



TECHNICAL NOTE

Issue 1.1
21/10/2020

Technical note for the implementation of the Real Time Quality Control of dissolved oxygen concentration by TAC

Change record

Issue	date	§	Description of change	Author
1.0	02/07/2020	all	Creation of the document	V. Racapé, J. E. Nilsen, H. Vindenes, V. Lien
1.1	21/10/2020		section 3 and 4 update to follow https://archimer.ifremer.fr/doc/00645/75704/	V. Racapé



This document details in depth the oxygen RTQC procedure for its implementation at the TAC level. The procedure is created to clean-up the database of coarse values minimizing the number of alerts to be viewed pending the more sophisticated REP step. The document is organized like this :

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Please, consider our recommendations regarding test application. The more eyes and experts there are, the faster we validate the RTQC procedure and improve data quality.

If you have any questions, comments or suggestions to improve this procedure, please contact us (virginie.racape@ifremer.fr, jan.even.oeie.nilsen@hi.no).



1. OXYGEN parameter name and unit

Oxygen observations come from various instruments or sources that's why dissolved oxygen concentration is defined either in ml/l (DOX1), or in mmol/m³ equivalent to µmol/l (DOXY), or in µmol/kg (DOX2 and DOX2_ADJUSTED) (Table 1). It is very important to keep oxygen data in the original format, that's mean:

ONE instrument = ONE unit as it is given by the provider

All thresholds are defined in ml/l, µmol/l and µmol/kg considering an averaged potential density of seawater of 1.025 kg/l and the conversion factor of **44.6596 µmol/mL** (SCOR WG 142, Bittig et al., 2016).

Table 1: Oxygen parameter name and unit

parameter name	Unit
DOX1 (ADJUSTED)	ml/l
DOXY	mmol/m ³ eq. to µmol/l
DOX2 (ADJUSTED)	µmol/kg

2. Quality control flag scale

Table 2 : Quality control (QC) flag scale

Code	Meaning	Comment
0	No QC performed	-
1	Good data	All QC tests passed
2	Probably good data	-
3	Bad data that are potentially correctable	These data are not to be used without scientific correction
4	Bad data	Data have failed one or more of the tests
5	Value changed	Data may be recovered after transmission error
6	Not used	-



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7	Nominal value	Data were not observed but reported (e.g., an instrument target depth)
8	Interpolated value	Missing data may be interpolated from neighbouring data in space or time
9	Missing value	The value is missing

3. OXYGEN RTQC procedure

3.1. Preprocessing

Before running the RTQC procedure, it is recommended:

For oxygen variables

- To check the number of units used to define oxygen for one profile (or time series). As we keep only the original format (cf. Section 1), two different units for one profile (or time series) suggest that oxygen has been measured by two different instruments.
- To check the well definition of valid oxygen observation following x, y, z and t axis.

For associated variables (temperature, salinity and depth or pressure at least)

- To run the corresponding RTQC procedure ([von Schuckmann et al., 2010](#))

3.2. Priority rules

Rule 1 : Priority to the adjusted parameter reading for platform

Rule 2 : Adjusted or non-adjusted consistency between all parameters for platform type PF (profiling float), GL (gliders) or SM (sea mammals)

- If one parameter of one station is adjusted, all other parameters must be adjusted, i.e. all parameters are defined by <PARAM_ADJUSTED>
- if <PARAM_ADJUSTED> is empty with <PARAM_ADJUSTED_QC> \neq Filled Value, the sensor cannot be adjusted. Don't use <PARAM>.

Rule 3 : Priority to vertical level <PRES>, that is the measured variable.

- If <PRES> and <DEPH> are available, used <PRES>
- If <PRES> is missing or empty, used <DEPH>



3.3. RTQC procedure

Each oxygen parameter (Table 1) must be checked by the RTQC procedure as an independent variable before integrating the Copernicus distribution.

The RTQC procedure, detailed below, gathers 3 tests together regarding metadata qualification and 9 tests together regarding oxygen qualification. Their applications depend on data and instrument/platform type (Table 3).

Table 3 : Applicable RTQC tests by platform type: Bottle (BO), CTD-O2 (CT), Mooring (MO), Mini Log (ML), Profiling float (PF), Ferry Box (FB), gliders (GL), Sea Mammals (SM) .

		PROFILE (PR)			TIME SERIES (TS)	
Application order	Platform type RTQC test	BO	CT, MO, ML, SM	PF*, GL*	FB, MO	BO
METADATA QUALITY CONTROL						
1	Impossible date test	X	X		X	X
1	Impossible location test	X	X		X	X
2	Missing value test	X	X	X	X	X
3	Land point test	X	X	X	X	X
OXYGEN DATA QUALITY CONTROL						
4	Negative pressure test	X	X		X	X
5	Metadata & hydrological QC test	X(dox2)	X(dox2)		X(dox2)	X(dox2)
6	Stuck Value test		X		X	
7	Regional Range test	X	X	X	X	X
8	Global Range test	X	X		X	X
9	Spike & Gradient test		X		X	
10	Saturation test	X	X	X	X	X
11	Flow test				X(FB)	

* Profiling floats as well as gliders follow ARGO recommendations with specific RTQC procedure documented in Thierry, Bittig et al. (2018) (<http://dx.doi.org/10.13155/46542>). The regional range test and the saturation test completes their internal procedure and are applied on profiling floats in delayed mode. The upper limit of the saturation test is also applied on profiling floats with real time oxygen data mode.



