COPERNICUS MARINE ENVIRONMENT MONITORING SERVICE

IN SITU TAC
CMEMS ELEMENT

REAL TIME QUALITY CONTROL OF BIOGEOCHEMICAL MEASUREMENTS WITHIN COPERNICUS MARINE IN SITU TAC

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CHANGE RECORD

Issue	Date	§	Description of Change	Contributors	Checked By
1.0	04/09/2020	all	First draft version	Virginie Racapé, Jan Even Øie Nilsen, Haavard Vindenes, Vidar Lien, Maria Sotiropoulou, Leonidas Perivioltis, Alex Gallardo, Marta de Alfonso, Fernando Manzano, Seppo Kaitala	
1.1	26/04/2021	2.1 & 3.1 & 3.4.5	add information about EMODnet chemistry ingestion	v.racapé	
2.0	05/09/2022	all	* new product name (§1) * add RTQC information for OSAT * evolution of spike test - regional range test - saturation test	BGC team	
3.0	29/09/2023		* add RTQC procedure for Nutrients variable (Nitrate, Phosphate, Silicate) * Change INSTAC by In Situ TAC * remove table automated - not automated results application and add information in sect. 3.2	v. racapé	

CONTENTS

1. Executive summary

1.1 Products covered by this document

The following document complements the Quality Information Document CMEMS-INS-QUID-013-030-036. It applies to the biogeochemical (BGC) data collected through the Copernicus Marine Service In Situ Thematic Assembly Center (In Situ TAC) and available in the following list of MYNRT products (Table 1). BGC variables covered by this document are listed in §2.2.

Table 1 : List of In Situ TAC MYNRT products for which this document is apply

Short Description	Product code	Area	Delivery Time
Global NRT	INSITU_GLO_PHYBGCWAV_DISCRETE_MYNRT_013_030	Global NRT	daily
Arctic NRT	INSITU_ARC_PHYBGCWAV_DISCRETE_MYNRT_013_031	Arctic NRT	daily
BAL NRT	INSITU_BAL_PHYBGCWAV_DISCRETE_MYNRT_013_032	BAL NRT	daily
IBI NRT	INSITU_IBI_PHYBGCWAV_DISCRETE_MYNRT_013_033	IBI NRT	daily
Western Black Sea NRT	INSITU_BS_PHYBGCWAV_DISCRETE_MYNRT_013_034	Western Black Sea NRT	daily
Med NRT	INSITU_MED_PHYBGCWAV_DISCRETE_MYNRT_013_035	Med NRT	daily
NWS NRT	INSITU_NWS_PHYBGCWAV_DISCRETE_MYNRT_013_036	NWS NRT	daily

1.2 Summary of the results

The In Situ TAC aggregates and provides to users a large panel of BGC variables together with useful metadata information on the platforms. The main parameters available in the MYNRT In Situ TAC products are dissolved oxygen concentration, nutrients (nitrate, silicate and phosphate), chlorophyll a (chl*a*), fluorescence and pH. Figure 1 shows the evolution of the platform file number for each BGC variable available in the MYNRT In Situ TAC products since the enter into service (EIS) in 2022. One file contains all the observations from the platform.

The present document is focused on the quality control procedure for dissolved oxygen concentration, named "oxygen" hereafter, and nutrients that are subject to contract. It will be progressively updated with other BGC parameters over the years (chl*a* is planned for november 2024).

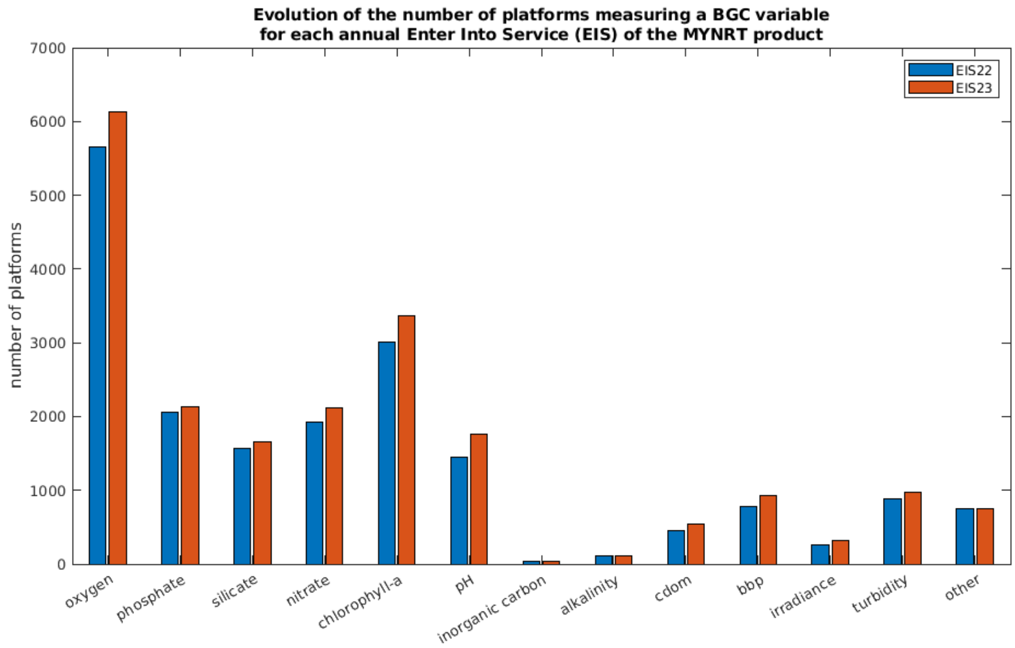

Figure 1 : Evolution of the number of platform measuring oxygen, phosphate, silicate, nitrate, chlorophyll a, pH, inorganic carbon, alkalinity, colored dissolved organic matter (cdom), particles backscattering (bbp), irradiance, turbidity and other minor BGC variables available in the MYNRT In Situ TAC products at each annual Enter Into Service (EIS) (from 2022 to 2023)

BGC variables are stored and made available within their original unit only (original units means unit in which observations were delivered). BGC variable unit depends either on the kind of sensor or chemical method used for measurement, or on the data provider (see Figures 2 and 3). The conservation of the original units supposes that one profile with 2 oxygen or nutrients parameters is measured by 2 different instruments (for example: 2 kinds of oxygen sensors).

The quality of the oxygen and nutrients observations are tested using the RTQC procedure (see §3.2) developed in collaboration by POKaPOK,IMR, Ifremer, HCMR and SYKE .

Quality control (QC) flags (see Table 5) are positioned to inform the users of the level of confidence attached to the observations. The accuracy of the in situ BGC observations depends on the platforms and sensors that have been used to acquire them (see Table 2).

1.3 Estimated Accuracy Numbers

Table 2 summarizes the accuracy of biogeochemical measurements that can be expected depending on the platforms and sensors. This is the best accuracy a user can expect for in situ data to which a quality flag “Good data” (QC=1) has been applied after the validation process. See document CMEMS-INS-QUID-013-030 -036 for more information for associated variables.

Table 2: Accuracy number for oxygen and nutrients parameter observation for the different platforms.

Data-type	**Oxygen**[1]	**Nutrients**[2] **(nitrate, silicate, phosphate)**
CTD	8 µM/5% 0.2 %	Discrete samples
PFL (profiling floats)	2% of saturation or 2mbar[3]	1 µmol/kg[4]
Moored buoy data: TRITON/TAO PIRATA/RAMA surface Subsurface	<8 µM or 5% Of concentration (Whichever is greater)	Not available
Glider	2% of saturation	1 µmol/kg[5]
Ferrybox	8 µM/5% 0.2 %	typically better 2% of the full scale. Repeatability: better than 2%

[1] Values given by a number of sensor providers, Aanderaa Instruments, Endress and Hauser

[2] Exemplary Systea MicroMac sensor. There is a limited number of different sensors available

[3] Thierry et al., 2021. Argo Quality control manual for dissolved oxygen concentration. http://dx.doi.org/10.13155/46542

[4] Johnson et al., 2023. BGC-Argo quality control manual for nitrate concentration. http://dx.doi.org/10.13155/84370

[5] Krahmann et al. OceanGlider Nitrate Standard Operating Procedure. https://oceangliderscommunity.github.io/Nitrate_SOP/README.html

2. Production Subsystem Description

2.1 Data sources

As detailed in CMEMS-INS-QUID-013-030-036, BGC data are collected through In Situ TAC, a distributed system built on the existing activities and services developed previously within the EC supported projects (MyOcean, Mersea, MFSTEP, Ferrybox, SEPRISE, etc.) and the activities carried out in the EuroGOOS Regional alliances (ROOSes) as well as EMODnet chemistry 2018 for Profile and 2021 for time series. In Situ TAC provides the interface between centers, distributing in situ measurements from national and international observing systems. It is a distributed center organized around 7 oceanographic regions: the global ocean and the 6 EUROGOOS regional alliances (see Fig. 1 of CMEMS-INS-QUID-013-030-036). In Situ TAC involves 16 partners from 9 countries in Europe.

