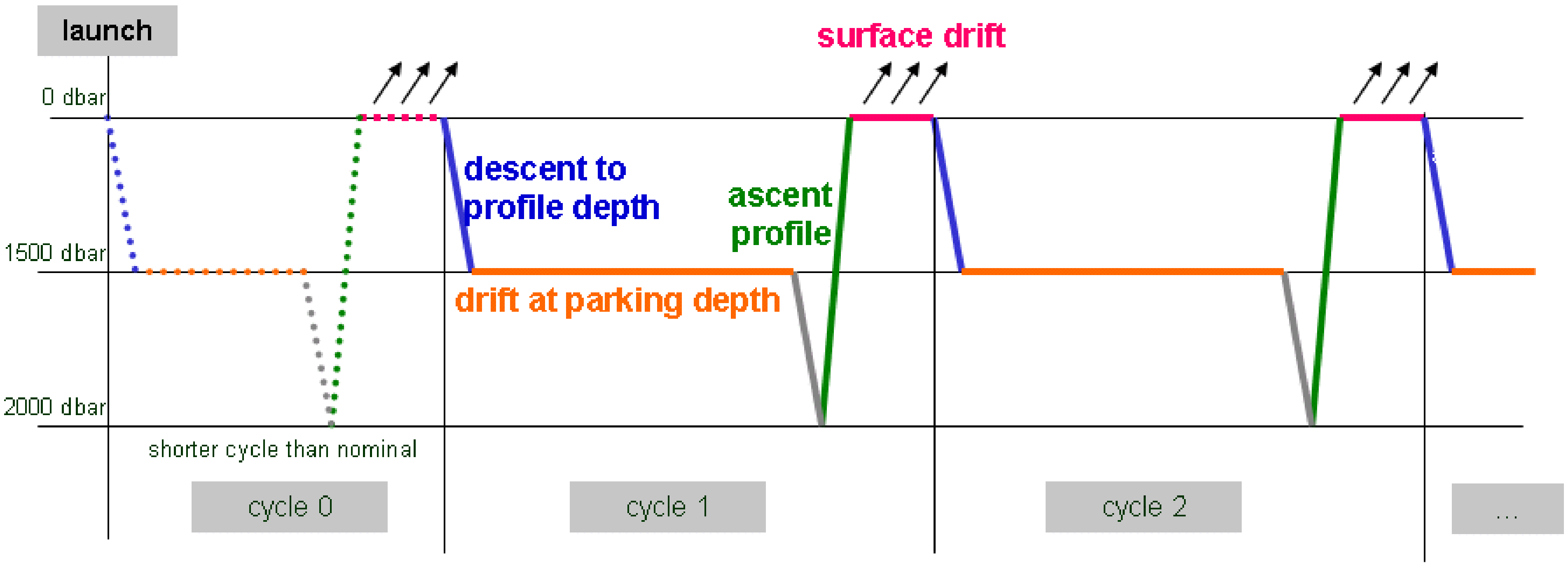
Management and QC procedures of oxygen data in the Argo data stream

V. Thierry

Cycle and profiles, files name



Data acquired during ascend or descent are stored in “profile” file exemple:

R5902269_001.nc PTS data for descending profiles

R5902269_001D.nc PTS data for descending profiles

BR5902269_001.nc BIO data for ascending profiles, including oxygen

Data acquired during drift at parking depth and at surface are stored in ”trajectory” file

5902269_Rtraj.nc PTS data during drift

5902269_BRtraj.nc BIO data during drift, including oxygen

Data format and data management
Parameters strored in the files

Final physical parameter: DOXY

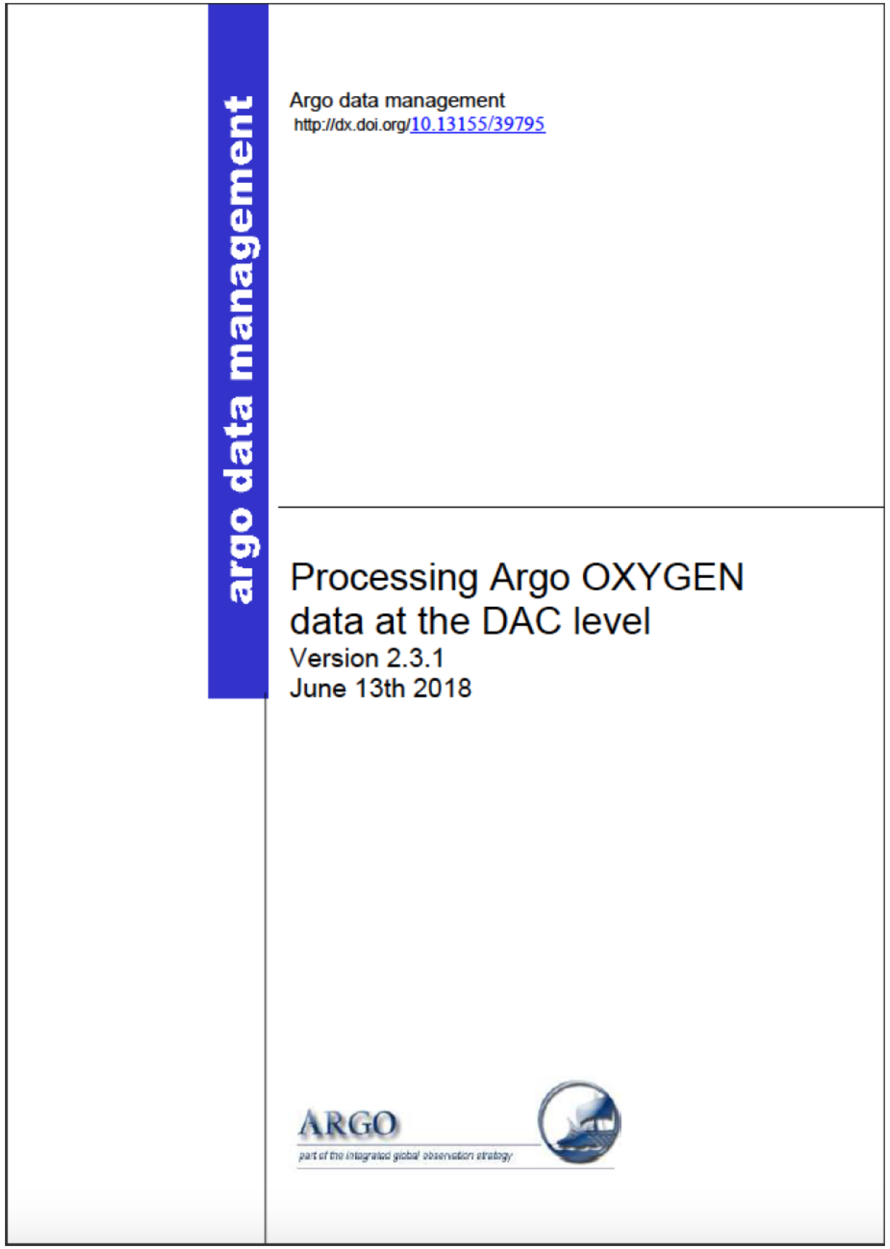
Unit: µmol/kg

Intermediate parameters (associated to different calibration equations /sensor described in the cookbook)