Saildrone (SM) is a new platform and needs feedback before integrating the table 3.

3.3.1. Impossible date and location test

The test requires that observation date and time are included in the specific range:

- Date no greater than today
- Hour in range 0 to 23
- Minutes in range 0 to 59
- Latitude in range -90 to 90
- Longitude in range -180 to 180

Actions

- If either <TIME> fails the test, then <TIME_QC> is marked as bad (QC=4).
- If <TIME> variable is missing, the test fails and passes to the next
- If either <LATITUDE> or <LONGITUDE> fails the test, then <POSITION_QC> is marked as bad (QC=4). Please, make sure that coordinates are defined with the good range (-180 to 180E, -90 to 90N).
- If <LATITUDE> or <LONGITUDE> are missing, the test fails and passes to the next

3.3.2. Land point test

Erroneous positioning data is not uncommon. Positions have been tested against both ETOPO2 elevation data and the Global Self-consistent Hierarchical High-resolution Shorelines (GSHHS) dataset (Wessel et al., 1996).

A 6 arc-minute global mask for near coast regions was created by detecting cells with any GSHHS full resolution coastline inside. The remaining cells are divided into two more masks, one for offshore and one for inland regions, with the aid of ETOPO2 elevation data. Some manual checking and editing of the latter two masks were done to ensure the robustness of these three masks.

For each file, as a first step the offshore mask is used to exclude lon/lat positions from further testing. Next, the inland mask is used to flag positions clearly inland from the coastline (QC=4). Then, full resolution GSHHS lon/lat (WGS84) coastline polygons for the geographical region covered by the remaining data are extracted (using the `m_map` package in Matlab; Pawlowicz, R., 2019). If these positions are widespread or many, clustering or simple longitude splitting of positions into several separate regions, is done to reduce computational load. Finally, each cluster is tested for the existence of positions within a land polygon (QC=4; see Figure 1).

Furthermore, flagged positions closer to the coastline than the resolution of the coastline, i.e., nearer than the distance between any of the two nearest coastline segments, are flagged as 'probably good data' (QC=2). It is found that the resolution of the coastline vector-data is the best indicator for coastline precision. The possibility of loss of sign or 'W' on longitudes or 'S' on latitudes, is not investigated.

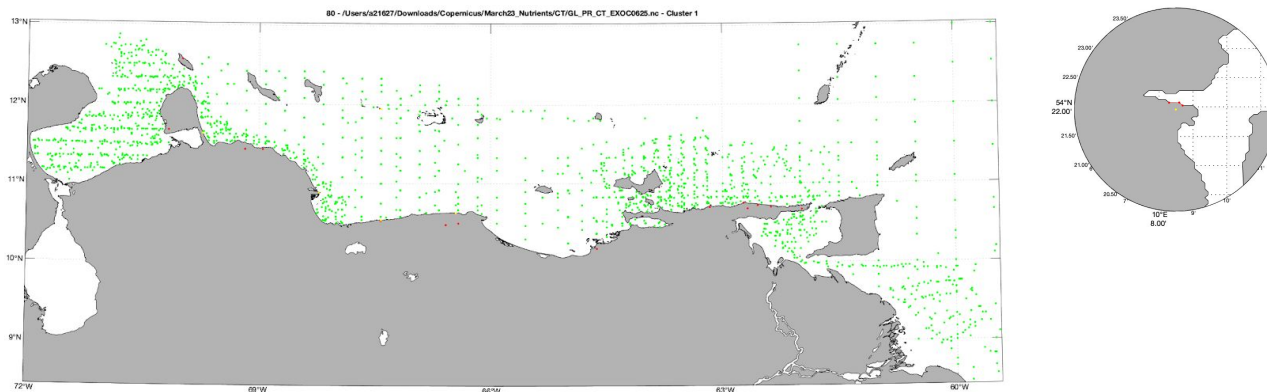


Figure 1: Example of the detection of on-land positions. a) Using GSHHS coast dataset on-land positions (red dots) and near coast 'probably good data' (yellow dots) are detected and flagged. b) Example showing the detection method for probably good positions, with nearest coastline points and line segments in red.

The test is shared by IMR (Institute of Marine Research) via the Even Nielsen's github: <https://github.com/evenrev1/evenQC>. Information to run the test is available in the script directly.

3.3.3. Missing value test

This test checks for missing values, usually called Fill Values in netcdf file. Any data matching this test should result in a bad value flag QC = 9 whereas data should have a flag QC different from 9.

3.3.4. Negative pressure test

The test checks that the oxygen measurement is carried out in the water column. The test checks thus if observations are associated with a pressure or depth greater than or equal to 0 (dbar or meter).