BGC data comes from a variety of sources (platforms) including manual CTD-O_2 measurements, bottle sampling, BGC-Argo profiling floats, ferrybox systems, gliders, sea mammals, moored buoys and saildrones. Due to the diverse sources, the nature of the data, e.g. the frequency in time, the spatial pattern and the depth varies a lot. For instance, CTD-O2 measurements and bottle sampling are typically collected along a transect, with measurements for a large number of depths (a depth profile). BGC-Argo data are similar in structure as they also consist of a collection of depth profiles, but here the location of the profiles follows the drift pattern of the float. Ferrybox data and buoy data, on the other hand, are time series collected at a fixed depth. Ferrybox data are collected with a relatively high frequency (typically, one measurement per minute) along a transect, while buoy data are from a single location.

2.2 BGC variables covered by the document

2.2.1 Dissolved oxygen concentration (DOX1, DOXY, DOX2, OSAT)

Oxygen data are stored within their original unit only (original unit = unit as it is delivered by provider). Oxygen unit depends either on the kind of sensor or the chemical method used for measurements, or the data provider (Figure 2 - bottom right). Dissolved oxygen concentration is thus defined either in ml/l, or in mmol/m^3 equivalent to µmol/l, or in µmol/kg or in percent (%), that's why four parameter names unit dependent (DOX1, DOXY, DOX2, OSAT) are available in the NRT products (Table 3).

User working on the MYNRT products can easily move from one unit to another one unit using the conversion factor of 44.6596 µmol/mL, the corresponding potential temperature and salinity to get the potential density of seawater referenced to a hydrostatic pressure of 0 dbar, or the solubility of oxygen in seawater (SCOR WG 142, Bittig et al., 2016). Unit standardization is a part of the reprocessing tools available in the In Situ TAC REP product.

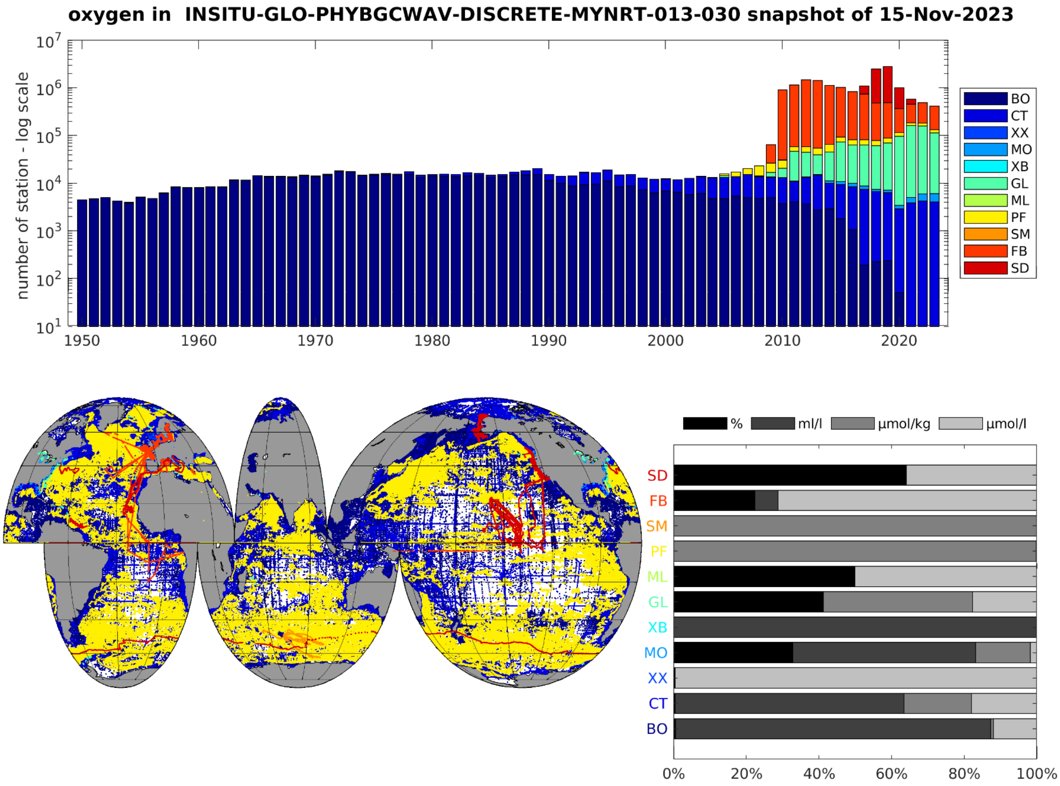

Figure 2 : Map shows the spatial distribution of profiles and time series including one oxygen data qualified by a QF flag 1 (Good data), or 2 (Probably good data), or 5 (value changed), 6 (below detection limit), or 8 (Interpolated value) at least. Oxygen data are collected either by CTD-02 (CT), or by profiling floats (PF), or by bottles (BO), or by gliders (GL), or by sea mammals (SM), or by mini-log system (ML), or by ferryboxes system (FB) or by mooring (MO), or by sail drones (SD),or by XBT sensors (XB), or by an unknown method (XX). Vertical histogram report the same distribution by year. Horizontal histogram shows the percent of profiles/time series including one oxygen with a QC 1, 2, 5, 6 or 8 in %, ml/l, µmol/l or µmol/kg per kind of platform file.

***Table 3:* Oxygen parameter names and units**

Parameter name	Unit	CF standard name
DOX1 (ADJUSTED)	ml/l	volume_fraction_of_oxygen_in_sea_water
DOXY (ADJUSTED)	mmol/m^3 eq. to µmol/l	mole_concentration_of_dissolved_molecular_oxygen_in_sea_water
DOX2 (ADJUSTED)	µmol/kg	moles_of_oxygen_per_unit_mass_in_sea_water
OSAT	%	fractional_saturation_of_oxygen_in_sea_water

Figure 2 represents the oxygen observations spatial and 1950-2023 temporal distribution as well. Most of the dissolved oxygen profiles included in the MYNRT products have been measured by bottle (BO) and CTD-O_2 (CT) during the last century and covered the global Ocean. This has progressively evolved over the last two decades with the implementation of the ARGO-O_2 profiling float network (PF). The spatial coverage of the profiling floats remains nevertheless insufficient.

2.2.2 Nutrient concentration : Nitrate (NTRA, NTAW), Silicate (SLCA, SLCW), Phosphate (PHOS, PHOW)

Nitrate, Phosphate and Silicate are the three nutrients quality controlled in real time by the In Situ TAC. As Oxygen, the nutrient data are stored within their original unit only (original unit = unit as it is delivered by provider). The nutrient unit depends either on the kind of sensor or the chemical method used for measurements, or the data provider (Figure 3 - bottom right). Nutrient observations are available either in $mmol/m^3$, equivalent to µmol/l (the mole concentration of dissolved molecules) or in µmol/kg (moles of nutrient per unit mass) that's why two parameter names unit dependent per variable (NTRA / NTAW, PHOS / PHOW, SLCA / SLCW) are available in the MYNRT products (Table 4). Except for argo nutrient data, most of the observations are provided in $mmol/m^3$ (Figure 3 - bottom right).

Figure 3 represents the spatial and 1950-2023 temporal distribution of nutrient observations as well. Nutrient measurements are essentially (if not exclusively) chemical (BO), but it is possible to find them in CTD (CT) instrument files to keep information with CTD-O_2 (CT) observations. BGC-ARGO profiling floats (PF) and GLIDER (GL) network measure nitrate only.