- TEMP_DOXY
- TEMP_VOLTAGE_DOXY
- VOLTAGE_DOXY
- FREQUENCY_DOXY
- COUNT_DOXY
- RPHASE_DOXY
- BPHASE_DOXY
- DPHASE_DOXY
- TPHASE_DOXY
- C1PHASE_DOXY, C2PHASE_DOXY
- MOLAR_DOXY
- PHASE_DELAY_DOXY
- MLPL_DOXY

Data format and data management
ARGO-O2 processing manual

- Define how to compute DOXY from raw data recorded and transmitted by the sensor
- **First part details the scientific basis** of the oxygen measurements and computation, describe the different sensors and associated calibration equations
  - ➔ in general copy/paste of the Oxygen Sensor manuals
  - ➔ take also into account SCOR WG142 results
- **Second part is the practical part for the DAC**. No need to be an expert to read and use this part. It provides the clear computational method for each case and the way to fill meta data and all required fields
- Thierry V., H. Bittig, D. Gilbert, T. Kobayashi, K. Sato, C. Schmid, 2018: Processing Argo OXYGEN data at the DAC level, v2.3.1, http://dx.doi.org/10.13155/39795


argo data management

Argo data management
http://dx.doi.org/10.13155/39795

Processing Argo OXYGEN data at the DAC level
Version 2.3.1
June 13th 2018

ARGO

Data format and data management

ARGO-O2 processing manual

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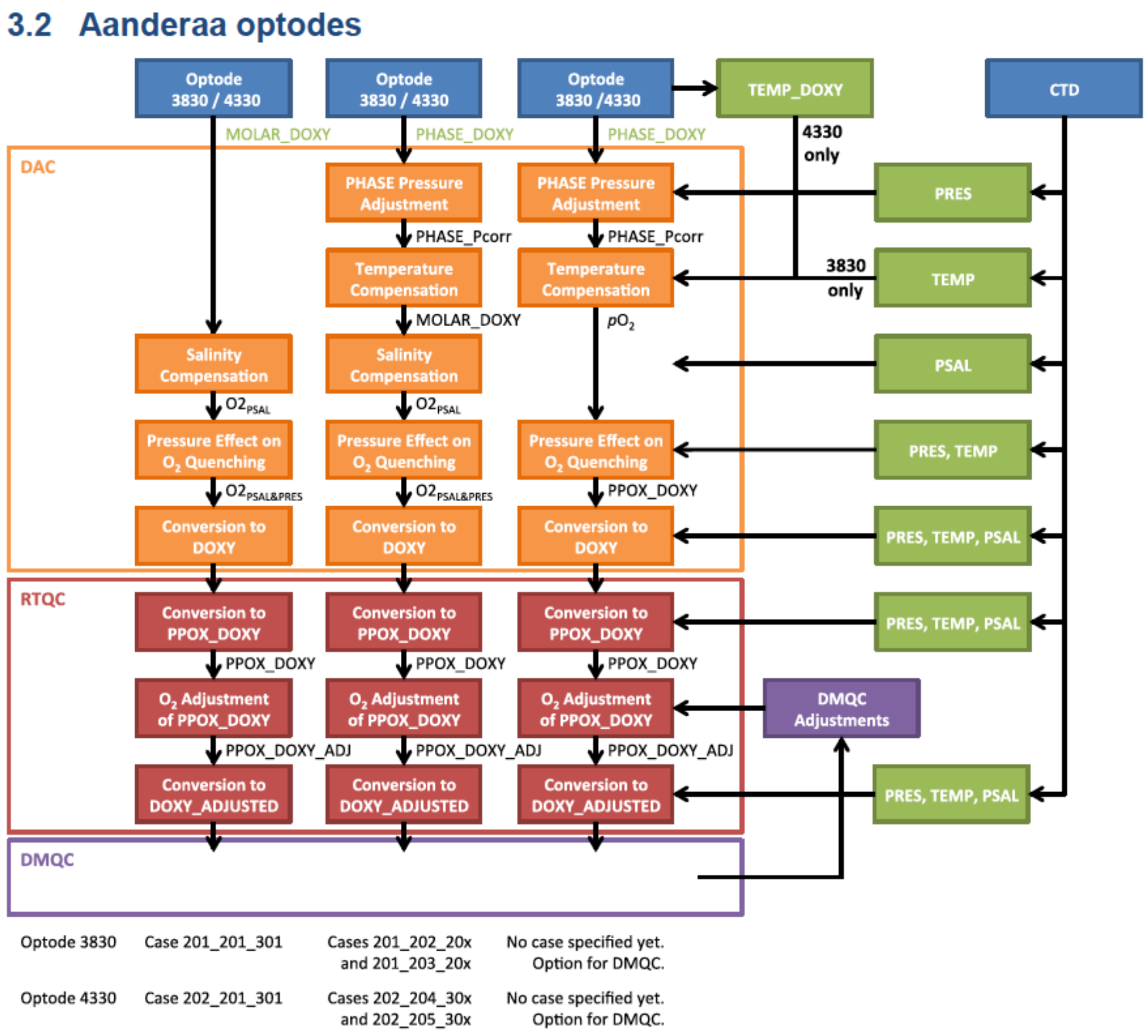

