COPERNICUS MARINE ENVIRONMENT MONITORING SERVICE

IN SITU TAC

CMEMS ELEMENT

Quality Control of Biogeochemical Measurements

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GLOSSARY AND ABBREVIATIONS

Additional terms:

BGC	Bio Geo Chemical
QC	Quality Control
CMEMS	Copernicus Marine and Environmental Monitoring Service

Applicable and Reference Documents

	Ref	Title	Date / Version

HISTORY

Previous versions of this document and up to version 2.5 were generated during MyOcean, MyOcean2 and MyOceanFO EU-projects. Starting in CMEMS, several updates have been performed but not officially released.

Version 3.1 is the first official release within CMEMS with focus on chlorophyll-a fluorescence.

The present Version 6 is the method used for the production of CMEMS INSITU_GLO_BGC_REP_OBSERVATIONS_013_046 release for the V4 of CMEMS in 2018

1 INTRODUCTION

An important step within CMEMS is to harmonize existing quality control and quality assurance procedures of the different areas involved. As the Copernicus service is thought to be available at any time and open to anyone, an agreement in good QC methods and procedures is vital to guarantee high data quality distributed to users via international exchange. The agreement on the implementation of uniform QC procedures has the potential to overcome the non- consistency within the existing datasets provided by the international community.

The detection of anomalous values of biogeochemical (BGC) parameters is challenging due to their inherent high spatial and temporal variability, e.g., diel Chl a fluorescence can vary by an order of magnitude or more due to changes in irradiance, self-shading, physiological states, community composition and cloud cover (Huot and Babin, 2010). In fact, the phytoplankton community composition can change the diel variability with as much as a factor 4. It is therefore a challenge to define regional tests to check data quality in sea regions that have different characteristics. The amount of data available for building regional climatology of BGC parameters is also very limited due to historically fewer observations. The lack of a common reference database for these parameters makes it difficult to identify anomalies at regional level.

Table 1 File occurrences with selected BGC parameters in the history repository on a total of 71068 files. Status from January 9, 2017.

Chlorophyll	2460
Oxygen	2635
Turbidity	1121
Nitrate	1044
Alkalinity	693
Phosphate	418
Silicate	398
Ammonium	311
CDOM	140
Carbon	1

The main focus of this document is to describe quality tests recommended to be commonly applied for biogeochemical (BGC) data from the various observational platforms available in the CMEMS service. Table 1 lists how many files from the history repository are expected to contain selected BGC parameters. While oxygen has the largest number of files, it is intentionally placed as second because this parameter is frequently reported in different units which are not always easy to convert. Therefore, this document will focus on Chl *a* measurements to provide examples of good practice in data handling Hence, chlorophyll has the highest frequency of occurrence and this is the reason why this parameter has been focused on.

The proposals for real time QC given within this document are built on the heritage from previous efforts, e.g. PABIM White Book (D'Ortenzio et al., 2010), Coriolis (Coatanoan and Petit de la Villéon, 2005), SeaDataNet (SeaDataNet, 2007) ECOOP (Tamm and Soetje, 2009), GOSUD (GOSUD, 2006), M3A (Basana et al., 2000), Argo (Argo, 2009), MyOcean T/S QC procedures (Schuckmann et al., 2010),

MyOcean Real Time Quality Control of biogeochemical measurements (Jaccard et al., 2015) as well as in-house expertise from contributors to this report.

This document presents quality assessment tools that can be applied as soon as data are delivered to the CMEMS production units, as well as reprocessing tools. The latter requires a certain knowledge about the type and structure of the data in order to build the control quality test.

In addition, a set of tools have been developed for the evaluation of the tests themselves and are likely to be applied on monthly and history repositories only. These evaluation tools are not expected to be implemented at production unit (PU) level, but applied by experts and scientists. The resulting analysis should confirm or provide an upgrade of the quality control tests implemented at PU level.

2 QUALITY CONTROL FLAGS

The in-situ data provided by the CMEMS In-situ Thematic Assembly Centre (In Situ-TAC) is thought to be used by different users, with different requirements. Thus, one of the goals of the RTQC procedure is the provision of known quality flags, which characterize the data.

These flags should always be part of data delivery, in order to maintain standards and to ensure data consistency and reliability. The QC flags for BGC data within CMEMS are based on the existing standards defined for other observational data sets. Table 2 indicates the flags and their specific meanings.

To avoid unnecessary failure in using the data sets, a clear guidance to the user of CMEMS in Situ-TAC data is necessary:

A data with QC flag = 0 indicates no QC has taken place, i.e. the data are not recommended to be used without a quality control carried out by the user.

A data with QC flag ≠ 1 for either position or date should tell the user to proceed with caution. The data should not be used without additional controls and checks carried out by the user.

Otherwise

- QC flag = 1, the data can be used safely without further analyses
- QC flag = 2, the data may be good for some applications but the users should verify this and document their results accordingly.
- QC flag = 3, the data are not usable as they are, but the CMEMS data center see potential for correcting the data in the delayed mode
- QC flag = 4, measurements should be rejected.

Quality control flag application policy (i.e. Argo, 2009): The QC flag value assigned by a test (see section 3) cannot override a higher value from a previous test.