Actions

- If <PRES(_ADJUSTED)> or <DEPH> is strictly less than (<) 0 then <DOX#_QC> is marked as bad (QC=4).
- If vertical level variable is missing, the test fails and passes to the next

3.3.5. Metadata and hydrological QC test

The test applies on profile with oxygen concentration expressed in $\mu\text{mol/kg}$. It checks that oxygen concentration has been converted with valid temperature, salinity and pressure, in other terms if <TEMP>, <PSAL> or <PRES> used for conversion is not qualified as doubtful (QC=3), or bad (QC=4) or with a Filled Value (QC = 9 or Filled Value).



Actions

- If temperature or salinity or vertical level is flagged as doubtful (QC=3), then $\langle \text{DOX2}(_ \text{ADJUSTED})_ \text{QC} \rangle = 3$
- If temperature or salinity or vertical level is flagged as bad (QC=4) or as missing (QC=9), then $\langle \text{DOX2}(_ \text{ADJUSTED})_ \text{QC} \rangle = 4$
- If one of the essential variables for the oxygen conversion into $\mu\text{mol/kg}$ (temperature, salinity or vertical level) is missing, the test fails and passes to the next.

Actions for bottle

- Regarding bottle sampling, if temperature or salinity is missing, the QC flag of $\langle \text{DOX2} \rangle$ in $\mu\text{mol/kg}$ is set to 2 “probably good data”. The bottle specification is due to the difference of the sampling resolution between bottles (low) and CTD (high). Salinity and temperature measurements from CTD are sometimes used to convert BGC parameters as oxygen from bottles into $\mu\text{mol/kg}$.

Additional comment regarding bottle

- Be careful with bottle data set. Because observations measured at the same level are not always collected in the same bottle or cast, providers write one line for one bottle or cast. As a consequence, vertical level is duplicate in the file and temperature and salinity are not in the same line. Please, remove duplicates if it is possible. This is not user-friendly.

3.3.6. Stuck value test

This test checks whether the values of N consecutive measurements are identically the same. The effect is to comment out periods of sensor malfunction. The value of N depends on the data type (PR or TS) and on the data sampling rate or the sensor acquisition (Table 4).

Vertical profile

For profile, N is fixed at 20 consecutive observations.

As observations coming from various instruments, platforms or sources, there are high heterogeneity in vertical sampling resolution (more or less than mixed layer depth, one point every 0.5 m or 20 m depth in the subsurface against 1 point every 500 m below 1000 m depth, ...) that returned lot of false detection. To have an automatic application with large success, a profile is checked if and only if there are more than 20 consecutive observations measured over a minimum layer of 800m and if the first observation of the profile is measured between 0 and 1000m depth. These conditions are useful to avoid profiles that sample the mixed layer or the bottom only.

Conditions to run the test

- (1) N valid observations ≥ 20 subsequent measurements
- (2) the difference between the minimum and maximum level (z) of one vertical profile that includes valid observations only (z and oxygen) is strictly greater than 800 m (or dbar)
 $\max(z) - \min(z) > 800$

- (3) The first value checked by the test is measured in the first part of the water column, above 1000m (or dbar)
 $\min(z) < 1000$

Recommendation

- Round oxygen observation to nearest decimal one to detect profile as reported by Figure 2 – right panel

