction (referred to as [PART 1] herafter)
- depending on what reference is used in the correction (climatology, continuous in-air measurements, reference profile, or predeployment in-air measurements), adjust the error estimate accordingly (referred to as [PART 2] herafter) and with consideration of the optodes base calibration accuracy (multi-point/SVU, or batch).

4.4.4.1 PART 1: Correction using oxygen partial pressure

DOXY_ADJUSTED corrected via the correction of the partial pressure PPOX as in Bittig et al. (2018).

SCIENTIFIC_CALIB_EQUATION	PPOX=f(DOXY); PPOX_DOXY_ADJUSTED=(SLOPE*(1+DRIFT/100*(profile_date_juld-launch_date_juld)/365)+INCLINE_T*TEMP)*(PPOX_DOXY+OFFSET); DOXY_ADJUSTED=f(PPOX_DOXY_ADJUSTED)
SCIENTIFIC_CALIB_COEFFICIENT	*OFFSET=a; SLOPE=b; DRIFT=c; INCLINE_T=d; launch_date_juld=yyyymmddHHMMSS*
SCIENTIFIC_CALIB_COMMENT	PPOX converted from DOXY; PPOX corrected [PART2]; DOXY_ADJUSTED converted from PPOX_DOXY_ADJUSTED; DOXY_ADJUSTED_ERROR recomputed from a PPOX_DOXY_ERROR = [xx] mbar

Where:

SLOPE: Oxygen slope/gain factor to correct for large ‘storage drift’ as it is summarized in PART 2.

DRIFT (% $year^{-1}$) to correct the potential small in-situ drift described in §4.2.1

INCLINE_T (°C^{-1}): temperature inclination of the gain factor, which can be observed in older, batch-calibrated optode (i.e. 3830 and 4330) because of incomplete temperature compensation. Please refers to Bittig et al. 2018 for details.

OFFSET: zero-offset, which can be observed in older, batch-calibrated optodes because of incomplete O2-phase-compensation

launch_date_juld: Corresponds to the LAUNCH_DATE given in the float’s meta file.

In many cases, INCLINE_T and OFFSET = 0.

Since only a linear drift in the slope is applied, the choice of reference date is arbitrary. To have a common guide accross all DACs and to allow array-wide monitoring/audits, the float’s launch date is chosen (from meta file).

4.4.4.2 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 adjustement must be specified. It can be WOA18 or CARS09 for instance.

DOXY_ADJUSTED_ERROR	equiv. 4-6 mbar (or specified by PI)
SCIENTIFIC_CALIB_COMMENT [PART 2]	[PART 1] by comparison to a climatology (WOA18) as in Takeshita et al. (2013); [PART 1]

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

3. 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	equiv. 4-6 mbar (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	equiv. 4-6 mbar (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	equiv. 4-6 mbar (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.

4. Correction based on a single in-air measurement

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

DOXY_ADJUSTED_ERROR	equiv. 4 mbar (or specified by PI)
SCIENTIFIC_CALIB_COMMENT [PART 2]	[PART 1] using a single in-air measurements before cycle 0; [PART 1]

Examples

Two examples of completely filled fields using one of the options 1–4 are shown here. The list 1–4 does not claim completeness and can be expanded by the respective PI.

- 2: Correction using oxygen partial pressure based on continuous in-air measurements

DOXY_ADJUSTED_ERROR	equiv. 2 mbar
SCIENTIFIC_CALIB_EQUATION	PPOX=f(DOXY); PPOX_DOXY_ADJUSTED=(SLOPE*(1+DRIFT/100*(profile_date_juld-launch_date_juld)/365)+INCLINE_T*TEMP)*(PPOX_DOXY+OFFSET); DOXY_ADJUSTED=f(PPOX_DOXY_ADJUSTED)
SCIENTIFIC_CALIB_COEFFICIENT	*OFFSET=a; SLOPE=b; DRIFT=c; INCLINE_T=d; launch_date_juld=yyyymmddHHMMSS*
SCIENTIFIC_CALIB_COMMENT	PPOX converted from DOXY; PPOX corrected using continuous in-air measurements as in Bittig and Körtzinger (2015); DOXY_ADJUSTED converted from PPOX_DOXY_ADJUSTED; DOXY_ADJUSTED_ERROR recomputed from a PPOX_DOXY_ERROR = 2 mbar