Table 2 Quality flag scale. Codes marked in red are mandatory following the RTQC procedure

Code	Meaning	Comment
0	No QC was performed	-
1	Good data	All real-time 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	-
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

A weakness of this QC notation is that it does not provide information about why the data is bad, or if all defined tests have been applied. Some tests have to be performed on consecutive measurements and will not provide the expected result if the time difference between the data points is larger than the events change rate. Hence, these tests cannot always be applied. Some other tests are based on extra information that is not provided for all datasets. Therefore, it is likely to meet situations where a measurement in a specific dataset is flagged as bad (QC=4) because one could apply an additional test on it. Moreover, another measurement from a similar dataset can be of much worse quality but flagged as good (QC=1) because not all tests could be executed.

Consequently, the information provided by these flags must be used with caution and not separated by the underlying data context. However, this kind of underlying information should be documented in the metadata or documentation of the dataset.

3 PARAMETER NAMING CONVENTION

Agreement on how to name the different BGC parameters and the units to use has been established and is presented in Table 3. This has been a first important step in the development of standardized tools for the quality control of such measurements.

Table 3 Naming conventions to use for the different BGC parameters

Name	Long Name	Unit	CF Standard Name
FLU2	Chlorophyll-a fluorescence	mg m^{-3}	mass_concentration_of_chlorophyll_a_fluorescence_in_sea_water
CPHL	Chlorophyll-a	mg m^{-3}	mass_concentration_of_chlorophyll_a_in_sea_water
DOXY	Dissolved oxygen	mmol m^{-3}, µmol l^{-1}, µM	mole_concentration_of_dissolved_molecular_oxygen_in_sea_water
DOX1	Dissolved oxygen	ml l^{-1}	volume_fraction_of_oxygen_in_sea_water
DOX2	Dissolved oxygen	µmol kg^{-1}	moles_of_oxygen_per_unit_mass_in_sea_water
OSAT	Oxygen saturation	%	fractional_saturation_of_oxygen_in_sea_water
TUR4	Turbidity	1, FNU, NTU, FTU	sea_water_turbidity
DPAR	downwelling photosynthetic active radiation	µmole m^{-2} s^{-1}	downwelling_photosynthetic_photon_flux_in_sea_water

3.1 Common Attributes

For all netCDF variables containing BGC data, the following set of attributes should be provided, if possible (Table 4). These come in addition to the standard required attributes. They are not present yet in the products, but it would be a good practice to provide them as this information is very relevant in the development, evaluation and improvement cycle of quality control tools.

Table 4 Parameter independent additional attributes to netCDF BGC variables.

Name	Description
last_calibration_date	The date in the format YYYY-MM-DD when the specific sensor was calibrated
calibration_method	A description or link to the method used to calibrate the sensor

The next sections specify in more details the parameter specific information to be included in the netCDF files.

3.2 FLU2: Chl-a Fluorescence

Measurements of Chl-a fluorescence are saved in variable FLU2. For historical reasons, using CPHL is also allowed for BioArgo platforms *only*, and in this case the netCDF variable must have attribute *sensing_method* set to **fluorescence.** If the latter is not provided or wrong, it will be considered as a Chl-a concentration, as those obtained from laboratory analysis from HPLC or spectrophotometry. Note that this exception is only accepted for data from BioArgo. All other must use FLU2.

3.2.1 Attributes

Name	Description
proxy_method	A description or a link to the method used to relate the fluorescence measurements to Chl-a concentration
last_proxy_method_date	The date in the format YYYY-MM-DD when the proxy relation to Chl-a concentration was generated.

3.2.2 Related Parameters

Downwelling photosynthetic active radiation (DPAR) if provided could be used in the future to improve quality control procedures.

3.3 CPHL: Chlorophyll-a Concentration

Chl-a concentration is described with CPHL. If possible, attribute *laboratory*_method and *laboratory*_analysis should be set to the laboratory method and analysis used.

3.3.1 Attributes

Name	Description
laboratory_technique	“HPLC”, “spectrophotometry”, “fluorometry_analysis”…
laboratory_method	e.g. if fluorometry, “acidification” or not; if HPLC, “using Van Heukelem & Thomas (2001)” or another reference

3.4 DOXY, DOX1, DOX2: Oxygen Concentration

DOXY, DOX1 and DOX2 are all oxygen concentrations in different units (see Table 3). DOXY is the most natural choice due to its relation to laboratory methods. DOX1 can be converted to DOXY knowing that 1 µmol of oxygen is equal to 0.022391 mg. DOX2 can also be converted using knowledge of density.

OSAT is another useful parameter about oxygen content in sea water and can be calculated from the dissolved oxygen concentration, temperature, pressure and salinity. Some sensors provide converted

values based on constant values or internal sensors. The latter are in many cases not as accurate as dedicated sensors for these specific auxiliary parameters. Full scientific information about dissolved oxygen is therefore achieved if information about internal auxiliary data and improved auxiliary data is provided. Moreover, whether the provided conversions arise from the internal or the improved auxiliary data should be provided. This minimal set of meta data can be easily provided in the variable attributes.