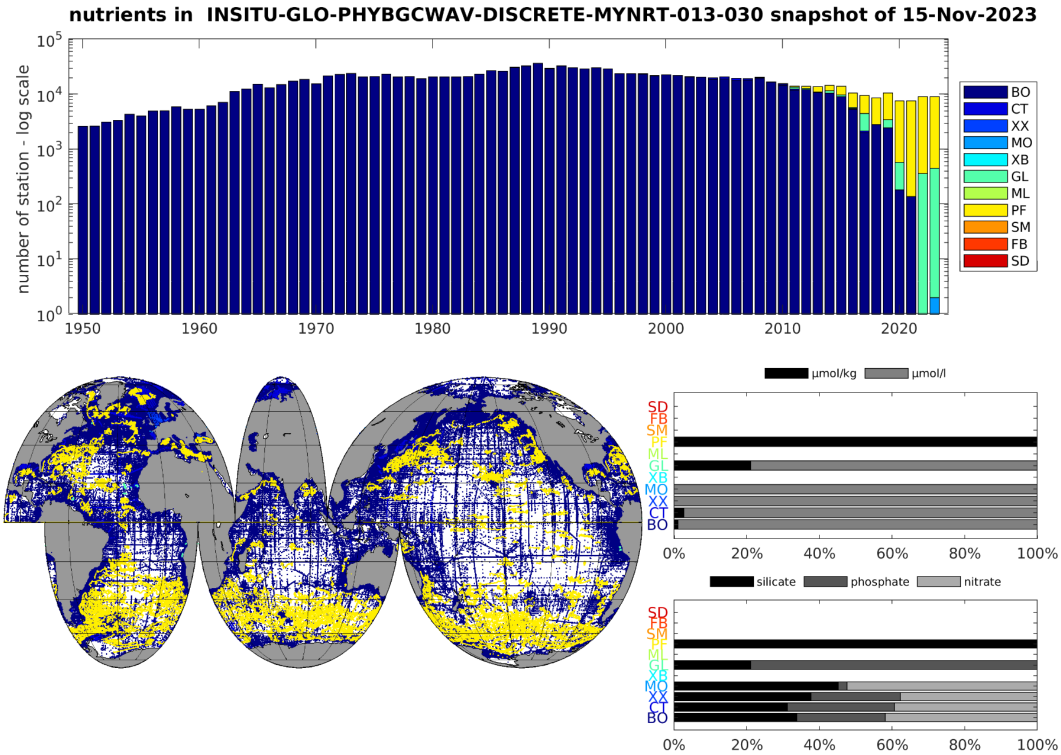

Figure 3 : Map shows the spatial distribution of profiles and time series including one silicate and/or nitrate and/or phosphate data qualified by a QF flag 1 (Good data), or 2 (Probably good data), or 5 (value changed), or 6 (below detection limit), or 8 (Interpolated value) at least. Nutrient data are collected either by CTD-02 (CT), or by profiling floats (PF), or by bottles (BO), or by gliders (GL), or by sea mammals (SM), or by mini-log system (ML), or by ferryboxes system (FB) or by mooring (MO), or by sail drones (SD), or by XBT sensors (XB), or by an unknown method (XX). Vertical histogram report the same distribution by year. Horizontal histogram on the top shows the percent of observation in µmol/l or µmol/kg with a QC 1, 2, 5, 6 or 8 per kind of platform file. Horizontal histogram on the bottom shows the percent of silicate, phosphate and nitrate in the dataset and per kind of platform file.

Table 4: **Nutrient parameter names and units**

Nutrient name	Parameter name	Unit	CF standard name
Nitrate (NO3-N)	NTRA (ADJUSTED)	$mmol/m^3$ eq. to µmol/l	mole_concentration_of_nitrate_in_sea_water
	NTAW (ADJUSTED)	µmol/kg	moles_of_nitrate_per_unit_mass_in_sea_water
Silicate (SIO4-SI)	SLCA (ADJUSTED)	$mmol/m^3$ eq. to µmol/l	mole_concentration_of_silicate_in_sea_water
	SLCW (ADJUSTED)	µmol/kg	moles_of_silicate_per_unit_mass_in_sea_water
Phosphate (PO4-P)	PHOS (ADJUSTED)	$mmol/m^3$ eq. to µmol/l	mole_concentration_of_phosphate_in_sea_water
	PHOW (ADJUSTED)	µmol/kg	moles_of_phosphate_per_unit_mass_in_sea_water

3. Validation framework

3.1 Quality control flags

The quality control (QC) flags and their meaning and their application for users are summarized in Table 5.

Table 5 : Quality control (QC) flag scale

Code	Meaning	Comment
0	No QC performed	-
1	Good data	All QC tests passed
2	Probably good data	These data should be used with caution
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	Value below detection/quantification	The level of the measured phenomenon was too small to be quantified/detected by the technique employed to measure it. The accompanying value is the quantification/detection limit for the technique or zero if that value is unknown
7	Nominal value	Data were not observed but reported (e.g., an instrument target depth)
8	Interpolated value	Missing data may be interpolated from neighboring data in space or time
9	Missing value	The value is missing

Currently, QC flag 6 qualifies BGC data from the EMODnet chemistry aggregated products only.

3.2 RTQC procedure

The overall RTQC procedure is generic. This gathers 4 tests together regarding metadata qualification and 8 tests together regarding BGC variable qualification. Test implementation and design depend on BGC data and platform file type (Table 6). Each BGC parameter listed in Tables 3 and 4 has been controlled as an independent variable. The only differences consist in the fact that threshold values change according to the chosen parameter. All tests listed in Table 6 are detailed in §3.3 and 3.4. Test results are automatically applied in general. A not automated result application is possible like for profiling floats or according to test performances.

Associated temperature, salinity and depth or pressure have been beforehand reprocessed following their corresponding RTQC procedure (von Schuckmann et al., 2010).

Table 6: Applicable RTQC tests by platform file type for oxygen (O2), nutrients (Nut, silicate-phosphate-nitrate) or nitrate (NO3) only: Bottle (BO), CTD-O2 (CT), Mooring (MO), Mini Log (ML), Profiling float (PF), Ferry Box (FB), gliders (GL), Sea Mammals (SM), Saildrone (SD), unknown platform (XX), XBT, XCTD or MBT profiles (XB).

		PROFILE (PR)					**TIME SERIES & TRAJECTORIES (TS)**	
Application order	**Platform type** **RTQC test**	**BO,XX**	**CT, MO, ML**	**PF**	**GL**	**SM**	**FB, MO,SD, XB**	**BO,XX**
Provider : reference of the QC procedure								
			X	1,2	3,4			
METADATA QUALITY CONTROL								
1	Impossible date test	X	X			X	X	X
1	Impossible location test	X	X			X	X	X
2	Missing value test	X	X	X	X	X	X	X
3	Land point test	X	X	X	X	X	X	X
OXYGEN DATA QUALITY CONTROL								
5	Negative pressure test	O2, Nut	O2, Nut			O2	O2, Nut	O2, Nut
6	Metadata & hydrological QC test		O2, NO3		O2, NO3	O2	O2, NO3	
7	Stuck Value test		O2, NO3		O2, NO3	O2	O2, NO3	
8	Regional Range test	O2, Nut	O2, Nut	O2, NO3 (adj)	O2, NO3 (adj)	O2 (adj)	O2, Nut	O2, Nut
9	Global Range test	O2, Nut	O2, Nut		O2, NO3	O2	O2, Nut	O2, Nut
10	Spike & Gradient test		O2		O2	O2	O2	
11	Saturation test			O2	O2			
4	QC3 raw data test			O2, NO3	O2, NO3	O2		

[1] O2 - Thierry, V., Bittig, H. and the Argo-BGC team (2021). Argo Quality Control Manual for Dissolved Oxygen Concentration, v2.1 http://dx.doi.org/10.13155/46542

[2] NO3 - Johnson, K. et al. (2023). BGC-Argo quality control manual for nitrate concentration. http://dx.doi.org/10.13155/84370

[3] O2 - López-García,, P., et al (2022) OceanGliders Oxygen SOP, Version 1.0.0. OceanGliders, 55pp. DOI: http://dx.doi.org/10.25607/OBP-1756. (GitHub Repository, OceanGliders Oxygen SOP. Available: https://oceangliderscommunity.github.io/Oxygen_SOP/README.html

[4] NO3 - Krahmann G. et al. Nitrate Standard Operating Procedure https://oceangliderscommunity.github.io/Nitrate_SOP/README.html

3.3 Description of metadata test

Metadata such as date, location, pressure and existing QC have been controlled following the tests described below.

3.3.1 Impossible date and location test

This metadata test checks whether the observation date, time, latitude and longitude from the profile data are within the following allowed ranges:

- Date no greater than today
- Month in range of 1 to 12
- Day in range expected for month
- Hour in range 0 to 23
- Minutes in range 0 to 59
- Latitude in range -90 to 90
- Longitude in range -180 to 180

If either of the metadata values fails the test by being outside the respective allowed range, the QC flag of the variable is set to 4 “Bad value”.

3.3.2 Automated test for on-land position

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 groups, is done to reduce computational load. Finally, each cluster is tested for the existence of positions within a land polygon (QC=4; Figure 4).