Data format and data management
ARGO-O2 processing manual

- Define how to compute DOXY from raw data recorded and transmitted by the sensor
- **First part details the scientific basis** of the oxygen measurements and computation, describe the different sensors and associated calibration equations
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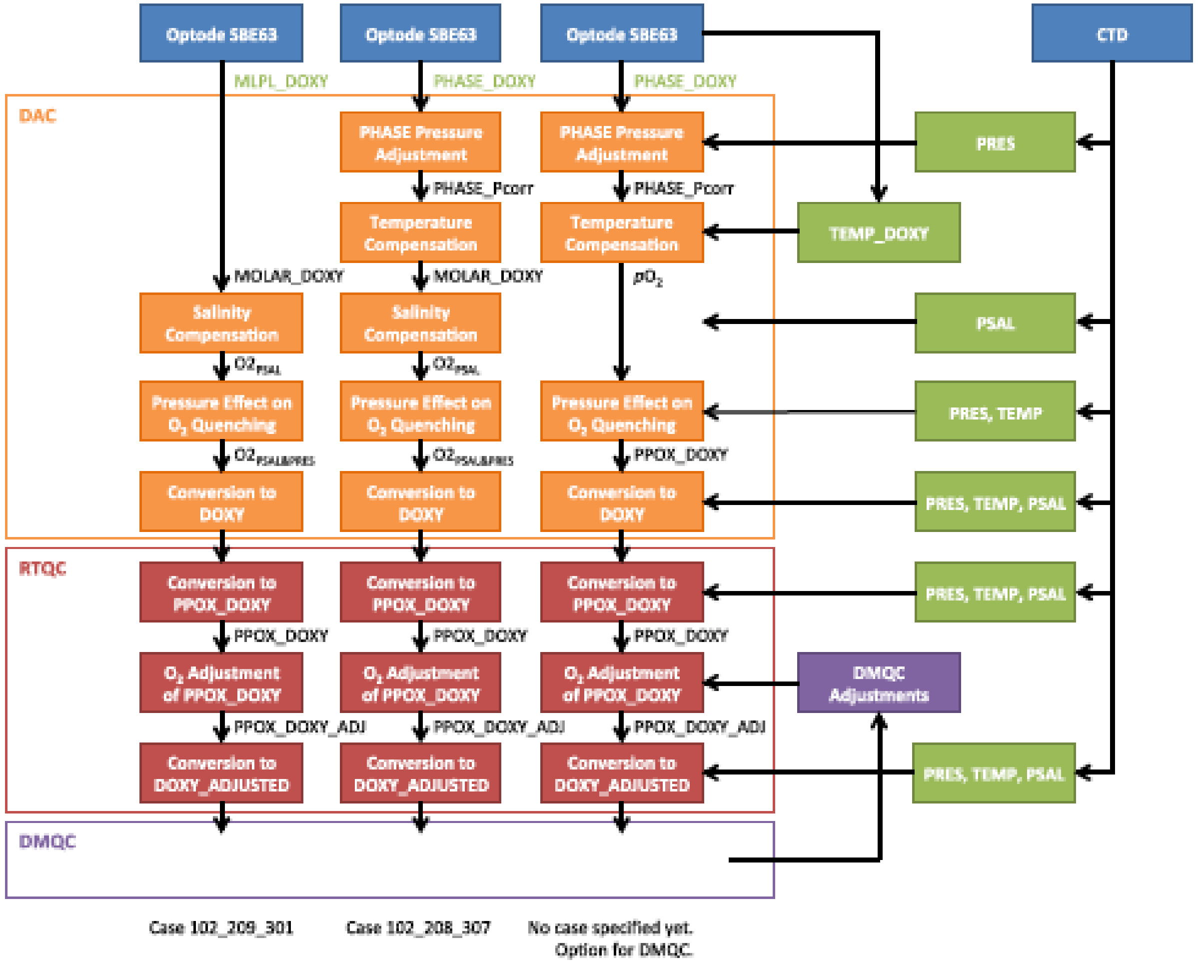
3.1 Seabird sensors

For the SBE43 IDO electrochemical sensor, there currently exists only one processing route (see §4.1.1). For the SBE63 optode with multiple processing paths, the recommended processing is illustrated below.



CASE_*SensorModelId_InputParamId_ComputationMethodId*

Sensor Model		Input parameter										
		201	202	203	204	205	206	207	208	209	210	211
		MOLAR_DOXY	BPHASE_DOXY	DPHASE_DOXY	TPHASE_DOXY	C1PHASE_DOXY & C2PHASE_DOXY	VOLTAGE_DOXY	FREQUENCY_DOXY	PHASE_DELAY_DOXY	MLPL_DOXY	LED_FLASHING_COUNT_DOXY & COUNT_DOXY	COUNT_DOXY
101	SBE43_IDO						**206 (7.2.1)**					
102	SBE43F_IDO							**206 (7.2.2)**				
103	SBE63_OPTODE								**307 (7.2.5)** 308 (7.2.6)	**301 (7.2.7)** 309 (7.2.8)		
201	AANDERAA_OPTODE_3830	**301 (7.2.11)**	**202 (7.2.12)** **204 (7.2.13)** 302 (7.2.14) 304 (7.2.15)	**202 (7.2.16)** **204 (7.2.17)** 302 (7.2.18) 304 (7.2.19)								
202	AANDERAA_OPTODE_4330 AANDERAA_OPTODE_4330F	**301 (7.2.22)**			202 (7.2.23) 203 (7.2.24) 204 (7.2.25) 205 (7.2.26) 302 (7.2.27) 303 (7.2.28) **304 (7.2.29)** **305 (7.2.30)**	202 (7.2.31) 203 (7.2.32) 204 (7.2.33) 205 (7.2.34) 302 (7.2.35) 303 (7.2.36) **304 (7.2.37)** **305 (7.2.38)**						
301	ARO_FT										**401 (7.2.40)**	

Table 5: Configurations for the calculation of DOXY as function of the sensor model and input parameter. The recommended configurations are highlighted in bold.

CASE_SensorModelId_InputParamId_ComputationMethodId

Sensor model			O₂ response model (~Type of calibration sheet)									
				optical sensors								
			electro-chemical sensors	internal calculation	20-term polynomial	28-term polynomial	28-term polynomial + 2 points adjustment	(old) Stern-Volmer	SVU Stern-Volmer	SVU Stern-Volmer + 2 points adjustment	SBE Stern-Volmer	JAC Stern-Volmer
Sensor model	101	SBE43_IDO	**206_206 (7.2.1)**									
	102	SBE43F_IDO	**207_206 (7.2.2)**									
	103	SBE63_OPTODE		**209_301 (7.2.7)**							**208_307 (7.2.5)**	
				209_309 (7.2.8)							208_308 (7.2.6)	
	201	AANDERAA_OPTODE_3830		**201_301 (7.2.11)**	**202_202 (7.2.12)**			**202_204 (7.2.13)**				
					202_302 (7.2.14)			202_304 (7.2.15)				
					203_202 (7.2.16)			**203_204 (7.2.17)**				
					203_302 (7.2.18)			203_304 (7.2.19)				
	202	AANDERAA_OPTODE_4330 or AANDERAA_OPTODE_4330F		**201_301 (7.2.22)**		204_202 (7.2.23)	204_203 (7.2.24)		204_204 (7.2.25)	204_205 (7.2.26)		
						204_302 (7.2.27)	204_303 (7.2.28)		**204_304 (7.2.29)**	**204_305 (7.2.30)**		
						205_202 (7.2.31)	205_203 (7.2.32)		205_204 (7.2.33)	205_205 (7.2.34)		
						205_302 (7.2.35)	205_303 (7.2.36)		**205_304 (7.2.37)**	**205_305 (7.2.38)**		
	301	ARO_FT										**210_401 (7.2.40)**

Table 6: Configurations for the calculation of DOXY as function of the sensor model and O2 response model. The recommended configurations are highlighted in bold.