3.4.1 Attributes

Attributes *used_** and *corrected* are necessary if the provided data is the result of a conversion. The other ones should be provided to let users apply the conversions.

used_salinity	The value used for the conversion. This can be a constant value (for some sensors) or the name of salinity variable in the same file. Default is PSAL.
used_temperature	The value used for the conversion. This is the name of temperature variable in the same file. Default is TEMP.
used_pressure	The value used for the conversion. This can be a constant value (for some sensors) or the name of pressure variable in the same file. Default is PRESS or DEPH.
salinity	Name of salinity variable in same file that should be used for conversion. Default is PSAL.
temperature	Name of temperature variable in same file that should be used for conversion. Default is TEMP.
pressure	Name of pressure variable in same file that should be used for conversion. Default is PRESS or DEPH.
compensated	YES or NO. Default assumes YES.

4 QC TESTS

4.1 Introduction

This section enumerates the tests to be implemented. It is mostly designed to be used by programmers.

Tests have been tagged in the following categories

RT **(Real Time)**	The test can be applied almost as soon as the measurement is received and dedicated for implementation on repositories latest, monthly and history.
REP **(Reprocessing)**	These tests require a certain amount of data both before and after the considered measurement and are therefore intended for implementation on reprocessing activities.

The first revision of these tests has been developed on the basis of existing data in the GLOBAL CMEMS repository in winter 2017. As a consequence, only measurements in the upper 10m were used since this layer contains by far the majority of all observations (Figure 1).

The second revision has been updated with a new snapshot of the same repository in September 2017.

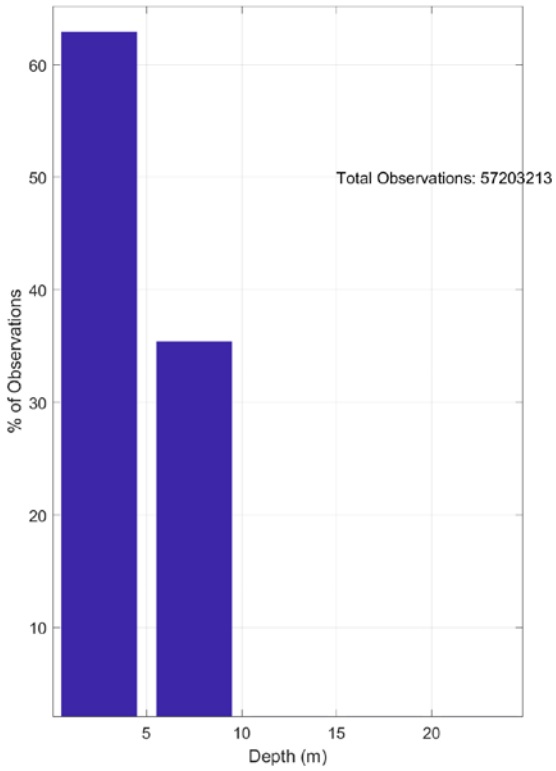

Figure 1 Depth occurrences of BGC parameters in January 2017 accounted for approximately 97% of the total observations within the top 10m.

4.2 Missing Value Test [RT, REP]

This tests 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

4.3 Frozen Value Test [RT, REP]

This test checks whether the values of N subsequent measurements are identically the same. If so, all of these should be marked as bad, QC=4.The effect is to comment out periods of sensor malfunction. The value of N will depend on the data sampling rate, on the sensor output and acquisition software.

Suggested values are provided in Table 5 and can be considered as a starting point to implement the test.

Table 5 Suggested number of consecutive measurements to take into account as a function the sampling time.

Δt ≤ 1min	N=10
Δt ≤ 5min	N=6
Δt ≤ 60min	N=3
Δt > 60min	N=2

4.4 Global Range Tests [RT, REP]

The purpose of this test is to comment out data that are far from values one can expect. For this test, one need minimal and maximal threshold values that can be applied on a global scale. Consequently, it is a very coarse control, but will in most circumstances detect sensor calibration errors or other malfunctions.

Thresholds must be obtained using statistical method on all available measurements. Any data not within the specified range should result in a bad value flag QC=4.

The high variability of BGC data can be caused by both high natural variations as well as sensor problems (e.g., biofouling, calibration). From the study of the data itself with no extra information, it is hard to separate natural variation from suspicious values.

This test checks whether the measured value is within a specified interval. Any value failing the test should be marked as bad, QC=4.

$$v_{\min} \leq v \leq v_{\max}$$

4.5 Local Range Tests [RT, REP]

This test is similar to the Global Range test, but with more specific thresholds based on regional and temporal scales. Any value failing the test should be marked as bad, QC=4.

$v_{\min} \leq v \leq v_{\max}$ Value for threshold limits rely on further analysis and expert knowledge from the selected areas.

A deeper analysis of the main BGC parameters (FLU2, CPHL, DOXY, DOX1, DOX2) has provided more detailed thresholds for the corresponding variables and covers now the global ocean as well as each region and period of the year.

The choice of thresholds has been based on the entire data set available from Copernicus, and in some cases (such as the Baltic) also on inter-comparison between sensor-based Chl a and measurements from bottle samples.

4.6 Spike Test [RT, REP]

Biogeochemical parameters may vary very much on all scales. Tests built on threshold limits would require very large threshold values and loose most of their effect. Moreover, BGC sensors based on optics often generate non-negligible noise. For example, this can be due to the presence of solid or gaseous particles in water affecting the optical properties of the water masses in the vicinity of the measured volume and hereby providing unwanted spikes. These oscillations depend on sensor technology but also local water masses and must be taken into account.