The possibility of loss of sign or ‘W’ on longitudes or ‘S’ on latitudes, is not investigated.

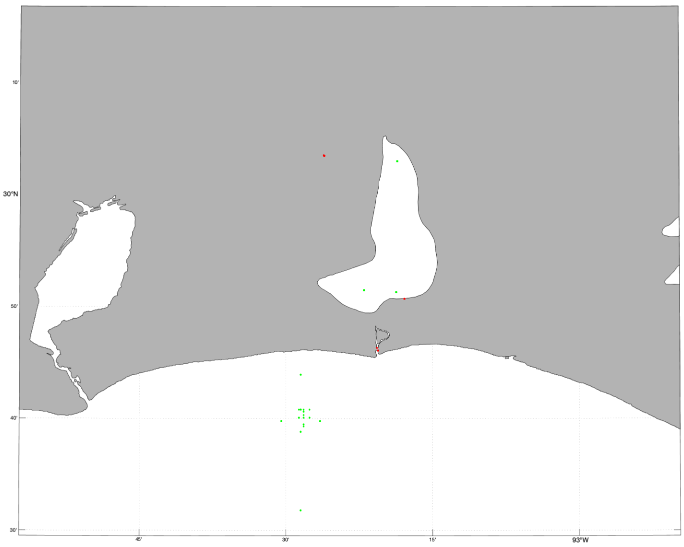

Figure 4: Example of the detection of on-land positions using the GSHHS coast dataset. Positions on land (red dots) are flagged as bad (QC=4).

The test is shared by IMR (Institute of Marine Research) via Jan Even Øie Nilsen's github: https://github.com/evenrev1/evenQC. Information on how to run the test is available in the script directly.[6]

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.

3.4 Description of BGC data test

Note that for the simple purpose of assigning variations to rather rough test criteria defined by depth at shallow water, meter and decibar (db) are here considered similar. Relevant information regarding test specificity is potentially mentioned with bracket in the subtitle

All thresholds used to control BGC data set are defined in ml/l (if relevant), 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). In some cases, oxygen concentration is converted into oxygen saturation using solubility coefficients derived from the data of Benson and Krause (1984) as fitted by Garcia and Gordon (1992, 1993).

[6] The near-coast functionality of the landpoint function is not to be used in RTQC.

3.4.1 Negative pressure test

This test checks whether the observation pressure or depth from the profile data is greater than or equal to 0, both for dbar and meter (depth/pressure is positive downwards). If PRES or DEPH is lower than 0 that means the corresponding bgc variable is potentially measured in the air. The QC flag of the BGC variables is set to 4 “Bad data”.

3.4.2 Metadata and hydrological QC test [µmol/kg]

The test is applied to profiles with BGC parameters expressed in µmol/kg that result from the conversion of a concentration per unit volume using the sea water density. The test checks that the BGC parameter has been converted with valid in situ temperature, salinity and pressure used to estimate the sea water density. If one of the QC flag of these three variables is marked as doubtful (QC=3), or bad (QC=4), the QC flag of the BGC parameter in µmol/kg is set to 3 or 4 respectively. ~~Except for data from bottle sampling, if one of the three variables, temperature, salinity or pressure, is missing, the QC flag of the BGC parameter in µmol/kg is set to 4. Regarding bottle sampling, if temperature or salinity is missing, the QC flag of the BGC parameter in µmol/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 measurement from CTD are sometimes used to convert BGC parameters as oxygen from bottles into µmol/kg.~~

Regarding the discrete chemical Oceanographic observations, Jiang et al. (2022) recommend to use the salinity and the “measurement temperature” to convert oxygen and nutrient variables into µmol/kg. In the case where the “measurement temperature” is missing, oxygen in mmol/m^3 or ml/l could be converted into µmol/kg using the in situ temperature because we assume that the oxygen fixation timing for measurement is close to the sampling timing. In contrast, the in situ temperature cannot be used for nutrient conversion because their “measurement temperature” corresponds to those of the laboratory that is constant between 20-22°C in general (22°C for Glodap, Lauvset et al., 2022). Because we don’t know the type of temperature used to convert the discrete BGC variables chemically measured, the test is not applied on data type BO (“Bottle”). In addition, phosphate and silicate are currently only discretes chemical oceanographic observations, the metadata and hydrological QC test is not applied on both variables.

ACTION : Except for the data-type BO (“Bottle”), if the QC of temperature, salinity and pressure is equal to 3 (or 4), oxygen qc and nitrate qc equal to 3 (or 4)

3.4.3 Stuck Value test

This test checks whether the values of N consecutive measurements are identically the same. If so, the QC flag of the BGC parameter for these N consecutive measurements, excepting the first one, is set up to 4 “bad data”. 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 7). For profile, N is fixed at 20 consecutive observations. To avoid false detection in the mixed layer or in the bottom layer, 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. For time series, N is in function of the time resolution and units. For oxygen in ml/l, we have in fact increased the N values associated with a short time resolution by a factor 15 (Table 7) in order to take into consideration the difference between two measurements acquired either with a sensor “DOX1” or with a sensor “DOXY”, (Δ0.01ml/l <> Δ0.446596 µmol/l). This factor of 15 results from a compromise between the ratio DOXY/DOX1 of 44.6596 µmol/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 7).

Table 7 : N consecutive measurements for a) profile and for b) time series. N is in function of time resolution (T. res) and oxygen units for time series.

	N consecutive measurements AND/OR time extension	
	(µmol/l or µmol/kg or %)	**(ml/l)**
a) 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)		
Time resolution (T. res) ≤ 1 min	N = 10	N = 150
1min < T. res ≤ 5 min	N = 6	N = 90
5 min < T. res ≤ 60 min	N = 3	After 12h, can be considered as bad
T. res > 60 min	N = 2	After 12h can be considered as bad with a N >= 4

ACTION : if N consecutive BGC values fail the test, their QC flags are set to 4-bad data except the first one.

3.4.4 Global Range test

This test applies a gross filter on observed BGC values. If one observation is out of the global range (Table 8), its QC flag is set up to 4 “bad data”. This test is applied on observation if and only if the regional range cannot run due to a missing variable (latitude or longitude) or badly positioned. Minimal and maximal control values are in keeping with the region range test (§3.4.5).

Table 8: Minimum and maximum control values allowed by the global range test for the BGC variables oxygen, nitrate, silicate and phosphate either in ml/l, µmol/l, µmol/kg and % (when it is relevant)

Parameters	ml/l	mmol/m³ or µmol/l	µmol/kg	%
oxygen	[-0.1 17.2]	[-5 769]	[-5 750]	[-5 180]
Phosphate		[-2.05 30.75]	[-2.00 30.00]	
Silicate		[-2.05 512]	[-2 499.51]	
Nitrate		[-2.05 550]	[-2 536.59]	

ACTION : If one observation from the list is out of the global range (Table 8), its QC flag is set up to 4 "bad data".

3.4.5 Regional Range test

This test is built to eliminate outliers in different geographical regions.

ACTION: If one observation from the list is out of the global range (Table 8), its QC flag is set up to 4 "bad data".

3.4.5.a. Dissolved oxygen concentration

The regions and limits are based on the gridded data set from WOA18 (Garcia et al., 2018; Figure 4). 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 individual bins. However, these numbers vary too much between neighboring bins to be used individually on a 1° by 1° basis. Instead, larger regions encompassing some typical behavior of ranges is sought.

There were initially 28 regions (Figure 5) each separated into 2 layers (Table 9) which have been defined according to an iterative manual process considering the following aspects:

- Geography, including known hydrographic regions.
- Latitude.
- More or less homogeneous regions in terms of O_2 level and variability.
- Unimodal distribution of bin mean values within each region and layer, i.e. capturing one type of O_2 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 seas which are not well characterized in WOA18.