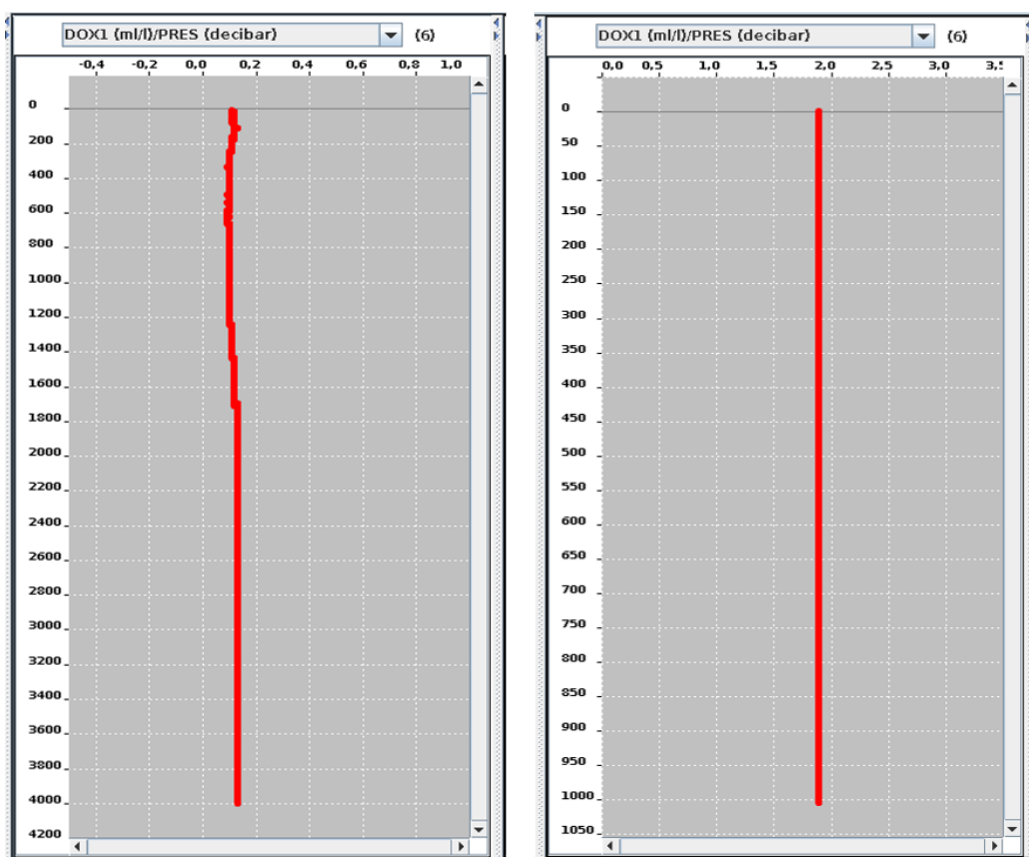


Figure 2 : Oxygen vertical profile in ml/l measured by ctd from 2 different platforms. If oxygen data is not rounded to the nearest decimal one, only the profile on the right will be detected by the stuck value test. The sensor on the left has a resolution of 0.02 masking the “stuck value” issue

Action

- If the N valid ($QC \neq 4$ or 9) and consecutive measurements fail the test, the QC flag of these data, excepting the first one, is set up to 4 “bad data”.
- If vertical level variable is missing, the test fails and passes to the next

Time series



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For time series, N is in function of the time resolution and units for oxygen measurements. For time series with oxygen concentration in ml/l , we have increased the N values by a factor 15 in order to take also into consideration the difference between two measurements acquired either with a sensor "DOX1" or with a sensor "DOXY", ($\Delta 0.01\text{ml/l} \leftrightarrow \Delta 0.446596 \mu\text{mol/l}$). This factor of 15 results from a compromise between the ratio DOXY/DOX1 of $44.6596 \mu\text{mol/ml}$ and the number of data available to apply the test. As this factor leads to a too late detection of the sensor malfunction in the case of long time resolution for oxygen in ml/l , we prefer to take into consideration the time extension as well and reduce the sensor acquisition to 12 hours (Table 4).

Table 4: N consecutive measurements for a) vertical profile and for b) time series. N is in function of time resolution (T. Res) and of oxygen units for time series

N consecutive measurements and/or time extension		
	DOXY and DOX2	DOX1
a) Vertical profile (PR)		
$N > 20$ consecutive measurements over a minimum layer of 800m with the first checked observation measured between 0 and 1000m depth		
b) Time Series (TS)		
T. Res ≤ 1 min	$N = 10$	$N = 150$
$1 \text{ min} < \text{T. Res} \leq 5 \text{ min}$	$N = 6$	$N = 90$
$5 \text{ min} < \text{T. Res} \leq 60 \text{ min}$	$N = 3$	After 12h, can be considered as bad
T. Res $> 60 \text{ min}$	$N = 2$	after 12h, can be considered as bad with a $N \geq 4$

Action

- If N valid oxygen observations from times series fail the test, these N valid oxygen observations ($\text{QC} \neq 4$ or 9) are marked as bad ($\text{QC}=4$).



- If <TIME> is marked as bad or is missing, the test fails and passes to the next

3.3.7. Regional range test

The test is built to eliminate outliers in different geographical regions. The regions and limits are based on the gridded data set from WOA18 (Garcia et al., 2018). These 1° by 1° by standard depths gridded data is provided with the sample mean, the standard deviation (std), and the sample size (N) for each bin. Thus a realistic range for measurements inside a specific bin can be estimated by the confidence interval (chosen at 99.9%) calculated using the inverse of the Student's T test at the degrees of freedom given by N. (N<5 is not accepted.) This results in estimates of realistic ranges for the bins. However, these numbers vary too much between neighbours to be used individually. Instead, larger regions encompassing some typical behaviour of ranges is sought.

There are currently 28 regions (Figure 3) each separated into 2 layers (see Table 6) are defined according to an iterative manual process considering the following aspects:

- Geography, including known hydrographic regions.
- Latitude.
- More or less homogeneous in terms of O₂ level and variability.
- Unimodal distribution of bin mean values within each region and layer, i.e. capturing one type of O₂ domain.
- A study of the vertical distribution of the bins' means and confidence intervals.
- Knowledge regarding other BGC parameters and biological processes that bind them.
- Knowledge regarding marginal sea not well characterized in WOA18.