Therefore, the suggested procedure is to test the statistical entropy change caused by the measurement in consideration, as described by UEDA (2009). It is based on a 2 steps estimation of the Akaike information criterion

$$U_t = \frac{1}{2} AIC = n_g \log(\sigma) - n_b \frac{\log(n!)}{n}\sqrt{2}$$

$$\sigma = \sqrt{\frac{\sum \left(x_i - \bar{x}\right)^2}{n_g}} \quad i = 1 \ldots n_g$$

where σ is the uncorrected standard deviation based on the z-score values x from good measurements, n_g the number of good measurements and n_b the number of potential outliers. This formula provides an estimate of the statistical entropy for the n points considered.

Consider the new data being x_0, the 2 previous measurements (x_{-1}, x_{-2}) and the 2 next measurements (x_{+1}, x_{+2}). Calculate U_t for the 4 previous and next measurements (x_{-1}, x_{-2}, x_{+1}, x_{+2}), yielding U_t with n_g=n=4 and n_b=0. Then apply the same formula with all 5 points, yielding U_{t0} with n_g=4, n_b=1 and n=5.

The value $dU = U_{t0} - U_t$ is used to evaluate whether the value x_0 is a potential outlier, and the value is marked as an outlier if $dU > dU_{crit}$. The literature states that $dU_{crit} = 0$ should be used. However, our experience with Ferrybox data is that dU > 0 for most of the data, so using $dU_{crit} = 0$ would lead to a very large number of observations being marked as bad. The reason for this is probably that for a Ferrybox sensor, the change rate of BGC events is relatively high compared to the sampling rate (also see note below). Consecutive measurements are typically around 400m apart (for a Ferrybox with 1 minute intervals between measurements) which may be quite much relative to size of phytoplankton “hotspots”. We found that setting dU_{crit} to the 97th percentile of the dU for the whole time series achieved more reasonable flagging, and therefore adopted this as a pragmatic approach (Figure 2).

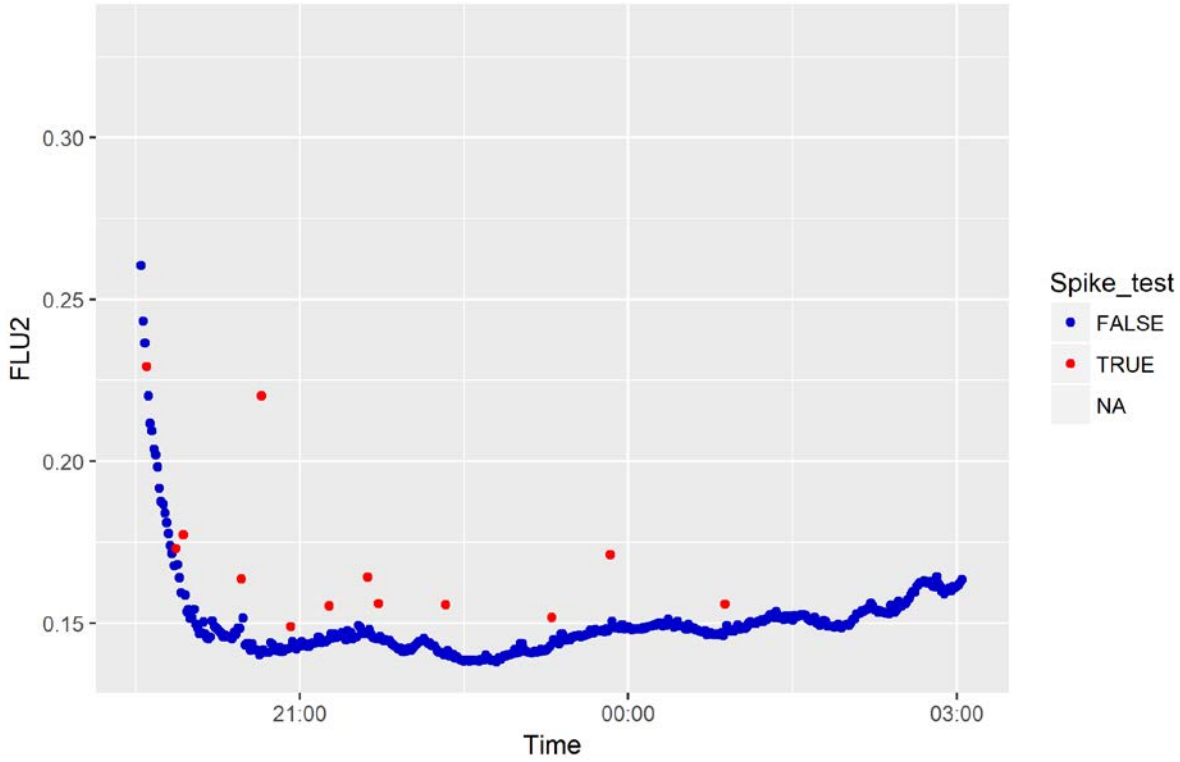

Figure 2 An example of spike detection.

