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Argo Quality Control Manual For dissolved oxygen concentration

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Argo Quality Control Manual For dissolved oxygen concentration

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History

Date (dd/mmm/yyyy)	Comment
8/July/2016	Creation of the document by Virginie
28/September/2016	Modification of some RT QC tests

Note: changes since last version are highlithed in yellow/

Reference Documents

Reference N°	Title	Link
#RD1	Argo Quality Control Manual for CTD and Trajectory Data	http://dx.doi.org/10.13155/33951
#RD2	Argo Quality Control Manual for Biogeochemical Data	http://dx.doi.org/10.13155/40879
#RD3	Argo user manual	http://dx.doi.org/10.13155/29825
#RD4	Processing Argo oxygen data at the DAC level	http://dx.doi.org/10.13155/39795

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
- The second level is the delayed-mode quality control system.

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

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

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

(a). B-Argo <PARAM>: these are the ocean state biogeochemical variables that will receive real-time qc tests, adjustment in real-time and delayed-mode adjustments. They are stored in both the b-files and the GDAC merged files.

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

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

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

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

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

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

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

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

1. Retrieve the data mode of the <PARAM> parameter (from DATA_MODE(N_PROF) in a c-file and from PARAMETER_DATA_MODE(N_PROF, N_PARAM) in a b-file or a m-file),
2. Access the data:
    - If the data mode is ‘R’: In <PARAM>, <PARAM>_QC and PROFILE_<PARAM>_QC,
    - If the data mode is ‘A’ or ‘D’: In <PARAM>_ADJUSTED, <PARAM>_ADJUSTED_QC, PROFILE_<PARAM>_QC and <PARAM>_ADJUSTED_ERROR.

Note that the data mode of a I-Argo parameter may depend on the DAC decision to include or not adjusted fields for I-Argo parameters in the b-Argo profile file:

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

2 Real-time quality control for dissolved oxygen concentration data and associated intermediate parameters

2.1 Introduction

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

At the present time, real-time tests are defined for the following biogeochemical and intermediate parameters related to dissolved oxygen concentration :

- DOXY,
- TEMP_DOXY

2.2 Argo real-time quality control tests for DOXY vertical profiles

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

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

The following tests are directly linked to DOXY, See Argo Quality Control Manual for Biogeochemical Data (#RD2).

6. Global range test

7. Regional range test

9. Spike test

11. Gradient test

12. Digit rollover test

13. Stuck value test

15. Grey list test

16. Gross temperature sensor drift

17. Visual QC

18. Frozen profile test

19. Deepest pressure test

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

2.2.2.1 For DOXY

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 bet set to 4

When PSAL_QC=4, DOXY_QC should be set 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.

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

A specific comment should however be set for PRES parameter

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

(see in Chapter 0 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 for DOXY on trajectories

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

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

2.3.1 Common Argo real-time quality control tests on trajectories

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

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

6. Global range test

7. Regional range test

2.3.2 Specific Argo real-time quality control tests on trajectories

2.3.2.1 For DOXY

57. DOXY specific Argo real-time quality control tests

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 bet set to 4

When PSAL_QC=4, DOXY_QC should be set 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

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

The following tests are directly linked to DOXY, See Argo Quality Control Manual for Biogeochemical Data (#RD2).

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

22. Near-surface mixed air/water test

2.4.2 Specific Argo real-time quality control tests for DOXY on near-surface data

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 bet set to 4

When PSAL_QC=4, DOXY_QC should be set 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

2.4.3 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.~~

~~The following tests are directly linked to DOXY, See Argo Quality Control Manual for Biogeochemical Data (#RD2).~~

No specific tests are defined on deep float data.

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

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 for DOXY data adjusted in Real-Time

No adjusted data in Real Time are defined yet for DOXY parameter.

4 Real-time quality control for DOXY data adjusted in Delayed-Mode

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

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

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

- <PARAM>_QC/<PARAM>_ADJUSTED_QC should be changed to '4' for bad and uncorrectable data that are not detected by the real-time tests; and
- <PARAM>_QC/<PARAM>_ADJUSTED_QC should be changed to '1' or '2' for good data that are wrongly identified as probably bad by the real-time tests.

4.2 Compulsory variables to be filled in a BD profile file

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

4.2.1 QC and ADJUSTED variables

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

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

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

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

If a data centre chooses to include these 3 adjusted variables for I-Argo <PARAM> in the B-profile file, then these 3 adjusted variables must be filled when the I-Argo <PARAM> has

been through the delayed-mode process, and PROFILE_<PARAM>_QC should be re-computed with <PARAM>_ADJUSTED_QC.

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

4.2.2 Scientific calibration information for each profile

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

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

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

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

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

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

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

For PARAMs that have been through delayed-mode qc

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.

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–3, $NewB_3$ = –8.17083e–3, $NewC_0$ = –4.88682e–7
SCIENTIFIC_CALIB_COMMENT	'Recomputation of the salinity compensation term according to SCOR WG 142 recommendations"

4.3.4 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] herafter)
- 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] herafter)

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 adjustement 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%
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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