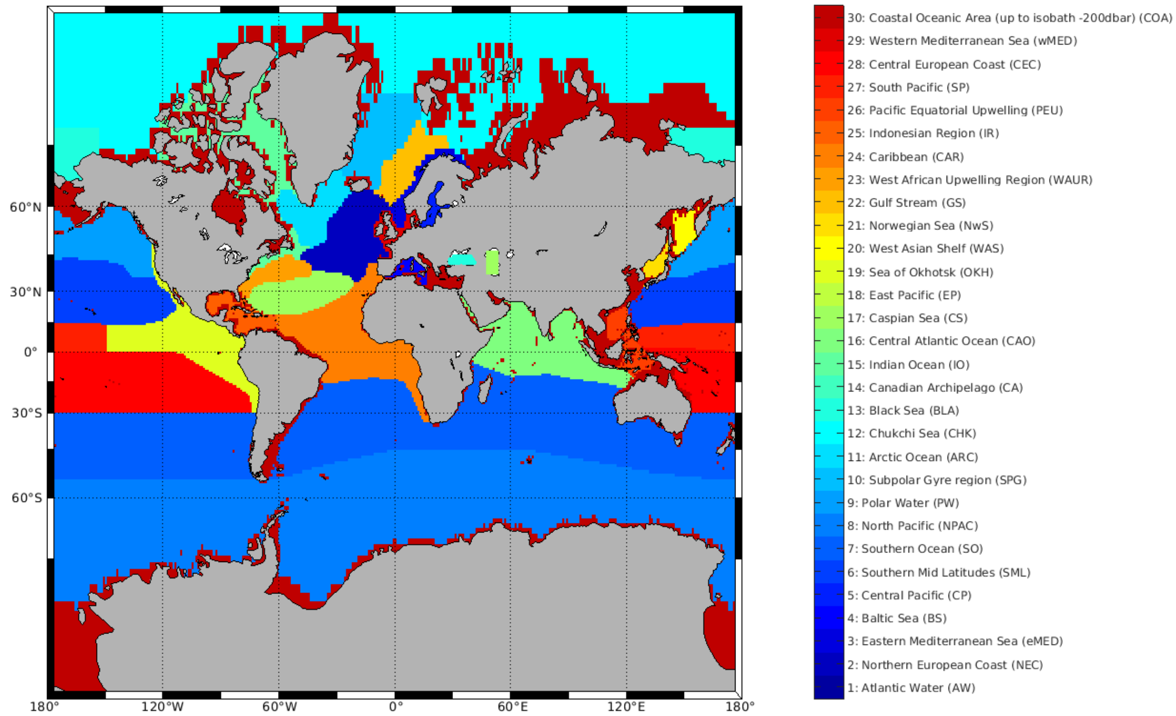

Figure 5: The current geographical regions used in the oxygen range test. The regions are also divided into 2 layers, with individual separation depths (see Table A1)

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). 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 µmol/kg (-0.1 ml/l or -5 µmol/l).

Regarding our expertise for the region, the Mediterranean Sea has been split into 2 subregions as well: the Eastern Mediterranean Sea (region 3) and the Western Mediterranean Sea (region 29).
Finally, Coastal Oceanic Area (region 30) has been added in order to take into account its specific characteristic as the rivers inputs or the strong diurnal to seasonal variability. This region extends from the coastline to the isobath 200dbar (from ETHOPO1) that corresponds approximately to the continental shelf extension, taking into account our 1°x1° grid. The allowed ranges for dissolved oxygen of all regions are reported in Table 9. If oxygen data is strictly outside the expected range at the grid point and those of these neighbors (Table 9), its QC flag is set to 4 (“bad data”).

Regarding OSAT, values in percent of saturation will first be converted into µmol/l or µmol/kg before applying the test.

Regional minimum and maximum acceptable values are listed in Annex 1 (table A1).

3.4.5.b. Nutrient concentration

The procedure for defining region, layer depth, and range is the same as for oxygen (previous section) using gridded WOA18 data as basis. For the nutrients tested, Nitrate, Phosphate, and Silicate, regions are initially based on Spalding domains. More regions are added as needed, and all regions changed and developed by the same iterative method as for oxygen, until acceptance. Figure 6 shows the resulting regions. The same geographical regions are found and used for all three nutrients, but the layer thicknesses vary.

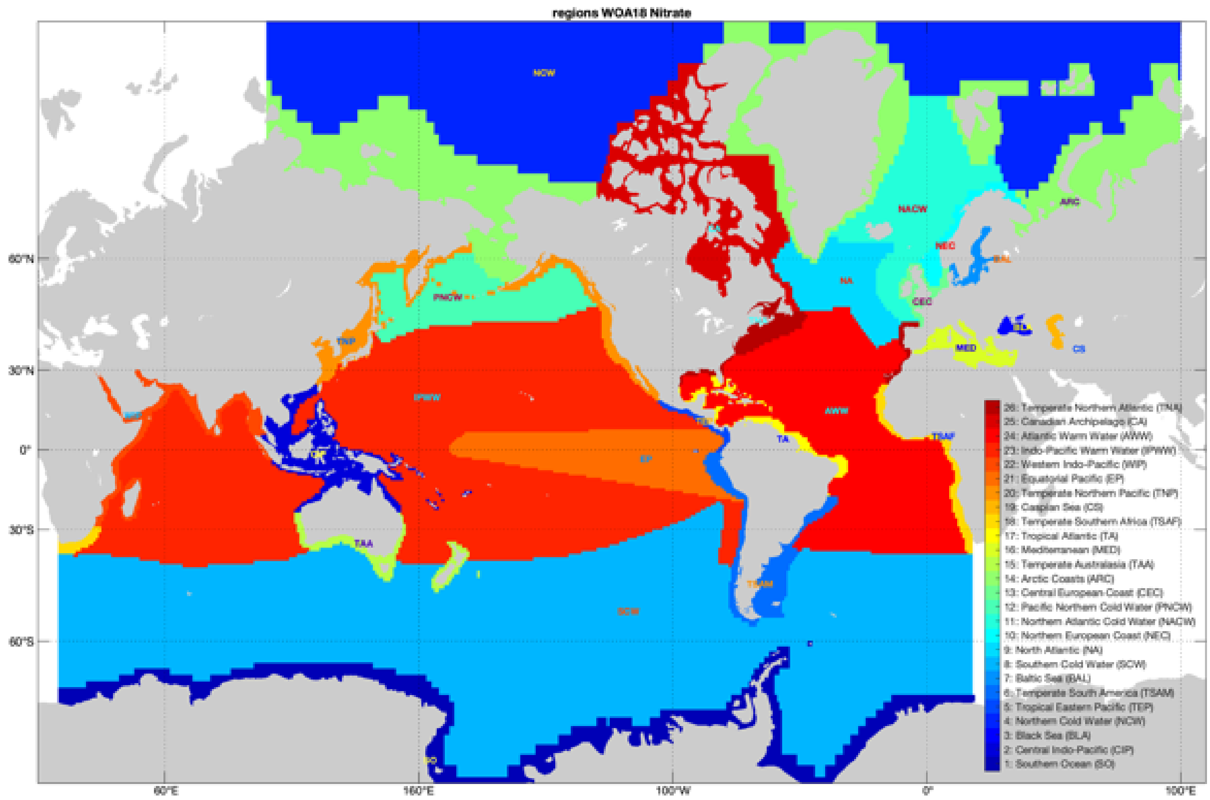

Figure 6: The current geographical regions used in the nutrients range test. The regions are also divided into 2 layers, with individual separation depths (see Tables A2 to A4)

The initial resulting ranges of this procedure were used for the quality control of the nutrients in the In Situ TAC reprocessed (REP) products (see the Quality Information Document CMEMS-INS-QUID-013-046 - version 2.6) for which alerts raised by the regional range test are visually controlled.

Due to an automatic application, the Regional Range test in NRT needs to be neither too wide to rule out outliers, nor too narrow to avoid over-flagging. In this context, we have first evaluated the required widening to adapt the REP regional ranges (visual inspection) to NRT conditions (automatic application). The widening (wdg) estimates how much the initial distance between the median and the threshold should be increased in order to remove false alerts (i.e. to include this measured value in the validity interval). For example, wdg = 0.2 means that the distance between the median and the threshold should be increased by 20% (i.e. multiplied by 1+0.2). The widening has been studied globally (that means same widening for all regions and for upper and lower layers) when it was possible.

In the second step, we have worked on the low threshold. Depending on regions, seasons, water masses could be characterized by a zero concentration (phytoplankton consumption) but the instrument inaccuracy could provide negative measurements. Such data could be marked as "value below the detection/quantification" (QC6); that is not always the case. To avoid over flagging with an automatic application of the regional range test in NRT, low thresholds below 0 mmol/m^3 have been set to -2,05 mmol/m^3 in order to match with -2 µmol/kg used by argo float for adjusted nitrate.

Finally and without satisfactory results, the regional range for Mediterranean sea has been set up to world ocean database minimum and maximum values in this region (see WOD user manual, 2018, Garcia et al., 2018).

Resulting ranges are listed in annex, in Table A2 through Table A4.

3.4.6 Spike and gradient test [Oxygen]

Spike and gradient tests from BGC argo recommendations (Thierry, Bittig et al., 2018) are combined here to detect single spikes along a vertical profile. 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 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 or front.