The value x_0 is a potential outlier if this condition happens should be marked as bad with flag QC=4.

Important note: as for the Frozen Value Test in section 5.3, this test requires consecutive values and will only work well if the sampling rate is considerably higher than the change rate of BGC events. Therefore, this test should not be applied if the time between consecutive measurements is above 60 minutes.

4.7 The Start Test [REP]

Some fluorescence time series from vessels show clear indications of having high values in the first period after the boat leaves the harbor. The reason is probably that there is algal growth in the stagnant water in the ferrybox system while the boat is in the harbor, and it takes some time to remove this stagnant water from the system. The telltale indication of this phenomenon is that fluorescence values are higher shortly after a trip has started than in the same area at the end of the previous trip. One example is given in Figure 3. However, it should be verified that the difference is not solely due to a diurnal effect, as fluorescence values typically have a peak around sunrise. This can be done with a GAM (Generalized Additive Model) regression of fluorescence values, including three independent variables: position (e.g. latitude), direction of travel, and time of day. The interaction between the two former terms, should be included, and the latter should be included as a cyclic cubic regression spline.

When the time of day did not remove the effect of vessel direction, the observations were flagged the following way:

(1) the transect was divided in suitable pieces. In the example in Figure 4, the transect was divided by latitude in 0.05 latitude bins.

(2) For each piece of the transect, we checked the difference between fluorescence values for each vessel direction. We used both the mean difference and the p-value of a statistical t-test.

(3) For each piece at the northern end of the transect, we flagged all southward observations as bad (QC = 4) if the mean difference was > 0.02 and the p-value was < 0.01. At the southern end of the transect, we flagged all northward observations using the same criteria.

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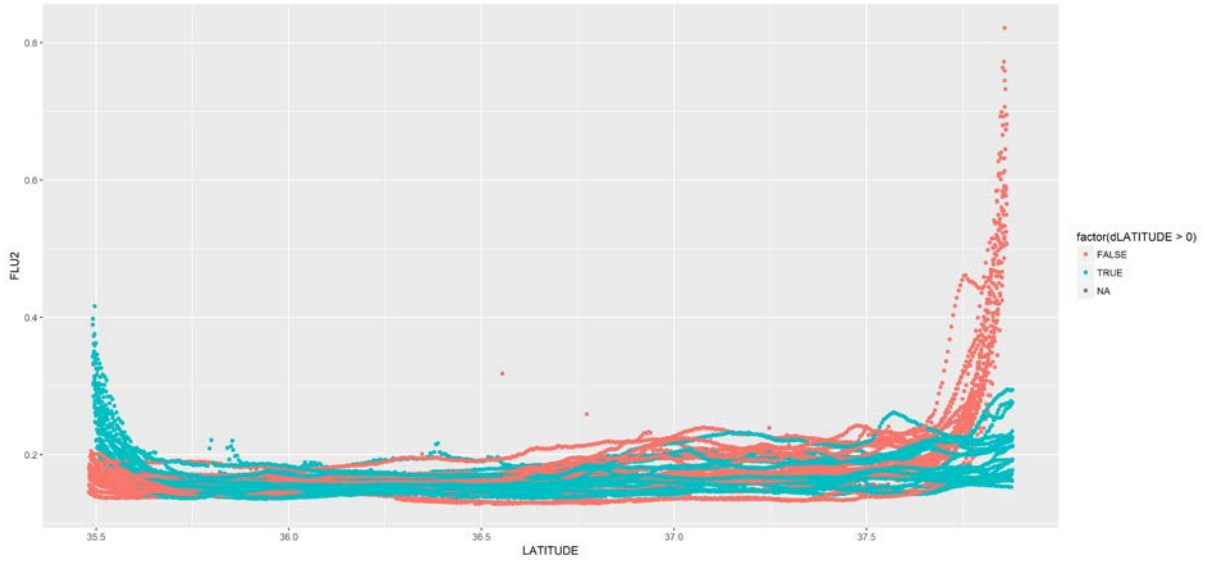

Figure 3 . Chl a fluorescence on the Athens- Heraklion line plotted relative to latitude (x axis) and direction of the vessel (southward = red, northward = blue). It can clearly be seen that for the same latitude, northward values are higher than southward values at the southern end of the transect, while the situation is opposite at the northern end of the transect. The effect of ship direction is particularly large at the northern harbour (Athens), probably because the vessel stays for a longer time at this harbour.

