DOXY: Updates to the Documentation

9th BGC-Argo, 21st ADMT, virtual

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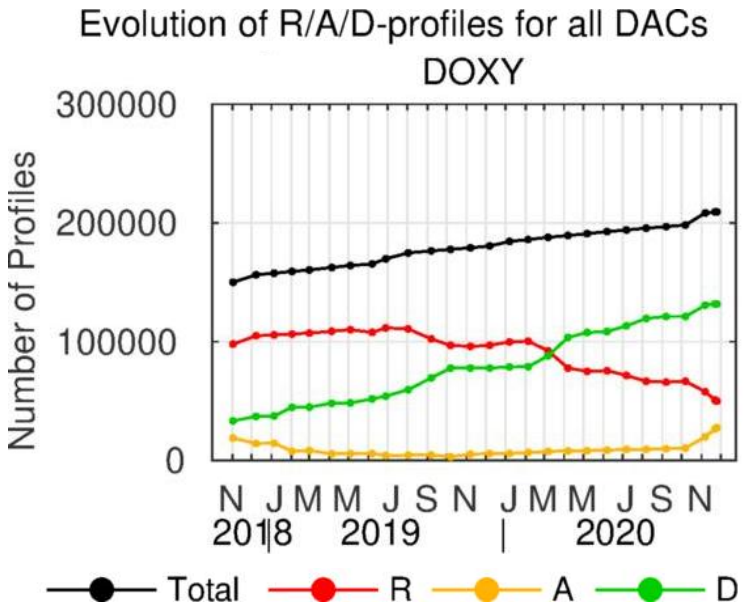
Topics:

- Common Adjustment Notation for DM and RT
- How to record Adjustments in SCIENTIFIC_CALIB_<...> section
- BGC-ADMT Decision to set DOXY_QC = ‘3’ (bad data) by default
- QC Flag Propagation Scheme with unadjusted/adjusted core/DOXY Data

Common Adjustment Notation for DM and RT

Motivation:

- Growing Number of Delayed Mode Quality controlled DOXY Data
- Known Biases in real-time unadjusted DOXY Data



- How to make Propagation of DM Adjustments to RT Adjustments easy for DACs?
- How to simplify across-DAC & across-DMQC Operator Coherence/Consistency?

-> Standardization of Adjustment Equation

Common Adjustment Notation for DM and RT

SCIENTIFIC_CALIB_EQUATION	PPOX_DOXY=f(DOXY); PPOX_DOXY_ADJUSTED=**OFFSET**+(**SLOPE***(1+**DRIFT**/100*(profile_date_juld–launch_date_juld)/365)+**INCLINE_T***TEMP)*PPOX_DOXY; 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_ADJUSTED_ERROR = [xx] mbar

Issue	Prevalence	Remedy
Bias in O_2 sensitivity	All Floats with Optodes	***SLOPE*** Factor on PPOX_DOXY
Ongoing change in O_2 sensitivity ("in situ drift")	Many Floats (>50 %)	Time-dependent ***DRIFT*** in Slope Factor on PPOX_DOXY
Improper/Incomplete Temperature Compensation	All 2nd Generation Floats[a]	Temperature-dependent Slope Factor by ***INCLINE_T***
Improper/Incomplete Oxygen Compensation at low O_2 values	All 2nd Generation Floats[a]	(Small) ***OFFSET*** on PPOX_DOXY
Improper/Incomplete Pressure Compensation	unknown (mostly Deep Argo-O_2?)	Refinement of *Pcoef3*; Addition of *INCLINE_P* ?

[a]: 1st Generation: Electrochemical SBE43; 2nd Generation: Batch-Foil calibrated Optodes; 3rd Generation: Multi-Point calibrated Optodes

How to record Adjustments in SCIENTIFIC_CALIB_<...> section

SCIENTIFIC_CALIB_EQUATION	PPOX_DOXY=f(DOXY); PPOX_DOXY_ADJUSTED=OFFSET+(SLOPE*(1+DRIFT/100*(profile_date_juld-launch_date_juld)/365)+INCLINE_T*TEMP)*PPOX_DOXY; 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_ADJUSTED_ERROR = [xx] mbar

Common Notation for most typical Corrections increases Consistency between DACs/DMQC Operators and makes DM Adjustment retrievable (parseable) for RT Adjustment at DAC.

Recommended for all future DOXY DMQC as well as for active Floats.
No enforcement (?).

Additional DM corrections (e.g., Pressure Compensation, Time Response, ...) could go in a second N_CALIB set of SCIENTIFIC_CALIB_<...> fields (?).