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

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

Where V2 is the observation to be tested, V1 and V3 are the valid values (≠QC9 or QC4) just above and below. Threshold values depend on the sampled oceanic layers and the vertical (Profile) or time (Time Series) resolution of the sampling.

3.4.6.a Profiles

V2 values are flagged as bad (QC4) when delta and grad exceed :

[ml/l µmol/l µmol/kg %]

- [1.5 52 50 13] for pressure less than 500 dbar and vertical resolution less than 2.05dbar
- [1.9 82 80 21] for pressure less than 500 dbar and vertical resolution less than 5.05dbar
- [0.6 26 25 6] for pressure greater or equal to 500 dbar and vertical resolution less than 20 dbar

3.4.6.b Time series

V2 values are flagged as bad (QC4) when delta and grad exceed :

[ml/l µmol/l µmol/kg %]

- [1.5 52 50 13] for pressure less than 500 dbar and time resolution less than 1.05min
- [1.9 82 80 21] for pressure less than 500 dbar and time resolution less than 5.05min
- [0.6 26 25 6] for pressure greater or equal to 500 dbar and time resolution less than 1.05min
- [1.5 52 50 13] for pressure less than 500 dbar and time resolution less than 5.05min

3.4.7 Saturation test [Oxygen]

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 overshot 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). In some cases like Chukchi Sea (region 12) or Baltic Sea (region 4) or Coastal Oceanic Area (region 30) and the Central European Coast (28) that is below isobath 200, upper saturation events could be temporarily higher than 150%. For these regions, the higher limit is fixed here at 180% (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% (Table 11). ~~Figure 6 shows the mask used to separate the open ocean area to the coastal area.~~

Oxygen observation measured in the ocean failing the test is visualized. Profile is marked as doubtful (QC = 3) if the sensor is negatively biased whereas it is marked as bad (QC = 4) if the sensor is positively biased (biofouling). Spike is however always marked as bad.

Table 11 : Regional control values for the saturation test

Region	**Oxygen saturation HIGHER ACCEPTED LIMIT**
Baltic Sea (reg. 4), Chukchi Sea (reg. 12), Coastal Oceanic Area (reg. 30), Central European Coast (28)	180%
Other regions	150 %
Region	**Oxygen saturation LOWER ACCEPTED LIMIT**
Other regions	50%

3.4.8 QC3 - raw data test

BGC argo and glider communities recommend setting the real time unadjusted oxygen qc flag to 3. This is because the majority of oxygen sensors deployed on this autonomous profiling platform (PF) suffer from bias in calibration generally occurring between the initial laboratory calibration and the float deployment and potentially correctable during the delayed mode treatment (Thierry, Bittig and al., 2021; López-García et al., 2022). Unfortunately, these recommendations are not always followed by providers. In this context, it was decided that the QC3 - raw data test checks if the unadjusted oxygen variables delivered in real time by the pre-cited platform (PF and GL) are set to QC 3 " doubtful data - potentially correctable".

Argo community provides the same recommendations for nitrate variables and for the same reason (Jonhson et al., 2021). Regarding the gliders (GL), it is not clearly noted setting the real time unadjusted nitrate qc flag to 3 in the Nitrate Standard Operating Procedure. However, the sections "post-recovery operations & calibrations" and "delayed mode processing & QC" of the document suggest a systematic bias of the raw nitrate delivered in real time. In addition, many gliders are equipped with UV spectrometers comparable to those mounted on argo platforms.
It was decided that the QC3 - raw data test checks if the unadjusted nitrate variables delivered in real time by the pre-cited platform (PF and GL) are set to QC 3 " doubtful data - potentially correctable".

Action : the QC of OXYGEN or NITRATE in R mode is set to 3

4. Validation Results

4.1 Oxygen saturation in surface

Percent oxygen saturation at the surface is a good indicator to inform users regarding the oxygen quality of the product. Air-sea O_2 exchanges are in fact very fast. While the physical and biological mechanisms may lead to under or over-saturation events as explained in §3.4.7, the surface ocean is close to the theoretical value of 100%. Figure 6 shows the spatial distribution of the oxygen saturation at the surface layer (0-10dbar) calculated from valid oxygen, temperature, salinity and pressure observations (QC 1, 2, 5 or 8) available in the COPERNICUS NRT products. While local hotspots are visible close to coasts and in the western part of the Atlantic Ocean, surface ocean in the real time is generally close to 100% except for well-known specific regions as Antarctic area, equatorial pacific or Baltic region.

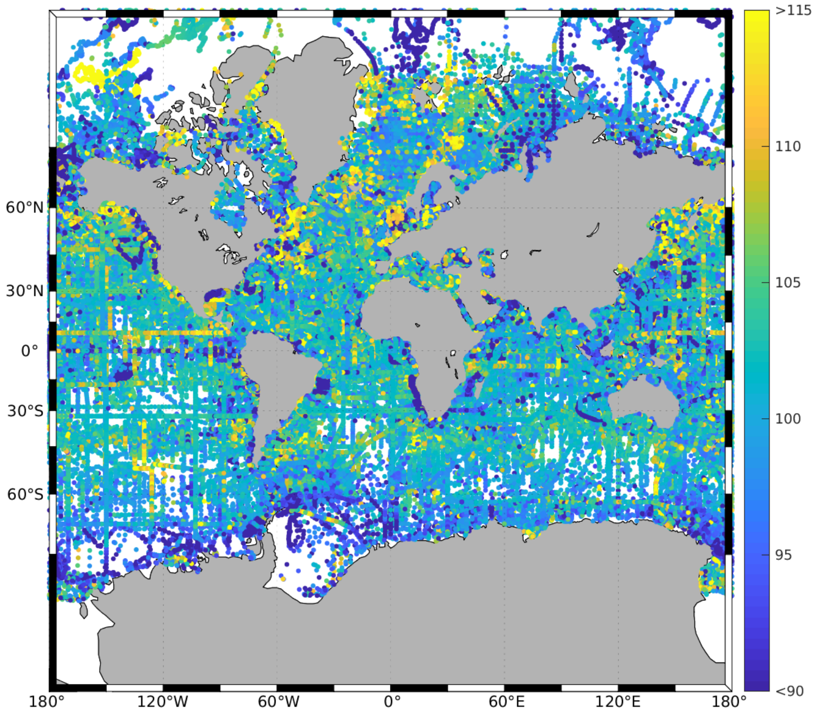

Figure 6: Distribution of the oxygen saturation (%) at the surface layer (0-10dbar) from the NRT COPERNICUS product INSITU_GLO_PHYBGCWAV-DISCRETE-MYNRT-013_030 (snapshot of the September 5th, 2022)

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6. Annex 1 - Regional minimum and maximum acceptable values for BGC variables

Table A1: Minimum and maximum control values for oxygen defined in ml/l, µmol/l and µmol/kg for each 30 regions separated into 2 layers by the specific upper layer depth noted in brackets.

Region (upper layer depth)	N° Abbr	Layer	DOX1 (ml/l) low	DOX1 (ml/l) high	DOXY (µmol/l) low	DOXY (µmol/l) high	DOX2 (µmol/kg) low	DOX2 (µmol/kg) high
Atlantic Water	1	upper	-0.1	9.9	-5	441	-5	430
(1600 m)	AW	lower	3.9	7.8	174	348	170	340
Northern European Coast	2	upper	-0.1	10.8	-5	482	-5	470
(100 m)	NEC	lower	2.3	10.1	102	451	100	440
eastern Mediterranean Sea	3	upper	-0.1	8.0	-5	359	-5	350
(100 m)	eMED	lower	-0.1	8.0	-5	359	-5	350
Baltic Sea	4	upper	-0.1	13.8	-5	615	-5	600
(50 m)	BS	lower	-0.1	13.8	-5	615	-5	600
Central Pacific	5	upper	-0.1	9.9	-5	441	-5	430
(900 m)	CP	lower	-0.1	4.8	-5	215	-5	210
Southern Mid Latitudes	6	upper	-0.1	12.6	-5	564	-5	550
(100 m)	SML	lower	-0.1	11.0	-5	492	-5	480
Southern Ocean	7	upper	-0.1	13.8	-5	615	-5	600
(100 m)	SO	lower	-0.1	13.1	-5	584	-5	570
North Pacific	8	upper	-0.1	13.8	-5	615	-5	600
(100 m)	NPAC	lower	-0.1	13.8	-5	615	-5	600
Polar Water	9	upper	2.1	13.8	92	615	90	600
(100 m)	PW	lower	4.6	9.6	205	430	200	420
Subpolar Gyre region	10	upper	-0.1	12.2	-5	543	-5	530
(100 m)	SPG	lower	-0.1	11.0	-5	492	-5	480
Arctic Ocean	11	upper	-0.1	13.8	-5	615	-5	600
(100 m)	ARC	lower	2.5	12.4	113	554	110	540
Chukchi Sea	12	upper	-0.1	17.2	-5	769	-5	750
(100 m)	CHK	lower	-0.1	9.0	-5	400	-5	390
Black Sea	13	upper	-0.1	13.8	-5	615	-5	600
(40 m)	BLA	lower	-0.1	13.8	-5	615	-5	600
Canadian Archipelago	14	upper	-0.1	13.8	-5	615	-5	600
(100 m)	CA	lower	-0.1	13.3	-5	595	-5	580
Indian Ocean	15	upper	-0.1	13.8	-5	615	-5	600
(100 m)	IO	lower	-0.1	9.2	-5	410	-5	400
Central Atlantic Ocean	16	upper	-0.1	7.8	-5	349	-5	340
(1400 m)	CAO	lower	3.4	7.6	154	338	150	330
Caspian Sea	17	upper	-0.1	13.8	-5	615	-5	600