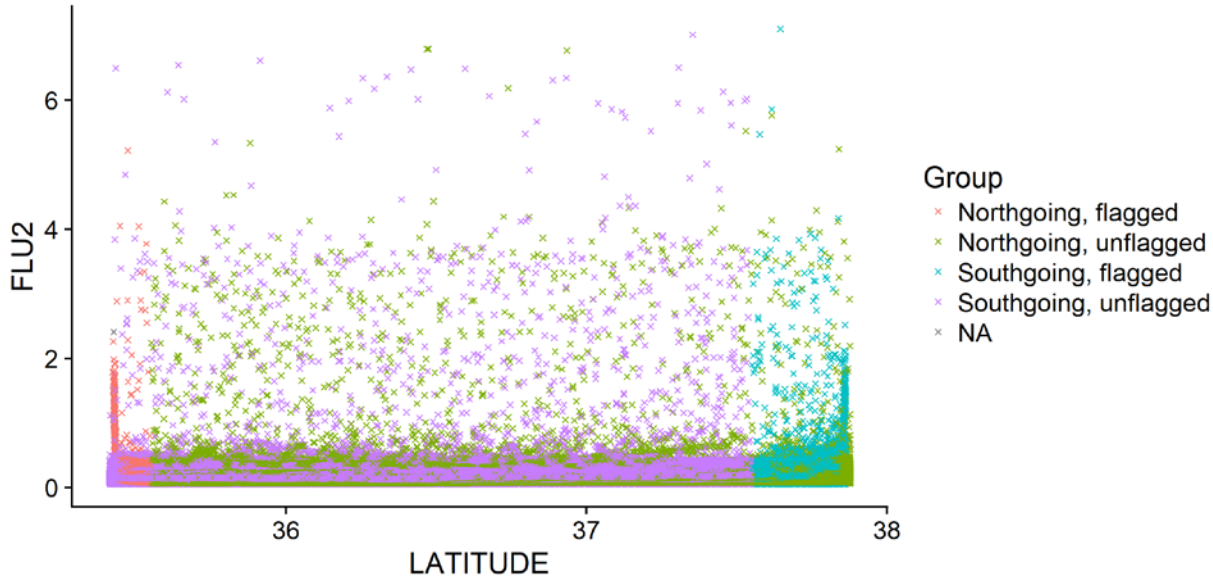

Figure 4. Flagging Chl a fluorescence values (as bad values, i.e. QC = 4) after applying the start test, flagging values where the mean difference was > 0.02 and the p-value was < 0.01.

4.8 Frozen Profile Test [RT, REP]

This test can detect an instrument that reproduces the same profile (with very small deviations) over and over again. It has been introduced for temperature and salinity data (e.g. Schuckmann et al 2010) It should be equally applicable to BGC data and was introduced in the first quality control tests for BGC data in MyOcean, 2009.

4.8.1 Step 1: Average Profiles

For each parameter derive an averaged profile by taking the median in 50 dbar slabs. This is necessary because the instruments do not sample at the same level for each profile. It is also preferable to use the median in order to reduce the effect of localized variation of BGC measurements. This yields the two new profiles

$$\overline{P_{prev}} \quad \overline{P_{next}}$$

4.8.2 Step 2 Compare Averaged profiles

Subtract the subsequent resulting profiles and compute the average, minimum and maximum values

$$\begin{aligned} \overline{\Delta P} &= \left\langle \overline{P_{next}} - \overline{P_{prev}} \right\rangle \\ \overline{\Delta P}_{\min} &= \min\left(\overline{\Delta P}\right) \\ \overline{\Delta P}_{\max} &= \max\left(\overline{\Delta P}\right) \end{aligned}$$

The test itself consist in checking these values against minimal thresholds. If all computed averages are less, the data must be flagged with flag QC=4.

4.9 Biofouling Test [REP]

Biofouling accumulates on the sensors, typically on a time scale of a few days. Often, this can be observed with steady increase of drifting values from the sensor. This bias is removed once the sensor is cleaned or replaced. Because the different platforms are maintained differently, a general rule is not obvious. In section 6 we suggest an experimental method for Chl a fluorescence that was derived from the CMEMS dataset. An evaluation will be required for improving results.

Detected biofouling events should be flagged with flag QC=3.

4.10 Ocean Colour Comparison [REP]

4.10.1 Concept

The main idea is to be in position to compare in-situ measurements of Chl a fluorescence against data from Ocean Colour with equivalent estimated quality. Depending on the observed relation between such pairs of points, a new quality flag is generated.

There is a risk of over- or under- estimate the data flags. Therefore, an adequate tuning is required and it depends on the nature of the in-situ data processed.

This method applies for Chl a fluorescence measurements performed at surface or very close to it (depths<3m). In-situ measurements are compared against L3 GlobColour products. Only good (QC=1) or probably good (QC=2) data is considered.

4.10.2 Procedure

In order to reduce the effects arising from the nature of the different data, a pseudo statistical approach has been chosen. The comparison is performed by using all OC and in situ data available within a specific area during defined time window. Tis is illustrated below (see Figure 6) with a box of 4x4 km. It corresponds to a megapixel of 16 GlobColour pixels and several measurements of ferrybox or of buoys.

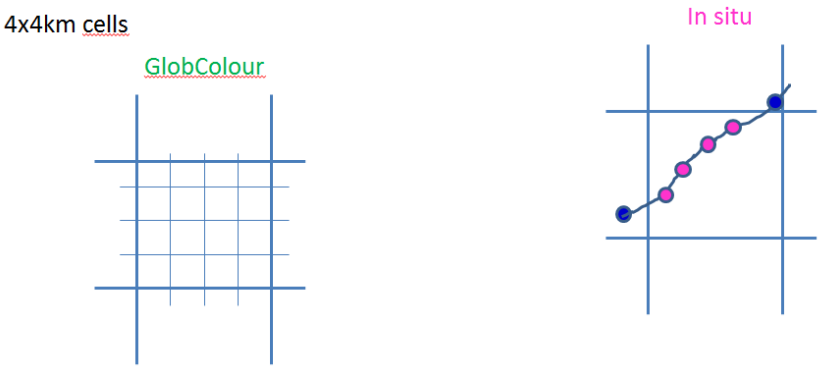

Figure 5 Joint exploitation of OC dataset and ferrybox and/or buoys data

A median and standard deviation is built on the megapixel from each dataset:

$$chla50_{insitu} \text{ and } \sigma_{insitu}$$
$$chla50_{sat} \text{ and } \sigma_{sat}$$

If known, the instrument standard deviation is quadratically added to σ_{insitu} and the uncertainty attached to the satellite product is quadratically added to σ_{sat}. Resulting values are compared and classified according to the situations described in Table 6.