DOXY_QC = '3' (bad data) by default

- Discussion about Standardization of QC flags for RT unadjusted BGC data by DACs earlier in 2020.
- Problem: Different DACs were interpreting and applying Argo quality flags differently for BGC:

ARGO USER'S MANUAL
Version 3.3
November 22nd 2019

E.g.

- Coriolis/Europe flagged RT unadjusted data a "1", intent on conveying to users: "This data has passed all real-time tests. Sensor is working." ("RTFM"-Approach)
- MBARI/SOCCOM flagged RT unadjusted data a "3", intent on conveying to users: "Caution: do not use data without correction." ("We know what's best for you"-Approach)

n	Meaning	Real-time comment	Delayed-mode comment
0	No QC was performed	No QC was performed.	No QC was performed.
1	Good data	All Argo real-time QC tests passed.	The adjusted value is statistically consistent and a statistical error estimate is supplied.
2	Probably good data		Probably good data.
3	Bad data that are potentially correctable	Test 15 or Test 16 or Test 17 failed and all other real-time QC tests passed. These data are not to be used without scientific correction. A flag '3' may be assigned by an operator during additional visual QC for bad data that may be corrected in delayed mode.	An adjustment has been applied, but the value may still be bad.
4	Bad data	Data have failed one or more of the real-time QC tests, excluding Test 16. A flag '4' may be assigned by an operator during additional visual QC for bad data that are not correctable.	Bad data. Not adjustable.
5	Value changed	Value changed	Value changed
6	Not used	Not used	Not used
7	Not used	Not used	Not used
8	Estimated value	Estimated value (interpolated, extrapolated or other estimation).	Estimated value (interpolated, extrapolated or other estimation).
9	Missing value	Missing value	Missing value

DOXY_QC = ‘3’ (bad data) by default

Argo Quality Control Manual for Dissolved Oxygen Concentration
Version 2.0
23th October 2018

Discussion in BGC-ADMT Task Team around:

- What do we have Documentation for?

> 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.

- What do QC Flags indicate? What can we transfer from core Argo and what not?
- If starting from Scratch: How would we design QC Flags?
- What Users do we have? (Operational; Research)
- What are their Needs? (‘good enough’ Data quickly; ‘Science-ready’ Data)
- How do Users behave? (Cannot prevent Data Misuse, but try to minimize the Risk: being clear & consistent across Argo)
- How do Sensors behave? (Core CTD: Likely good for Operational; Deep CTD: Likely need Correction for Operational; BGC: Likely need Correction for Operational; All Sensors: Need DMQC before being ‘Research-ready’)
- What is ‘good enough’ in R-/A-mode?

DOXY_QC = '3' (bad data) by default

Bottom Line:

- What is 'good enough' (for Operational Use) in R-mode?
  EITHER: we need to **universally flag** sensors known to likely be bad by default
  OR: we need RT-tests that are **robust and sufficient** to allow a **good flag**

Decision by BGC Argo Data Management Task Team, May 26, 2020:

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'.

Argo Quality Control Manual for Dissolved Oxygen Concentration
Version 2.1
20th November 2020
draft

QC Flag Propagation: Question

DOXY RT Test 57 defines how TEMP and PSAL QC Flags impact DOXY QC Flags:

> 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 set to 3** because in general PSAL is not bad enough to justify to put a QC=4 to DOXY.

This Test applies both to real-time unadjusted R-mode DOXY_QC and to **real-time adjusted A-**/ delayed-mode adjusted D-mode DOXY_ADJUSTED_QC

- What happens to DOXY when PTS is in A-/D-mode? Which ..._QC field is used for which ..._QC result?

	DOXY in 'R'	DOXY in 'A'/'D'-mode
PTS <PARAM> in 'R'	<PARAM>_QC for DOXY_QC; DOXY_ADJUSTED_QC empty	<PARAM>_QC for DOXY_QC; <PARAM>_QC for DOXY_ADJUSTED_QC
PTS <PARAM> in 'A'/'D'	<PARAM>**_ADJUSTED**_QC for DOXY_QC; DOXY_ADJUSTED_QC empty	<PARAM>**_ADJUSTED**_QC for DOXY_QC; <PARAM>_ADJUSTED_QC for DOXY_ADJUSTED_QC

- Should <PRES/TEMP/PSAL>_ADJUSTED_QC be used for DOXY_QC when available (e.g., in 'A')?
- Should <PRES/TEMP/PSAL>_ADJUSTED be used for DOXY Calculation when available (e.g., in 'A')?
- Remember: Value of DOXY_ADJUSTED is commonly based on Value of DOXY! No Re-Calculation from Sensor Data with <PTS>_ADJUSTED involved.