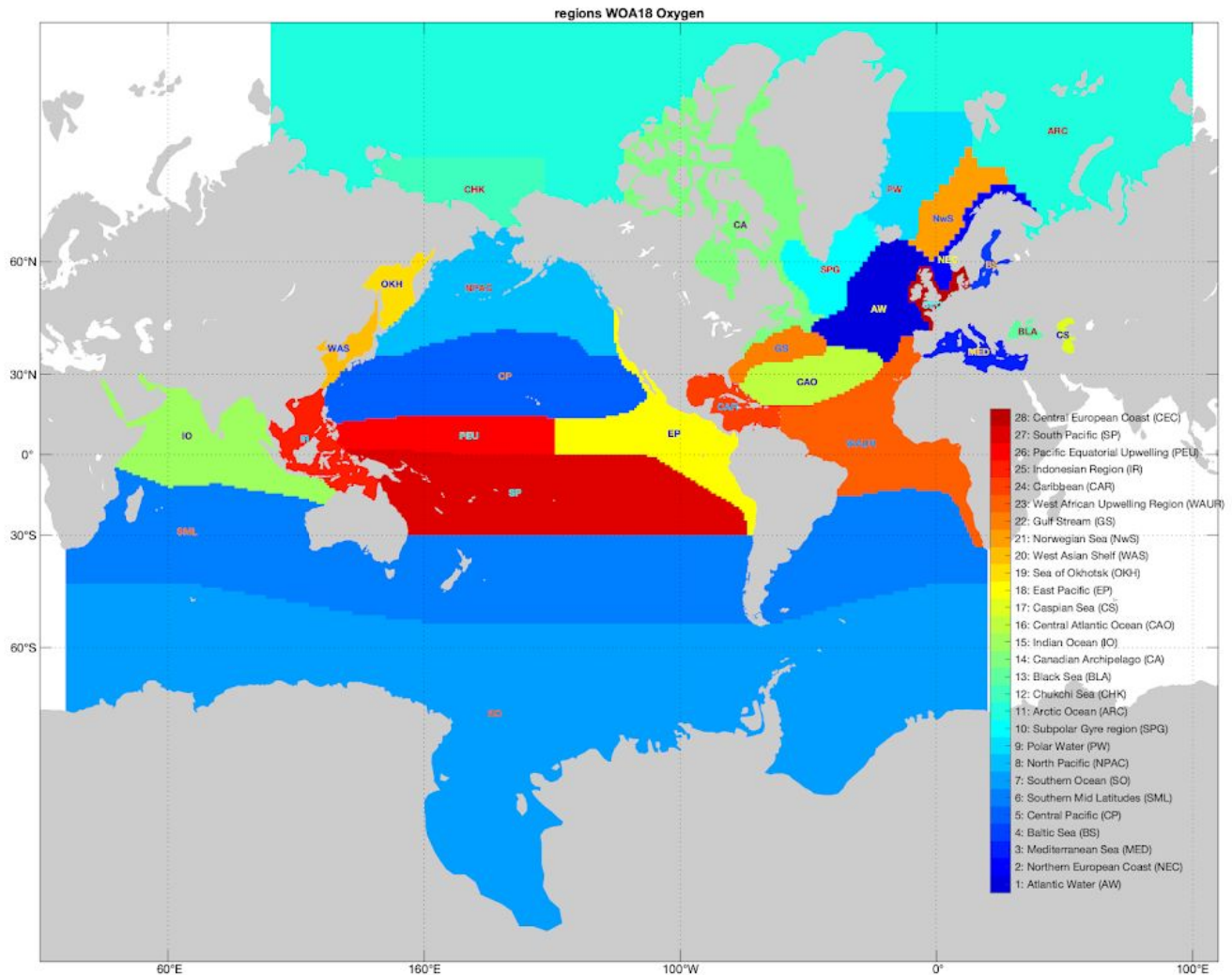


Figure 3: The current geographical regions used in the oxygen range test. The regions are also divided into two layers, with individual separation depths (see Table 6).

The initial selection of range for a region is objectively set as between the 0.1 percentile of all the region's lower ranges and the 99.9 percentile of its upper ranges. Thereafter a visual inspection of vertical profiles of boxplots of the ranges of individual bins allows for some adjustment, as well as selection of the best vertical separation of the two layers. In addition, a double check against GLODAP bottle data (Olsen et al., 2016) is done. Minimal and maximal control values are in keeping with the global range test (3.3.5) except for 1 well known area for supersaturation events: Chukchi Sea (Copdispoti and Richards, 1971; Lowry et al., 2015). In addition, and to not mask oxygen decrease in response to climate change (e.g. Bopp et al., 2013) or biological activity enhanced by nutrient discharge (Breitburg et al., 2018), each lower limit of potential interested regions is nevertheless fixed at $-5 \mu\text{mol/kg}$ (-0.1 ml/l or $-5 \mu\text{mol/l}$) (Table 6).



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Table 6 : Minimum and maximum control values defined in ml/l, $\mu\text{mol/l}$ and $\mu\text{mol/kg}$ for each 28/29 regions separated into 2 layers by the specific upper layer depth noted in brackets.