	/100)+D3*S]; Ts2=ln[(298.15-TEMP)/(273.15+TEMP)]; Pcorr=1+((Pcoef2*TEMP+Pcoef3)*PRES)/1000; DOXY=O2/rho, where rho is the potential density [kg/L] calculated from CTD data
PREDEPLOYMENT_CALIB_COEFFICIENT	Spreset=*0*; Pcoef1=*Pcoef1*, Pcoef2 =*Pcoef2*, Pcoef3=*Pcoef3*; B0=*B0*, B1=*B1*, B2=*B2*, B3=*B3*; C0=*C0*; PhaseCoef0=*PhaseCoef0*, PhaseCoef1=*PhaseCoef1*, PhaseCoef2=*PhaseCoef2*, PhaseCoef3=*PhaseCoef3* ; c0=*c0*, …, c27=*c27*; m0=*m0*, …, m27=*m27*; n0=*n0*, …, n27=*n27*; ConcCoef0 = *ConcCoef0*, ConcCoef1= *ConcCoef1*; A0 = *A0*, A1 = *A1*, A2 = *A2*, A3 = *A3*, A4 =*A4*, A5 = *A5*; D0=*D0*, D1=*D1*, D2=*D2*, D3=*D3*
PREDEPLOYMENT_CALIB_COMMENT	see TD269 Operating manual oxygen optode 4330, 4835, 4831; see Processing Argo OXYGEN data at the DAC level, Version 2.2 (DOI: http://dx.doi.org/10.13155/39795)

7.2.29 CASE_202_204_304

Sensor: AANDERAA_OPTODE_4330

Sensor output: uncalibrated phase in degree TPHASE_DOXY

Calculation: Stern-Volmer conversion of raw data to oxygen concentration on umol/L with TEMP_DOXY from the oxygen sensor + pressure and salinity compensation with TEMP, PRES and PSAL from the CTD + unit conversion

Calculation input:

- PRES, PSAL and TEMP, pressure, salinity and temperature from the CTD
- TPHASE_DOXY from the oxygen sensor
- TEMP_DOXY, the temperature from the oxygen sensor
- P_{coef1}, P_{coef2}, P_{coef3}, the pressure compensation coefficients (default P_{coef1}=0.1, P_{coef2}=0.00022, P_{coef3}=0.0419)
- *B0, B1, B2, B3* and *C0* the salinity compensation coefficient (default B0 = -6.24523e-3; B1 = -7.37614e-3; B2 = -1.03410e-2; B3 = -8.17083e-3; C0 = -4.88682e-7)
- *D0, D1, D2 and D3* the pH20 computation coefficient (default D0 = 24.4543, D1 = -67.4509, D2 = –4.8489, D3 = –5.44e–4)
- S_{preset} = 0
- rho, the potential density of water [kg/L] at zero pressure and at the potential temperature computed from PRES, TEMP and PSAL (from CTD) (UNESCO, 1983 [RD3] and Millero, 1981 [RD11])
- $PhaseCoef_0$, $PhaseCoef_1$, $PhaseCoef_2$ and $PhaseCoef_3$ coefficients provided in the optode calibration certificate. If they are not, then uses *PhaseCoef0=0, PhaseCoef1=1, PhaseCoef2=0, PhaseCoef3=0* (see §9.2.2.3 in ANNEX A for an example).
  For calibrations after Apr. 2017, PhaseCoef0=0 must be verified by recalculation of the calibration data, as it may not figure on the calibration certificate.
- *ci* coefficients provided in the optode calibration certificate (see §9.2.2.3 in ANNEX A for an example)

Calculation output:

- DOXY in umol/kg

Equations:

$$Phase\_Pcorr = TPHASE\_DOXY + P_{coef1} \times PRES/1000$$

$$CalPhase = PhaseCoef_0 + PhaseCoef_1 \times Phase\_Pcorr + PhaseCoef_2 \times Phase\_Pcorr^2 + PhaseCoef_3 \times Phase\_Pcorr^3$$

$$MOLAR\_DOXY = [((c_3 + c_4 \times TEMP\_DOXY)/(c_5 + c_6 \times CalPhase)) - 1]/K_{SV}$$

$$K_{SV} = c_0 + c_1 \times TEMP\_DOXY + c_2 \times TEMP\_DOXY^2$$

$$O2_{PSAL\&PRES} = MOLAR\_DOXY \times [S_{corr}] \times [P_{corr}]$$

$$S_{corr} = A(TEMP, PSAL, S_{preset}) \times e^{\left((PSAL)\times(B0+B1.T_s+B2.T_s{}^2+B3.T_s{}^3)+C_0\times(PSAL^2)\right)}$$

$$A(TEMP, PSAL, S_{preset}) = \frac{1013.25 - pH_2O(TEMP, S_{preset})}{1013.25 - pH_2O(TEMP, PSAL)}$$

$$pH_2O(TEMP, S] = 1013.25 \times e^{\left(D_0 + D_1\times\left(\frac{100}{TEMP+273.15}\right) + D_2\times ln\left(\frac{TEMP+273.15}{100}\right) + D_3\times S\right)}$$

$$P_{corr} = 1 + \frac{(P_{coef2} \times TEMP + P_{coef3}) \times PRES}{1000}$$

$$T_s = ln((298.15 - TEMP)/(273.15 + TEMP))$$

$$DOXY[umol/kg] = O2_{PSAL\&PRES}/rho$$

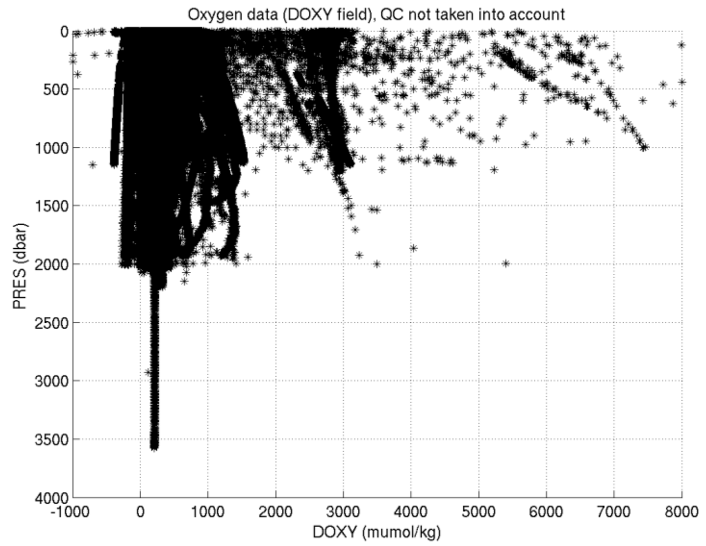
Float sensor information	
Name	**Value**
SENSOR	OPTODE_DOXY
SENSOR_MAKER	AANDERAA
SENSOR_MODEL	AANDERAA_OPTODE_4330
SENSOR_SERIAL_NO	*Sensor serial number*