- 3 isobaric: Correction using oxygen concentration based on a reference profile and an isobaric match

DOXY_ADJUSTED_ERROR	equiv. 6 mbar
SCIENTIFIC_CALIB_EQUATION	PPOX=f(DOXY); PPOX_DOXY_ADJUSTED=(SLOPE*(1+DRIFT/100*(profile_date_juld-launch_date_juld)/365)+INCLINE_T*TEMP)*(PPOX_DOXY+OFFSET); DOXY_ADJUSTED=f(PPOX_DOXY_ADJUSTED)
SCIENTIFIC_CALIB_COEFFICIENT	*OFFSET=a; SLOPE=b; DRIFT=c; INCLINE_T=d; launch_date_juld=yyyymmddHHMMSS*
SCIENTIFIC_CALIB_COMMENT	PPOX converted from DOXY; PPOX corrected by comparison to a single reference profile (isobaric match as in Takeshita et al. (2013)) on cycle 0; DOXY_ADJUSTED converted from PPOX_DOXY_ADJUSTED; DOXY_ADJUSTED_ERROR recomputed from a PPOX_DOXY_ERROR = 6 mbar

4.4.4.3 Additional corrections beyond the common SCIENTIFIC_CALIB_EQUATION

In some cases, additional correction steps beyond the framework of the common SCIENTIFIC_CALIBRATION_EQUATION (§4.4.4) may be warranted.

E.g., oxygen optodes on Deep Argo floats may require a refined pressure correction coefficient to reproduce both surface O2 data (e.g. from in air measurements) and deep ocean O2 data (e.g., in a reproducibly stable deep water mass).

Analoguous to core Argo delayed mode QC, such additional corrections can be performed by the float PI and recorded in the SCIENTIFIC_CALIB section by expansion of the N_CALIB dimension. Thus, the common SCIENTIFIC_CALIBRATION_EQUATION (e.g., in N_CALIB = 1) can be used alongside additional corrections (e.g., in N_CALIB = 2).

4.4.5 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’.

4.4.5.1 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'

4.4.5.2 A delayed-mode procedure is applied to the intermediate parameters

To be defined when relevant.

4.5 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.

The tool 'Scoop-Argo: visual quality control for Argo NetCDF data files' (http://dx.doi.org/10.17882/48531) exists as one option to help with the visual QC process.

4.6 Further delayed-mode tasks for DOXY

In addition to O2 adjustment as suggested above and general visual QC, delayed-mode QC for DOXY should try to address:

- Correction of the oxygen optode time response if time stamps are available (see e.g., Bittig and Körtzinger 2017, Bittig et al. 2014).

- If no time stamps are available, correction of the oxygen optode time response may still be feasible using a mean float ascent velocity as input (see figures 2/3 of https://dx.doi.org/10.5194/os-13-1-2017 and https://dx.doi.org/10.5194/os-2016-75-AC1, respectively).

- The presence of a so-called 'O2 hook' at the base of the profile (first ~50 dbar), i.e., significantly lower O2 observations as suggested by the O2 gradient at slightly shallower depths / as indicated from climatological data

- Optode foil batch calibrations that use a two-point slope and offset scaling on phase show a high uncertainty in the characterization of the O2-T-response of the sensors (Bittig et al., 2018). Re-fitting the data with a different two-point scaling can improve the O2-T-response calibration.

Re-calculation of oxygen using such re-fitted calibration data should be considered for optodes with foil batch calibration ("Aanderaa polynomial standard calibration").

5 References for DOXY

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