Table 6 Classification rules for inter-comparison of in situ measurements with ocean colour.

Initial QC		Comparison status	
In situ QC	OC QC	 Overlap of the [-σ,+σ] intervals	 No overlap of the [-σ,+σ] intervals
1	1	Final QC: in situ 1	Final QC: in situ 3
2	1		

4.11 Summary

Table 7 lists the applicable QC tests by platform. A non-exhaustive list of platform types is given in the second row as examples.

Information in this table must be applied within the context of the data. For example, there are surface gliders types that will not provide *profile* datasets. Therefore, this platform is present in both columns *Profiles* and *Time Series*.

A separate column for non-continuous sampling is introduced as *Isolated Samples*.

Table 7 Applicable QC tests by platform

	***Profiles*[1]**	***Time Series/Trajectories***	***Isolated Samples***
	PF, GL, CT, SF, XB, SM	***GL, MO, RF, FB, TS, ML***	***BO***
Missing Value	x	x	x
Frozen Value	x	x	
Global Range	x	x	x
Local Range	x	x	x
Spike	x[1]	x	
Frozen Profile	x		
Biofouling		x	
Start		x	
Ocean Color	x	x	x

[1] If not mentioned otherwise, consecutive points in a profile are within that profile, and not from profile to profile.

5 FLU2

5.1 Data Selection

Tests in this section can be applied on variables satisfying that the unit for the variable is `mg m-3` or an equivalent.

It should be noted that fluorescence measured by Bio-Argo floats are recorded as CPHL with the attribute `sensing_method` set to `fluorescence`

1. The variable name is either
    a. FLU2 or
    b. CPHL with the attribute `sensing_method` set to `fluorescence`
2. In addition, the unit for the variable, in either case is `mg m-3` or an equivalent.

5.2 Global Range Tests

Small negative values of Chl a can also occur, and explained mainly by instrumental and electronic "noise" or a small drift in the calibration.

Based on this, global limits for FLU2 are defined in Table 8.

Table 8 Global thresholds for FLU2

	Min	Max
FLU2 (mg m^{-3})	-0.1	80

5.3 Local Range Test

Limits for FLU2 and CPHL are listed in Table 9 and Table 10, respectively.

Table 9 Ranges for FLU2.

	Month		Longitude		Latitude		Depth		Range test	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Global	1	9	-180	180	-30	90	0	200	-0,1	20
Global	10	12	-180	180	-30	90	0	200	-0,1	10
Global	1	12	-180	180	-90	-30	0	200	-0,1	10
Global	1	12	-180	180	-90	90	200	10000	-0,1	0,5
Arctic	1	2					0	200	-0,1	2
Arctic	3	4					0	200	-0,1	12
Arctic	5	9					0	200	-0,1	6
Arctic	10	12					0	200	-0,1	2
Arctic	1	12					200	10000	-0,1	0,5
North Sea	1	6					0	200	-0,1	14
North Sea	7	8					0	200	-0,1	8
North Sea	9	12					0	200	-0,1	12
North Sea	1	12					200	10000	-0,1	0,5
Baltic	1	2	23,22	30,2	59,5	60,3	0	200	0,5	25
Baltic	3	5	23,22	30,2	59,5	60,3	0	200	1,5	77,6
Baltic	6	9	23,22	30,2	59,5	60,3	0	200	0,5	36,8
Baltic	10	12	23,22	30,2	59,5	60,3	0	200	0,5	25
Baltic	1	2	19,88	23,21	58,4	59,6	0	200	0,5	6
Baltic	3	5	19,88	23,21	58,4	59,6	0	200	1,5	31
Baltic	6	9	19,88	23,21	58,4	59,6	0	200	0,5	13
Baltic	10	12	19,88	23,21	58,4	59,6	0	200	0,5	25
Baltic	1	2	12,27	17,09	54,5	56,2	0	200	0,5	7,6
Baltic	3	5	12,27	17,09	54,5	56,2	0	200	1,5	27,3
Baltic	6	9	12,27	17,09	54,5	56,2	0	200	0,5	20,5
Baltic	10	12	12,27	17,09	54,5	56,2	0	200	0,5	25
Celtic Sea	1	12					0	200	-0,1	12
Celtic Sea	1	12					200	10000	-0,1	0,5
Bay of Biscay	1	12					0	200	-0,1	12
Bay of Biscay	1	12					200	10000	-0,1	0,5
Mediterranean	1	6					0	200	-0,1	25
Mediterranean	7	12					0	200	-0,1	20
Mediterranean	1	12					200	10000	-0,1	0,5
Black Sea	1	12					0	200	-0,1	25
Black Sea	1	12					200	10000	-0,1	0,5

Table 10 Ranges for CPHL using the fluorescence method.