Float parameter information	
Name	**Value**
PARAMETER	TPHASE_DOXY
PARAMETER_SENSOR	OPTODE_DOXY
PARAMETER_UNITS	degree
PARAMETER_ACCURACY	??
PARAMETER_RESOLUTION	??
Float calibration information	
Name	**Value**
PREDEPLOYMENT_CALIB_EQUATION	none
PREDEPLOYMENT_CALIB_COEFFICIENT	none
PREDEPLOYMENT_CALIB_COMMENT	Phase measurement with blue excitation light; see TD269 Operating manual oxygen optode 4330, 4835, 4831

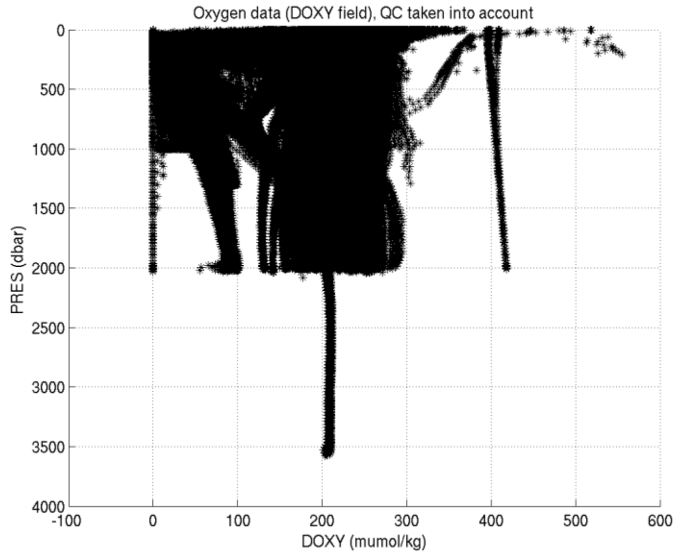
Float parameter information	
Name	**Value**
PARAMETER	DOXY
PARAMETER_SENSOR	OPTODE_DOXY
PARAMETER_UNITS	umol/kg
PARAMETER_ACCURACY	10
PARAMETER_RESOLUTION	0.1
Float calibration information	
Name	**Value**
PREDEPLOYMENT_CALIB_EQUATION	Phase_Pcorr=TPHASE_DOXY+Pcoef1*PRES/1000; CalPhase=PhaseCoef0+PhaseCoef1*Phase_Pcorr+PhaseCoef2*Phase_Pcorr^2+PhaseCoef3*Phase_Pcorr^3; MOLAR_DOXY=[((c3+c4*TEMP_DOXY)/(c5+c6*CalPhase))-1]/KSV; KSV=c0+c1*TEMP_DOXY+c2*TEMP_DOXY^2; O2=MOLAR_DOXY*Scorr*Pcorr; Scorr=A*exp[PSAL*(B0+B1*Ts+B2*Ts^2+B3*Ts^3)+C0*PSAL^2]; A=[(1013.25-

Real-time QC tests
What is already existing

- **Automatic tests done on real time data to assess QC flag to DOXY**
- QC flag = 0 : no QC performed
- QC flag = 1 : good data
- QC flag = 2 : probably good data
- QC flag = 3 : probably bad data
- QC flag = 4 : bad data



- **Agreement of real-time QC tests for O2 data in 2012**
  - Global range test + Spike test + Gradient test + Stuck value test
  - Clear efficiency of the tests at that time
- **Need to improve those tests to better reflect the data quality (on going work)**
  - Known bias (QC=3?)
  - Need to detect sensor drift or failure



Adjustment

- Raw data= real-time data
  - DOXY: Raw O2 value computed from intermediate parameters recorded by sensor and computed from calibration equation and coefficient
  - DOXY_QC: QC flags assessed by RT QC tests

- Adjusted data
  - DOXY_ADJUSTED: O2 value that went through an adjustment process. The data are corrected (or not) of any sensor bias or drift
  - DOXY_ADJUSTED_QC
  - **Adjustment in real-time (parameter data mode='A')** based on automatic procedure, adjusted data available in real-time (**B5902269_001.nc)**

  - **Adjustment in delayed mode (parameter data mode='D')** done by a delayed mode operator, adjusted data available with some delay. Best data based on current knowledge (**BD5902269_001.nc)**