(100 m)	CS	lower	-0.1	13.8	-5	615	-5	600
East Pacific	18	upper	-0.1	13.8	-5	615	-5	600
(100 m)	EP	lower	-0.1	9.9	-5	441	-5	430
Sea of Okhotsk	19	upper	-0.1	13.8	-5	615	-5	600
(100 m)	OKH	lower	-0.1	13.1	-5	584	-5	570
West Asian Shelf	20	upper	-0.1	13.8	-5	615	-5	600
(100 m)	WAS	lower	-0.1	9.4	-5	420	-5	410
Norwegian Sea	21	upper	4.8	9.2	215	410	210	400
(100 m)	NwS	lower	5.1	8.7	226	390	220	380
Gulf Stream	22	upper	-0.1	11.7	-5	523	-5	510
(1500 m)	GQ	lower	4.8	7.3	215	328	210	320
West African Upwelling Region	23	upper	-0.1	11.5	-5	513	-5	500
(1500 m)	WAUR	lower	3.4	7.1	154	318	150	310
Caribbean	24	upper	-0.1	8.5	-5	379	-5	370
(1500 m)	CA	lower	2.8	9.0	123	400	120	390
Indonesian Region	25	upper	-0.1	9.2	-5	410	-5	400
(100 m)	IR	lower	-0.1	7.3	-5	328	-5	320
Pacific Equatorial Upwelling	26	upper	-0.1	8.5	-5	379	-5	370
(100 m)	PEU	lower	-0.1	9.0	-5	400	-5	390
South Pacific	27	upper	-0.1	9.4	-5	420	-5	410
(100 m)	SP	lower	-0.1	10.6	-5	472	-5	460
Central European Coast	28	upper	-0.1	11.9	-5	533	-5	520
(100 m)	CEC	lower	-0.1	8.0	-5	359	-5	350
western Mediterranean Sea	29	upper	-0.1	9.0	-5	405	-5	395
(100 m)	wMED	lower	-0.1	9.0	-5	405	-5	395
Coastal Oceanic Area	30	upper	-0.1	17.2	-5	769	-5	750
(50 m)	COA	lower	-0.1	17.2	-5	769	-5	750

Table A2: Minimum and maximum control values for nitrate defined in µmol/l and µmol/kg for each 30 regions separated into 2 layers by the specific upper layer depth noted in brackets.

Region (upper layer depth)	**N° Abbr**	**Layer**	**NTRA (µmol/l) low**	**NTRA (µmol/l) high**	**NTAW (µmol/kg) low**	**NTAW (µmol/kg) high**
Southern Ocean	1	upper	-2.05	550	-2	536.59
(100 m)	SO	lower	9.17	51.83	8.95	50.57
Central Indo-Pacific	2	upper	-2.05	550	-2	536.59
(100 m)	CIP	lower	-2.05	105.78	-2	103.2
Black Sea	3	upper	-2.05	550	-2	536.59
(100m)	BLA	lower	-2.05	33.54	-2	32.72
Northern Cold Water	4	upper	-2.05	550	-2	536.59
(300m)	NCW	lower	-2.05	32.25	-2	31.46
Tropical Eastern Pacific	5	upper	-2.05	550	-2	536.59
(100m)	TEP	lower	-2.05	83.65	-2	81.8
Temperate South America	6	upper	-2.05	550	-2	536.59
(100m)	TSAM	lower	-2.05	92.88	-2	90.61
Baltic Sea	7	upper	-2.05	550	-2	536.59
(50m)	BAL	lower	-2.05	24.51	-2	23.91
Southern Cold Water	8	upper	-2.05	550	-2	536.59
(1000m)	SCW	lower	2.14	55.86	2.09	54.5
North Atlantic	9	upper	-2.05	550	-2	536.59
(100m)	NA	lower	-2.05	38.7	-2	37.76
Northern European Coast	10	upper	-2.05	550	-2	536.59
(100m)	NEC	lower	-2.05	39.99	-2	39.01
North Atlantic Cold Water	11	upper	-2.05	550	-2	536.59
(100m)	NACW	lower	-2.05	36.12	-2	35.24
Pacific Northern Cold Water	12	upper	-2.05	550	-2	536.59
(100m)	PNCW	lower	-2.05	104.49	-2	101.94
Central European Coast	13	upper	-2.05	550	-2	536.59
(100m)	CEC	lower	-2.05	27.09	-2	26.43
Arctic Coasts	14	upper	-2.05	550	-2	536.59
(200m)	ARC	lower	-2.05	79.98	-2	78.03
Temperate Australasia	15	upper	-2.05	550	-2	536.59
(100m)	TAA	lower	-2.05	70.95	-2	69.22
Coastal Mediterranean	16	upper	-2.05	30.75	-2	30.00
(100m)	Coast MED	lower	-2.05	30.75	-2	30.00
Tropical Atlantic	17	upper	-2.05	550	-2	536.59
(100m)	TA	lower	-2.05	86.43	-2	84.32
Temperate Southern Africa	18	upper	-2.05	550	-2	536.59

(100m)	TSAF	lower	-2.05	54.18	-2	52.86
Caspian Sea	19	upper	-2.05	550	-2	536.59
(100m)	CS	lower	-2.05	2.58	-2	2.52
Temperate Northern Pacific	20	upper	-2.05	550	-2	536.59
(200m)	TMP	lower	-2.05	86.43	-2	84.32
Equatorial Pacific	21	upper	-2.05	550	-2	536.59
(200m)	EP	lower	2.82	69.18	2.75	67.49
Western Indo-Pacific	22	upper	-2.05	550	-2	536.59
(100m)	WIP	lower	-2.05	70.95	-2	69.22
Indo-Pacific Warm Water	23	upper	-2.05	550	-2	536.59
(100m)	IPWM	lower	-2.05	96.75	-2	94.39
Atlantic Warm Water	24	upper	-2.05	550	-2	536.59
(100m)	AW	lower	-2.05	74.82	-2	73
Canadian Archipelago	25	upper	-2.05	550	-2	536.59
(200)	CA	lower	-2.05	33.54	-2	32.72
Temperate Northern Atlantic	26	upper	-2.05	550	-2	536.59
(100m)	TNA	lower	-2.05	89.01	-2	86.84
Alboran Sea	27	upper	-2.05	30.75	-2	30.00
(500m)	ALB	lower	-2.05	30.75	-2	30.00
Western Mediterranean 1	28	upper	-2.05	30.75	-2	30.00
(1100m)	West1 MED	lower	-2.05	30.75	-2	30.00
Western Mediterranean 2	29	upper	-2.05	30.75	-2	30.00
(1100m)	West2 MED	lower	-2.05	30.75	-2	30.00
Eastern Mediterranean	30	upper	-2.05	30.75	-2	30.00
(5200m)	East MED	lower	-2.05	30.75	-2	30.00

Table A3: Minimum and maximum control values for silicate defined in µmol/l and µmol/kg for each 30 regions separated into 2 layers by the specific upper layer depth noted in brackets.