Region (upper layer depth)	Layer	(ml/l)		($\mu\text{mol/l}$)		($\mu\text{mol/kg}$)	
		low	high	low	high	low	high
Atlantic Water	upper	-0.1	9.9	-5	441	-5	430
(1600 m)	lower	3.9	7.8	174	348	170	340
Northern European Coast	upper	-0.1	10.8	-5	482	-5	470
(100 m)	lower	2.3	10.1	102	451	100	440
Mediterranean Sea*	upper	-0.1	11.5	-5	512.5	-5	500
(100 m)	lower	-0.1	11.5	-5	512.5	-5	500
Baltic Sea	upper	-0.1	13.8	-5	615	-5	600
(50 m)	lower	-0.1	13.8	-5	615	-5	600
Central Pacific	upper	-0.1	9.9	-5	441	-5	430
(900 m)	lower	-0.1	4.8	-5	215	-5	210
Southern Mid Latitudes	upper	-0.1	12.6	-5	564	-5	550
(100 m)	lower	-0.1	11.0	-5	492	-5	480
Southern Ocean	upper	-0.1	13.8	-5	615	-5	600
(100 m)	lower	-0.1	13.1	-5	584	-5	570
North Pacific	upper	-0.1	13.8	-5	615	-5	600
(100 m)	lower	-0.1	13.8	-5	615	-5	600
Polar Water	upper	2.1	13.8	92	615	90	600
(100 m)	lower	4.6	9.6	205	430	200	420
Subpolar Gyre region	upper	-0.1	12.2	-5	543	-5	530
(100 m)	lower	-0.1	11.0	-5	492	-5	480
Arctic Ocean	upper	-0.1	13.8	-5	615	-5	600
(100 m)	lower	2.5	12.4	113	554	110	540
Chukchi Sea	upper	-0.1	17.2	-5	769	-5	750
(100 m)	lower	-0.1	9.0	-5	400	-5	390
Black Sea	upper	-0.1	13.8	-5	615	-5	600
(40 m)	lower	-0.1	13.8	-5	615	-5	600
Canadian Archipelago	upper	-0.1	13.8	-5	615	-5	600



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(100 m)	lower	-0.1	13.3	-5	595	-5	580
Indian Ocean	upper	-0.1	13.8	-5	615	-5	600
(100 m)	lower	-0.1	9.2	-5	410	-5	400
Central Atlantic Ocean	upper	-0.1	7.8	-5	349	-5	340
(1400 m)	lower	3.4	7.6	154	33	150	330
Caspian Sea	upper	-0.1	13.8	-5	615	-5	600
(100 m)	lower	-0.1	13.8	-5	615	-5	600
East Pacific	upper	-0.1	13.8	-5	615	-5	600
(100 m)	lower	-0.1	9.9	-5	441	-5	430
Sea of Okhotsk	upper	-0.1	13.8	-5	615	-5	600
(100 m)	lower	-0.1	13.1	-5	584	-5	570
West Asian Shelf	upper	-0.1	13.8	-5	615	-5	600
(100 m)	lower	-0.1	9.4	-5	420	-5	410
Norwegian Sea	upper	4.8	9.2	215	410	210	400
(100 m)	lower	5.1	8.7	226	390	220	380
Gulf Stream	upper	-0.1	11.7	-5	523	-5	510
(1500 m)	lower	4.8	7.3	215	328	210	320
West African Upwelling Region	upper	-0.1	11.5	-5	513	-5	500
(1500 m)	lower	3.4	7.1	154	318	150	310
Caribbean	upper	-0.1	8.5	-5	379	-5	370
(1500 m)	lower	2.8	9.0	123	400	120	390
Indonesian Region	upper	-0.1	9.2	-5	410	-5	400
(100 m)	lower	-0.1	7.3	-5	328	-5	320
Pacific Equatorial Upwelling	upper	-0.1	8.5	-5	379	-5	370
(100 m)	lower	-0.1	9.0	-5	400	-5	390
South Pacific	upper	-0.1	9.4	-5	420	-5	410
(100 m)	lower	-0.1	10.6	-5	472	-5	460
Central European Coast	upper	-0.1	11.9	-5	533	-5	520
(100 m)	lower	-0.1	8.0	-5	359	-5	350



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*Regarding our expertise for the region, Mediterranean sea has been split into 2 subregions, the Eastern Mediterranean Sea and the Western Mediterranean Sea. The allowed ranges for dissolved oxygen are reported below:

Eastern Mediterranean Sea (lat: 28 to 45.8 lon: 16.26 to 37.0) [-0.1 8]ml/l [-5 359] μ mol/l [-5 350] μ mol/kg

Western Mediterranean Sea (lat: 28 to 45.8 lon: -5.61 to 16.25) [-0.1 9]ml/l [-5 405] μ mol/l [-5 395] μ mol/kg

Min/Max gridded product

All minimum and maximum control values, as well as the geographical definition of each region are available in the gridded product "regions_WOA18_Oxygen.mat" on the INSTACT github (https://github.com/CopernicusMarineIn situ/O2_RTQC_procedure/RegionalRangeTest). File description is available in Table 7.

Table 7 : "regions_WOA18_Oxygen.mat" file description

Name	Size	Class	Description
LAT	180 x 360	Int16	Latitude [-90 90]
LON	180 x 360	Int16	Longitude [-180 180]
REGION	180 x 360	Int16	Region index (0 = land, 1 = Atlantic Water ... to 28)
region	1 x 28	Cell	Gather all regional information together. Each cell is a structure with following fields : abbr, full, high, low, upper_layer_depth See description below (Example)

Example of Cell description for region 1 Atlantic Water

region{1}

struct with fields

abbr : 'AW'

full : 'Atlantic Water'

high : [2x3 double]

low : [2x3 double]

upper_layer_depth : 1600

region{1}.high

High limit in



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	ml/l	$\mu\text{mol/l}$	$\mu\text{mol/kg}$
upper layer	9.9	441	430
Low layer	7.8	348	340

Actions

- If an oxygen observation is strictly outside the expected range (Table 6), then its quality flag is marked as bad (QC=4).