QC procedures described in two cookbooks

argo data management

Argo data management

DOI: http://dx.doi.org/10.13155/40879

Argo Quality Control Manual
For Biogeochemical Data

Version 1.0

1st March 2016

ARGO

part of the integrated global observation strategy

argo data management

Argo data management

DOI: http://dx.doi.org/10.13155/46542

Argo Quality Control Manual
for Dissolved Oxygen Concentration

Version 2.0

23th October 2018

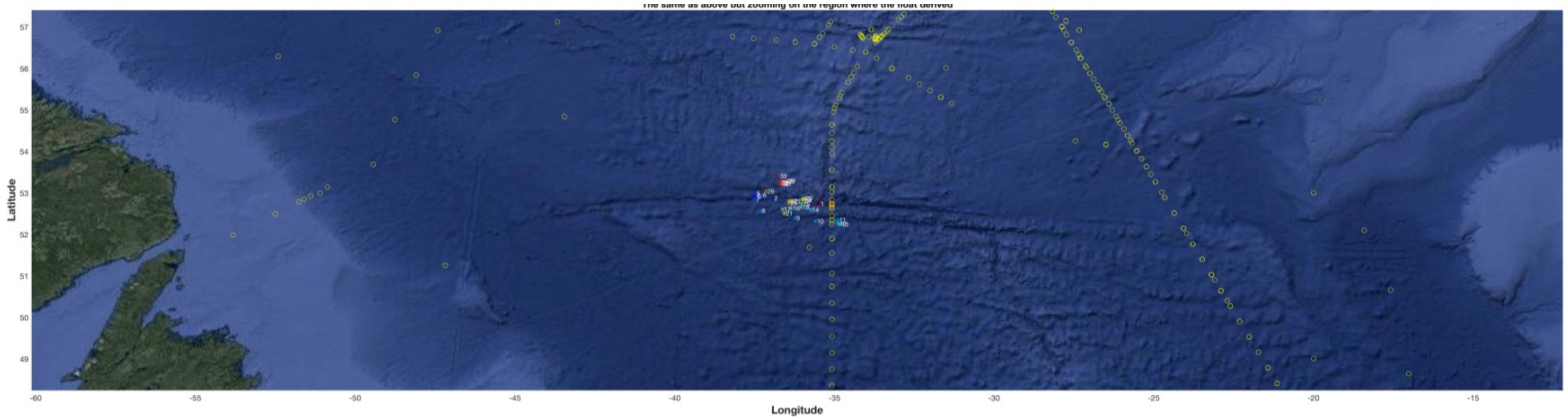
ARGO

part of the integrated global observation strategy

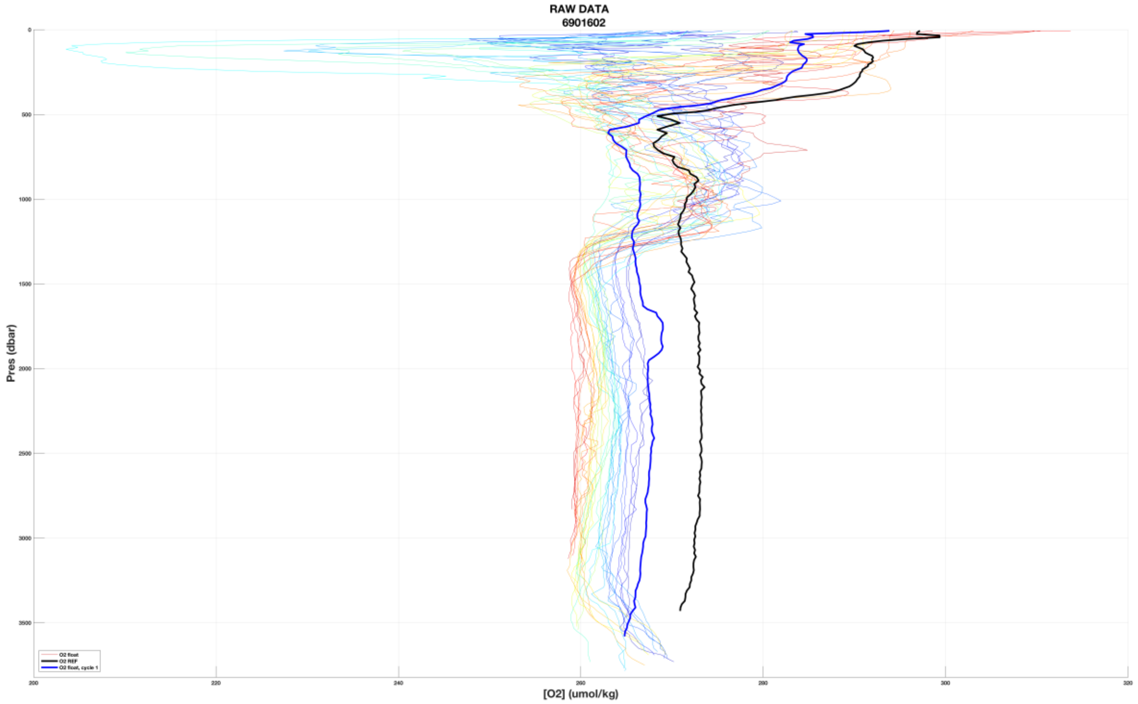
Delayed mode adjustment

- Based on reference data : WOA, ship-based calibrated profile, in air measurements
- Methods described in Takeshita et al. (2013), Johnson et al. (2015), Bittig et al. (2018), etc..
- Existing tool
  - Sage-O2 (US)
  - LOCODOX (France)

LOCODOX

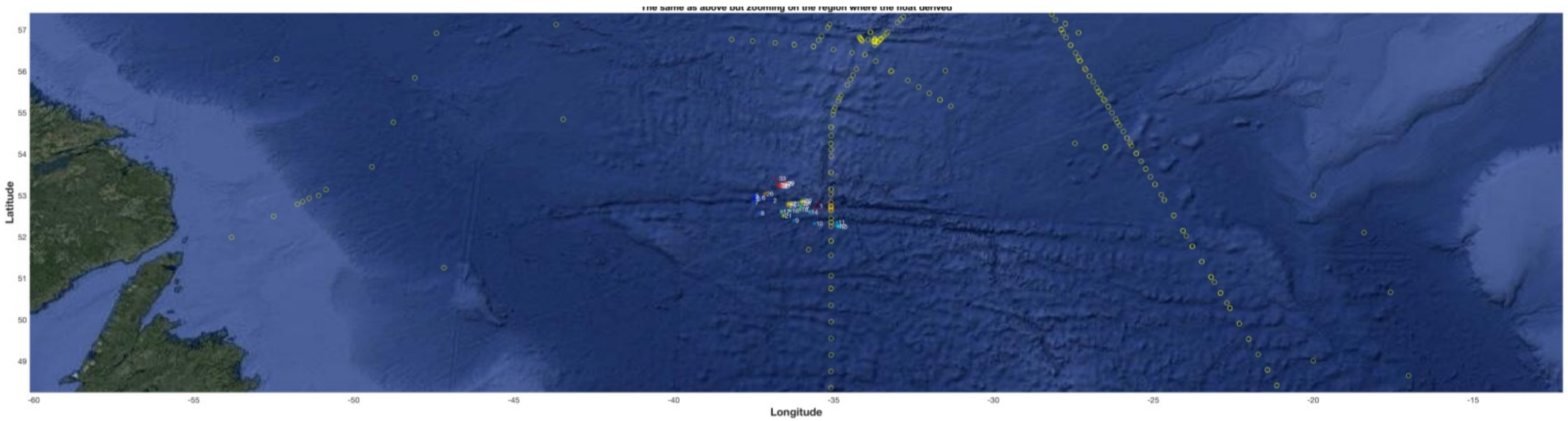


The same as above but zooming on the region where the float derived
57
56
55
54
53
52
51
50
49
Latitude
-60
-55
-50
-45
-40
-35
-30
-25
-20
-15
Longitude

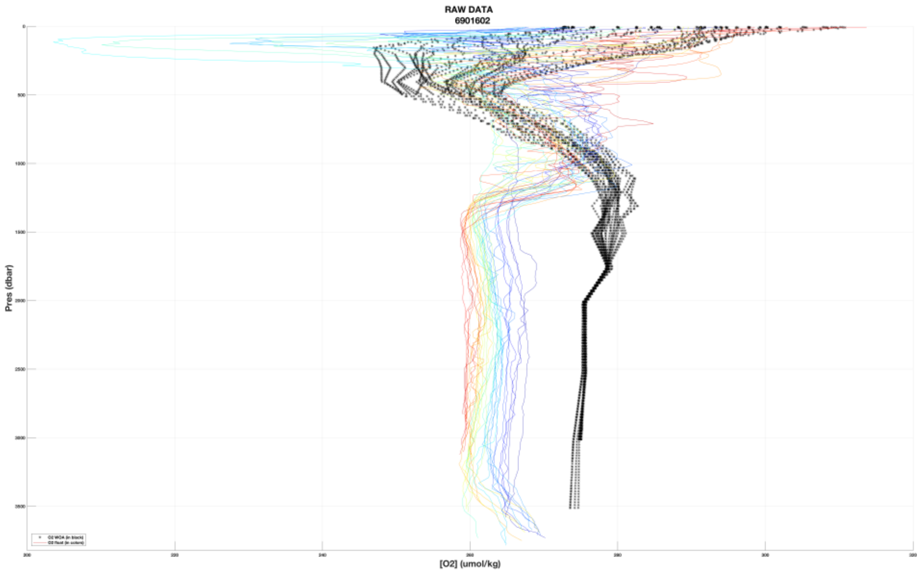


RAW DATA
6901602
0
500
1000
1500
2000
2500
3000
3500
Pres (dbar)
200
220
240
260
280
300
320
[O2] (umol/kg)
O2 float
O2 REF
O2 float, cycle 1