Region (upper layer depth)	N° Abbr	Layer	SLCA (µmol/l) low	SLCA (µmol/l) high	SLCW (µmol/kg) low	SLCW (µmol/kg) high
Southern Ocean	1	upper	-2.05	410	-2	400
(100 m)	SO	lower	-2.05	410	-2	400
Central Indo-Pacific	2	upper	-2.05	246	-2	240
(100 m)	CIP	lower	-2.05	410	-2	400
Black Sea	3	upper	-2.05	266	-2	259.51
(100m)	BLA	lower	-2.05	512	-2	499.51
Northern Cold Water	4	upper	-2.05	206	-2	200.98
(300m)	NCW	lower	-2.05	62	-2	60.49
Tropical Eastern Pacific	5	upper	-2.05	184	-2	179.51
(100m)	TEP	lower	-2.05	370	-2	360.98
Temperate South America	6	upper	-2.05	164	-2	160
(100m)	TSAM	lower	-2.05	430	-2	419.51
Baltic Sea	7	upper	-2.05	144	-2	140.49
(50m)	BAL	lower	-2.05	500	-2	487.8
Southern Cold Water	8	upper	-2.05	390	-2	380.49
(1000m)	SCW	lower	-2.05	410	-2	400
North Atlantic	9	upper	-2.05	62	-2	60.49
(100m)	NA	lower	-2.05	164	-2	160
Northern European Coast	10	upper	-2.05	42	-2	40.98
(100m)	NEC	lower	-2.05	62	-2	60.49
North Atlantic Cold Water	11	upper	-2.05	62	-2	60.49
(100m)	NACW	lower	-2.05	144	-2	140.49
Pacific Northern Cold Water	12	upper	-2.05	410	-2	400
(100m)	PNCW	lower	-2.05	512	-2	499.51
Central European Coast	13	upper	-2.05	82	-2	80
(100m)	CEC	lower	-2.05	42	-2	40.98
Arctic Coasts	14	upper	-2.05	472	-2	460.49
(200m)	ARC	lower	-2.05	164	-2	160
Temperate Australasia	15	upper	-2.05	62	-2	60.49
(100m)	TAA	lower	-2.05	328	-2	320
Coastal Mediterranean	16	upper	-2.05	82	-2	80
(100m)	Coast MED	lower	-2.05	82	-2	80
Tropical Atlantic	17	upper	-2.05	124	-2	120.98
(100m)	TA	lower	-2.05	184	-2	179.51

Temperate Southern Africa	18	upper	-2.05	144	-2	140.49
(100m)	TSAF	lower	-2.05	370	-2	360.98
Caspian Sea	19	upper	-2.05	124	-2	120.98
(100m)	CS	lower	-2.05	184	-2	179.51
Temperate Northern Pacific	20	upper	-2.05	390	-2	380.49
(200m)	TMP	lower	-2.05	512	-2	499.51
Equatorial Pacific	21	upper	-2.05	164	-2	160
(200m)	EP	lower	-2.05	370	-2	360.98
Western Indo-Pacific	22	upper	-2.05	184	-2	179.51
(100m)	WIP	lower	-2.05	370	-2	360.98
Indo-Pacific Warm Water	23	upper	-2.05	206	-2	200.98
(100m)	IPWM	lower	-2.05	512	-2	499.51
Atlantic Warm Water	24	upper	-2.05	82	-2	80
(100m)	AW	lower	-2.05	328	-2	320
Canadian Archipelago	25	upper	-2.05	206	-2	200.98
(200)	CA	lower	-2.05	308	-2	300.49
Temperate Northern Atlantic	26	upper	-2.05	102	-2	99.51
(100m)	TNA	lower	-2.05	288	-2	280.98
Alboran Sea	27	upper	-2.05	82	-2	80
(500m)	ALB	lower	-2.05	82	-2	80
Western Mediterranean 1	28	upper	-2.05	82	-2	80
(1100m)	West1 MED	lower	-2.05	82	-2	80
Western Mediterranean 2	29	upper	-2.05	82	-2	80
(1100m)	West2 MED	lower	-2.05	82	-2	80
Eastern Mediterranean	30	upper	-2.05	82	-2	80
(5200m)	East MED	lower	-2.05	82	-2	80

Table A4: Minimum and maximum control values for phosphate defined in µmol/l and µmol/kg for each 30 regions separated into 2 layers by the specific upper layer depth noted in brackets.

Region (upper layer depth)	N° Abbr	Layer	PHOS (µmol/l) low	PHOS (µmol/l) high	PHOW (µmol/kg) low	PHOW (µmol/kg) high
Southern Ocean	1	upper	-2.05	7.50	-2	7.32
(100 m)	SO	lower	-2.05	6.75	-2	6.59
Central Indo-Pacific	2	upper	-2.05	5.55	-2	5.41
(100 m)	CIP	lower	-2.05	9.60	-2	9.37
Black Sea	3	upper	-2.05	10.80	-2	10.54
(100m)	BLA	lower	-2.05	21.45	-2	20.93
Northern Cold Water	4	upper	-2.05	7.65	-2	7.46
(300m)	NCW	lower	-2.05	4.20	-2	4.1
Tropical Eastern Pacific	5	upper	-2.05	9.00	-2	8.78
(100m)	TEP	lower	-2.05	7.80	-2	7.61
Temperate South America	6	upper	-2.05	9.45	-2	9.22
(100m)	TSAM	lower	-2.05	8.85	-2	8.63
Baltic Sea	7	upper	-2.05	4.50	-2	4.39
(50m)	BAL	lower	-2.05	30.00	-2	29.27
Southern Cold Water	8	upper	-2.05	7.8	-2	7.61
(1000m)	SCW	lower	-2.05	5.85	-2	5.71
North Atlantic	9	upper	-2.05	4.95	-2	4.83
(100m)	NA	lower	-2.05	4.05	-2	3.95
Northern European Coast	10	upper	-2.05	3.45	-2	3.37
(100m)	NEC	lower	-2.05	3.75	-2	3.66
North Atlantic Cold Water	11	upper	-2.05	4.35	-2	4.24
(100m)	NACW	lower	-2.05	3.75	-2	3.66
Pacific Northern Cold Water	12	upper	-2.05	9.90	-2	9.66
(100m)	PNCW	lower	-2.05	10.50	-2	10.24
Central European Coast	13	upper	-2.05	5.40	-2	5.27
(100m)	CEC	lower	-2.05	4.65	-2	4.54
Arctic Coasts	14	upper	-2.05	9.45	-2	9.22
(200m)	ARC	lower	-2.05	5.85	-2	5.71
Temperate Australasia	15	upper	-2.05	4.95	-2	4.83
(100m)	TAA	lower	-2.05	6.45	-2	6.29
Coastal Mediterranean	16	upper	-2.05	30.75	-2	30.00
(100m)	Coast MED	lower	-2.05	30.75	-2	30.00
Tropical Atlantic	17	upper	-2.05	4.80	-2	4.68
(100m)	TA	lower	-2.05	6.75	-2	6.59
Temperate Southern Africa	18	upper	-2.05	6.90	-2	6.73

(100m)	TSAF	lower	-2.05	8.25	-2	8.05
Caspian Sea	19	upper	-2.05	30.75	-2	30.00
(100m)	CS	lower	-2.05	30.75	-2	30.00
Temperate Northern Pacific	20	upper	-2.05	8.80	-2	8.49
(200m)	TMP	lower	-2.05	9.30	-2	9.07
Equatorial Pacific	21	upper	-2.05	10.20	-2	9.95
(200m)	EP	lower	-2.05	7.95	-2	7.76
Western Indo-Pacific	22	upper	-2.05	9.60	-2	9.37
(100m)	WIP	lower	-2.05	8.55	-2	8.34
Indo-Pacific Warm Water	23	upper	-2.05	9.00	-2	8.78
(100m)	IPWM	lower	-2.05	8.40	-2	8.20
Atlantic Warm Water	24	upper	-2.05	6.15	-2	6.00
(100m)	AW	lower	-2.05	7.05	-2	6.88
Canadian Archipelago	25	upper	-2.05	5.55	-2	5.41
(200)	CA	lower	-2.05	4.35	-2	4.24
Temperate Northern Atlantic	26	upper	-2.05	4.05	-2	3.95
(100m)	TNA	lower	-2.05	6.90	-2	6.73
Alboran Sea	27	upper	-2.05	30.75	-2	30.00
(500m)	ALB	lower	-2.05	30.75	-2	30.00
Western Mediterranean 1	28	upper	-2.05	30.75	-2	30.00
(1100m)	West1 MED	lower	-2.05	30.75	-2	30.00
Western Mediterranean 2	29	upper	-2.05	30.75	-2	30.00
(1100m)	West2 MED	lower	-2.05	30.75	-2	30.00
Eastern Mediterranean	30	upper	-2.05	30.75	-2	30.00
(5200m)	East MED	lower	-2.05	30.75	-2	30.00