For information:

Upper layer = all observations with a vertical level \leq upper layer depth

Lower layer = all observations with a vertical level $>$ upper layer

Index region is determined as the closest gridded point from observation with a valid index ($\neq 0$). If observation is between 2 (or more) gridded points with different index regions, check the two (all) sets of thresholds.

- Regional Range test depends on the x, y and z position of an observation and their quality flag. If $\langle \text{LATITUDE} \rangle$ or $\langle \text{LONGITUDE} \rangle$ is missing or if $\langle \text{POSITION_QC} \rangle$ equal 4, then the regional range test cannot run.

☐ RUN the Global range test

If the vertical reference is missing or marked as bad (QC=4), then the regional range test cannot run layer by layer.

☐ RUN the regional range test taking into consideration the less restrictive low limit (= the lowest low value) and the less restrictive high limit (= the highest high value) of the two layers.

3.3.8. Global range test

This test applies a gross filter on observed oxygen values (Table 5) **if and only if the regional range test cannot run due to a missing variable (latitude or longitude) or badly positioned.**

Table 5: minimum and maximum control values allowed by the global range test for oxygen variable in ml/l, $\mu\text{mol/l}$ and $\mu\text{mol/kg}$ if the regional range test cannot run.

ml/l (DOX1)	$\mu\text{mol/l}$ (DOXY)	$\mu\text{mol/kg}$ (DOX2)
[-0.1 13.8]	[-5 615]	[-5 600]

Action

- If one oxygen observation is strictly less than the minimum value control (e.g. $< -5 \mu\text{mol/kg}$) or is strictly greater than the maximum value control (e.g. $> 600 \mu\text{mol/kg}$), then its quality flag is marked as bad (QC=4).



3.3.9. Spike test and gradient test

Vertical profile

Spike and gradient tests are combined to detect single spike along vertical profile. The two tests are designed according to ARGO recommendations for profiling float (Thierry, Bittig et al., 2018). The spike test checks the difference between sequential measurements (*delta*) according to equation (1). Based on eq. (1), one measurement significantly different from adjacent ones is a spike in both size and gradient. It is definitively a spike if the difference between vertically adjacent measurements (*grad*) given by equation (2) is too steep. This second step is useful to avoid false detection in strong gradient areas like oxycline.

$$\text{delta} = | V2 - (V3 + V1) / 2 | - | (V3 - V1) / 2 | \quad (1)$$

$$\text{grad} = | V2 - (V3 - V1) / 2 | \quad (2)$$

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

Recommendations

- The test does not consider differences in depth. Keep all oxygen observations of the vertical profile, including QC9 and QC4, and check them as individual observations.
- Run the test if there are strictly more than 3 observations

Actions

- V2 measured above 500dbar (vertical level < 500) is a spike and flagged as bad (QC=4) if *delta* & *grad* are strictly greater than 50 µmol/kg (51 µmol/l or 1.1 ml/l)
- V2 measured at or below 500dbar (vertical level ≥ 500) is a spike and flagged as bad (QC=4) if *delta* & *grad* are strictly greater than 25 µmol/kg (26 µmol/l or 0.6 ml/l)
- If the vertical level observation is missing or marked as bad (QC=4), use the less restrictive thresholds of each test to validate them
delta & *grad* are strictly greater than 50 µmol/kg (51 µmol/l or 1.1 ml/l)

Time series

The test recommended by Jaccard et al., 2018 returns too many false alerts. Because the spike and gradient tests defined previously for profile do not consider differences in depth, it's easy to adapt the test for time series. Detection is not optimal but efficient.

3.3.10. Saturation test

The test checks the upper limit of dissolved oxygen content at the surface calculated from the recommendations of the SCOR WG 142 (Bittig et al., 2016). The limit is the oxygen concentration expected in a water parcel at equilibrium with air at ambient conditions of temperature, salinity, air pressure, and hydrostatic pressure. This theoretical value of 100% in surface may be overshoot by biological production and

entrainment of air through wave breaking and mixing. The upper limit of the saturation test allowed in the ocean is fixed here at 150% above the first 10 meter depth (20 m depth if no data are measured above, Table 11). While the physical and biological mechanisms cited above may lead to under-saturation events, very small oxygen saturation values at the surface are impossible in the open ocean. In this context, and to detect potential sensor biases, the saturation test applied on data collected in the open ocean checks that the dissolved oxygen content is not too far from the theoretical maximum value as well. Currently the low limit in the first 10 m depth is fixed at 50%. Figure 4 shows the mask used to separate the open ocean area to the coastal area.