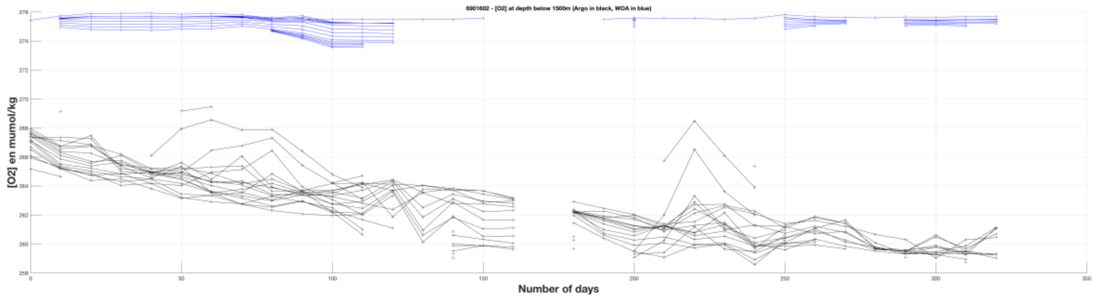
LOCODOX



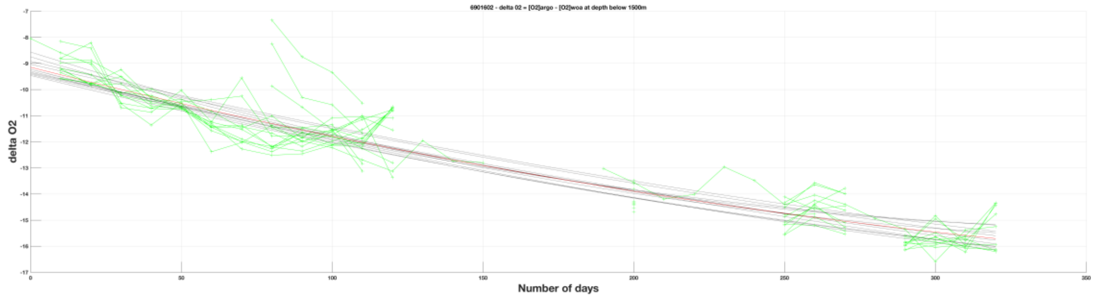
The same as above but zooming on the region where the float derived
Latitude
Longitude



RAW DATA
6901602
Pres (dbar)
[O2] (umol/kg)

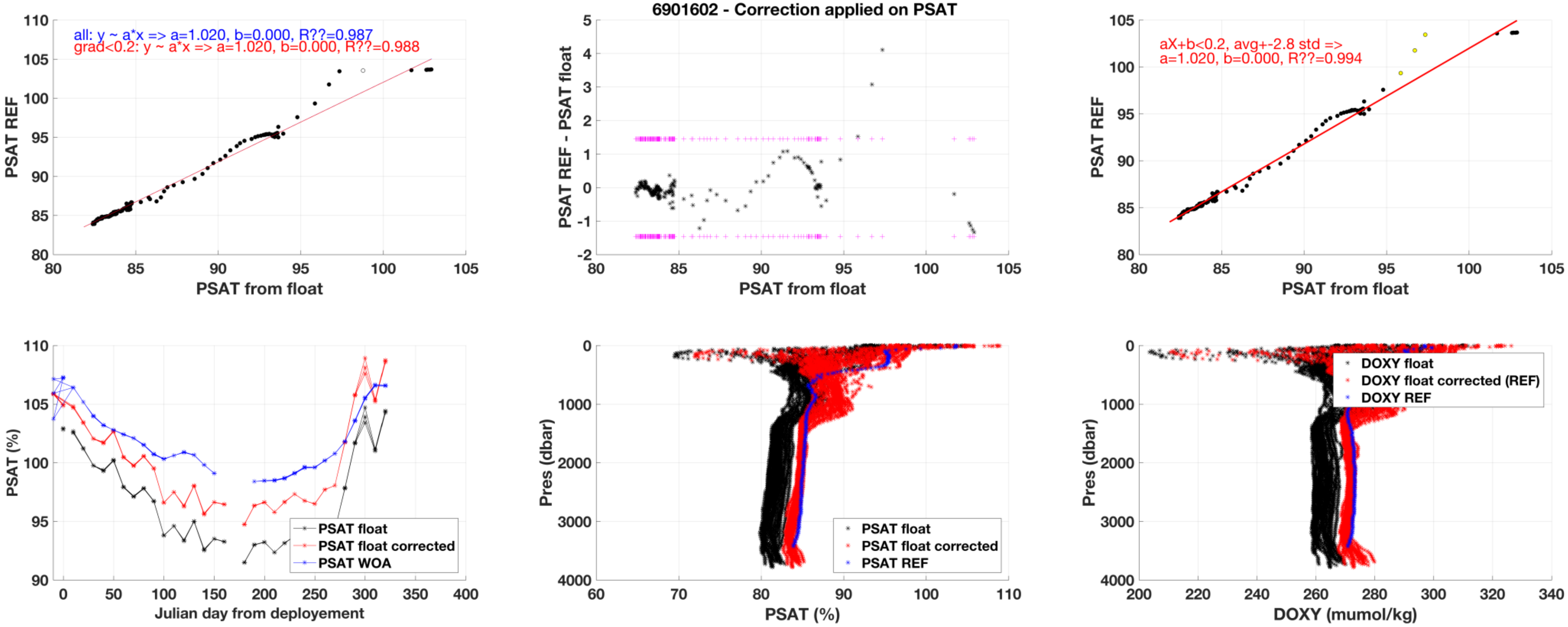


6901602 - [O2] at depth below 1500m (Argo in black, WOA in blue)
[O2] en mumol/kg
Number of days

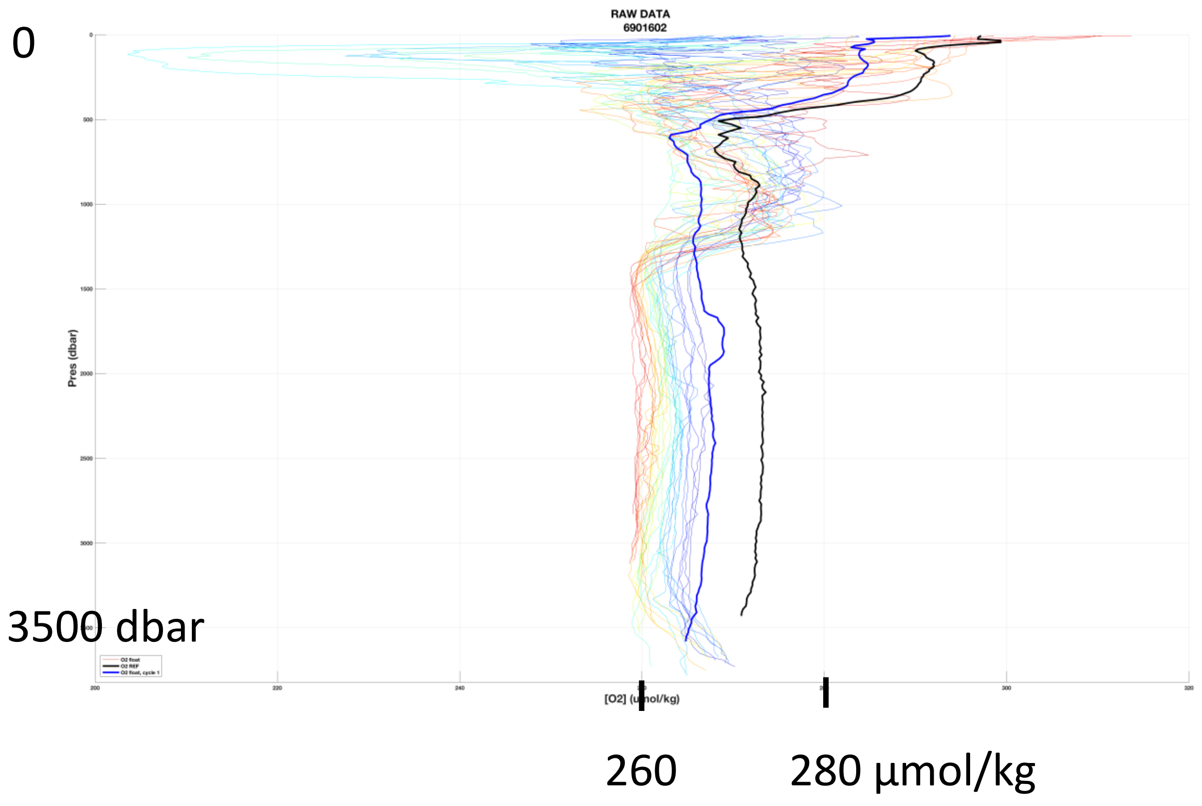


6901602 - delta 02 = [O2]argo - [O2]woa at depth below 1500m
delta O2
Number of days

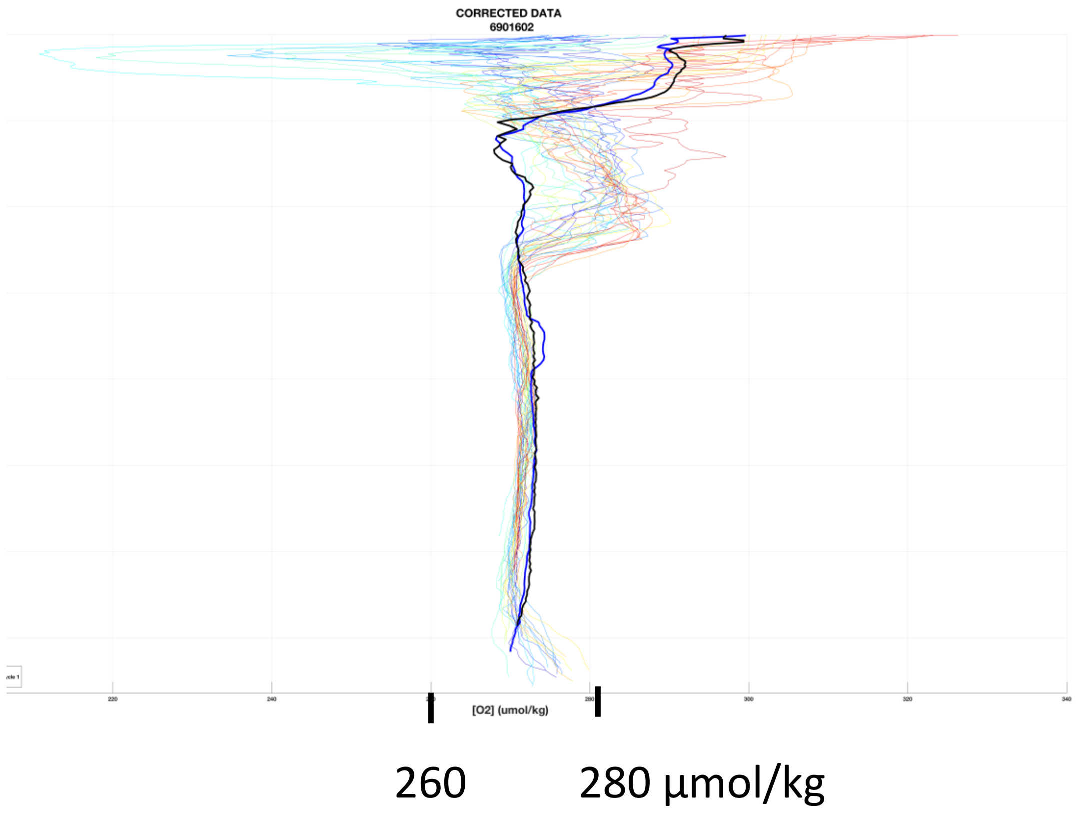
LOCODOX


all: y ~ a*x => a=1.020, b=0.000, R??=0.987
grad<0.2: y ~ a*x => a=1.020, b=0.000, R??=0.988
PSAT REF
PSAT from float
6901602 - Correction applied on PSAT
PSAT REF - PSAT float
aX+b<0.2, avg+-2.8 std =>
a=1.020, b=0.000, R??=0.994
PSAT (%)
Julian day from deployement
PSAT float
PSAT float corrected
PSAT WOA
Pres (dbar)
PSAT REF
DOXY float
DOXY float corrected (REF)
DOXY REF
DOXY (mumol/kg)

LOCODOX



0
RAW DATA
6901602
Pres (dbar)
3500 dbar
[O2] (umol/kg)
260
280 µmol/kg



CORRECTED DATA
6901602
[O2] (umol/kg)
260
280 µmol/kg

Real-time adjustment

- Need to be implemented
- Based on last estimate of DM adjustment
  - This will be tested for and discussed at the next ADMT meeting
- Based on in air measurement
  - Still need to work on that, in particular the correction in the deep layers
- Based on WOA
  - Not very satisfactory