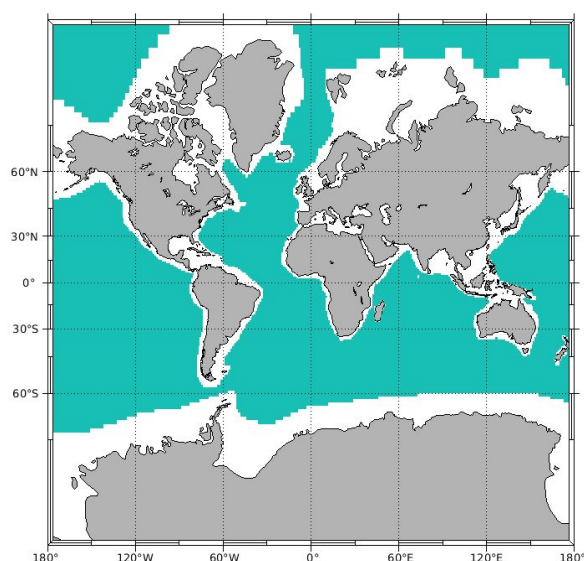


Figure 4: Water green color shows the mask used in the saturation test to separate the open ocean area from the coastal area.

Table 8: Regional control values for the saturation test

Region	Location	Oxygen saturation control value
Open Ocean	off_shelf_and_rivers_mask.mat / OFFSHELF = 1	[50-150%]

off_shelf_and_rivers_mask.mat : Useful gridded product to separate the coastal area (OFFSHELF = 0) from the open Ocean (OFFSHELF=1). The product is available here: https://github.com/CopernicusMarineInsitu/O2_RTQC_procedure/SaturationTest/

Action

- Convert oxygen concentration measured in the first 10m (dbar) (or 20m or dbar if no data are available above) into oxygen saturation following recommendations of the SCOR WG 142

Profile from Bottle (each measurement is independent of each other)

- If **ONE** observation is strictly outside the saturation ranges (table 8), then **its quality flag** is marked as bad (QC=4)

Profile from Sensor

- If observation(s) is (are) strictly higher than the oxygen saturation control values (Table 8), either it is a **spike** >> **observation quality flag** is marked as bad (QC=4) or it is due to **biofouling** (all profile that is false) >> **profile quality flag** is marked as bad (QC=4)
- If observation(s) measured in the open ocean is (are) strictly lower than the oxygen saturation control value (<50%), Either it is a **spike** >> **observation quality flag** is marked as bad (QC=4) or it is a **sensor bias** (all profile that is shifted) >> **profile quality flag** is marked as doubtful (QC=3)

Time series

- If **ONE** observation is strictly higher than the oxygen saturation control values (Table 8), then **its quality flag** is marked as bad (QC=4)
- If **ONE** observation measured in the open ocean is strictly lower than the oxygen saturation control value (<50%), then its **quality flag** is marked as bad (QC=4) (equivalent to a spike)
- If several observations measured in the open ocean is strictly lower than the oxygen saturation control value (<50%), then their **quality flag** is marked as doubtful (QC=3) (≈ suspicion of sensor bias)
- If one useful variable to position in space or time the observation or convert it into oxygen saturation is missing, the test fails and passes to the next.

3.3.11. Flow test for ferry box**not yet documented****4. Recommendations for RTQC application**

Some tests need visualization during one or two year more. Please report to table 9 and specific recommendations below for the RTQC applications.

Table 9 : Recommendation for RTQC application

		AUTOMATIC		VISUAL INSPECTION	
Application order	data type RTQC test	Profile	Time Series	Profile	Time series
METADATA QUALITY CONTROL					



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1	Impossible date test	X	X		
1	Impossible location test	X	X		
2	Missing value test	X	X		
3	Land point test	X	X		
OXYGEN DATA QUALITY CONTROL					
4	Negative pressure test	X	X		
5	Metadata & hydrological QC test	X	X		
6	Stuck Value test			X	X
7	Regional Range test	X	X	X	X
8	Global Range test	X	X		
9	Spike & Gradient test			X	X
10	Saturation test			X	X
11	Flow test				

4.1. Specific recommendation for Stuck Value test

We don't have enough feedback yet for the time series to validate definitively the test.

4.2. Specific recommendations for Regional Range test

We need feedback from regional leaders to validate definitively regional oxygen ranges. Please take extra care a) with boundaries between region 28-Central European Coast, region 22-Gulf stream and region 14-Canadian Archipelago (the NAC variability is not well represented), b) with region 2-northern European Coast and R25 -Central european coast because we have not enough feedback yet, and c) with all data measured close to the coast.

If you have recommendations for the Black Sea to refine their ranges, please tell us.

4.3. Specific recommendations for saturation test

In the absence of an easy flag scheme, this test requires the action of an operator to qualify the data. Its implementation will eliminate a lot of coarseness.

4.4. Specific recommendations for spike and gradient test

These both tests need more visualization to improve it. For information, all alerts returned by the spike and gradient test for time series has been validated but the test doesn't catch all spikes.

Give us feedback on your experiences to improve RTQC procedure. The more eyes and experts there are, the faster we validate the RTQC procedure and improve data quality.



5. At the end of the RTQC procedure

Before to be distributed, check:

- That all QC differs from zero for all oxygen variables. If RTQC procedure runs with success, that means no alerts lead to mark oxygen value as doubtful (QC=3) or bad (QC=4), then oxygen quality is marked as good data (QC = 1).
- That all oxygen variables reported for one profile are not empty with QC=9.

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