	Month		Longitude		Latitude		Depth		Range test	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Global	1	3	-180	180	60	90	0	200	-0,1	10
Global	4	6	-180	180	60	90	0	200	-0,1	20
Global	7	12	-180	180	60	90	0	200	-0,1	10
Global	1	12	-180	-120	30	60	0	200	-0,1	10
Global	1	12	-120	-30	30	60	0	200	-0,1	20
Global	1	12	-30	180	30	60	0	200	-0,1	10
Global	1	12	-180	-60	0	30	0	200	-0,1	5
Global	1	12	-60	180	0	30	0	200	-0,1	7,5
Global	1	12	-180	-90	-30	0	0	200	-0,1	5
Global	1	6	-90	-60	-30	0	0	200	-0,1	5
Global	7	9	-90	-60	-30	0	0	200	-0,1	15
Global	10	12	-90	-60	-30	0	0	200	-0,1	5
Global	1	6	-60	30	-30	0	0	200	-0,1	15
Global	7	12	-60	30	-30	0	0	200	-0,1	10
Global	1	12	30	120	-30	0	0	200	-0,1	5
Global	1	12	120	180	-30	0	0	200	-0,1	10
Global	1	3	-180	-60	-90	-30	0	200	-0,1	7,5
Global	4	6	-180	-60	-90	-30	0	200	-0,1	15
Global	7	12	-180	-60	-90	-30	0	200	-0,1	7,5
Global	1	6	-60	30	-90	-30	0	200	-0,1	15
Global	7	9	-60	30	-90	-30	0	200	-0,1	10
Global	10	12	-60	30	-90	-30	0	200	-0,1	15
Global	1	6	-60	180	-90	-30	0	200	-0,1	15
Global	7	9	-60	180	-90	-30	0	200	-0,1	10
Global	10	12	-60	180	-90	-30	0	200	-0,1	15
Global	1	12	-60	180	-90	-30	200	10000	-0,1	0,5
Arctic	1	12					0	200	-0,1	10
Arctic	1	12					200	10000	-0,1	0,5
North Sea	1	12					0	200	-0,1	10
North Sea	1	12					200	10000	-0,1	0,5
Baltic	1	12					0	200	-0,1	10
Baltic	1	12					200	10000	-0,1	0,5
Celtic Sea	1	12					0	200	-0,1	10
Celtic Sea	1	12					200	10000	-0,1	0,5
Mediterranean	1	12					0	200	-0,1	10
Mediterranean	1	12					200	10000	-0,1	0,5
Bay of Biscay	1	12					0	200	-0,1	10
Bay of Biscay	1	12					200	10000	-0,1	0,5
Black Sea	1	12					0	200	-0,1	10
Black Sea	1	12					200	10000	-0,1	0,5

5.4 Frozen Profile Test

The thresholds to be used for data from variable FLU2 are

$$\overline{\Delta P} < 0.02 \mu g / l$$
$$\overline{\Delta P}_{\min} < 0.001 \mu g / l$$
$$\overline{\Delta P}_{\max} < 0.3 \mu g / l$$

5.5 Biofouling Test

For chlorophyll-a fluorescence, biofouling leads to a steady increase of measured values. However, variations may still be superimposed. When the sensor is cleaned, values drop quickly to a much lower level. In a natural bloom, data variance will tend to increase less. Moreover, the lower 5th percentile is expected to increase slower than the median value.

We have developed a test for indicating possible biofouling events. However, the “signature” of biofouling is not easy to describe mathematically in a way that separates them form normal bloom events, and the flags set by the test should be checked by an expert. The test, described in detail in chapter 6.5.1, can shortly be described as follows: first, we calculate the 5th percentile and the median value for each 6-hour period of data, reducing each day of data to 8 values (step 1). These are then analysed over windows of 6 days in step 2-4. The percentile and median values are first normalized for each 6-day period (step 2). Then, two numbers (denoted features) are calculated for each period; the first indicates whether there was an apparent increase in fluorescence values during the first 5 days, the second indicates whether there was a sudden decrease from day 5 to day 6 (step 3). From these two features, we calculate a coefficient $P_{biofoul}$ which indicate the probability that day 5 marks the end of a biofouling period (i.e. sensor cleaning; step 4). When steps 2-4 are repeated (with overlap) for every 6-day period, it results in a list of possible biofouling end points, indicated by high values of $P_{biofoul}$. For each of these end points, one goes back in time to find the start of the possible biofouling period (step 5). The possible biofouling periods are then shown graphically (step 6) for evaluation by an expert. In practice, the expert looks over the graphs and notes in a spreadsheet which events (marked by numbers in the graphs) that appears to be actual biofouling. This spreadsheet is then used as input to an R script which performs the actual flagging of the raw data.

Figure 5 shows an example of graphical presentation of possible biofouling events, used for later expert judgement. Because the start and end of periods are recorded by the procedure, the expert needs only to make a simple decision whether or not s/he accepts each preliminary flag, minimizing the time use of the expert. Measurements during biofouling events should be flagged as potentially correctable, QC=3.

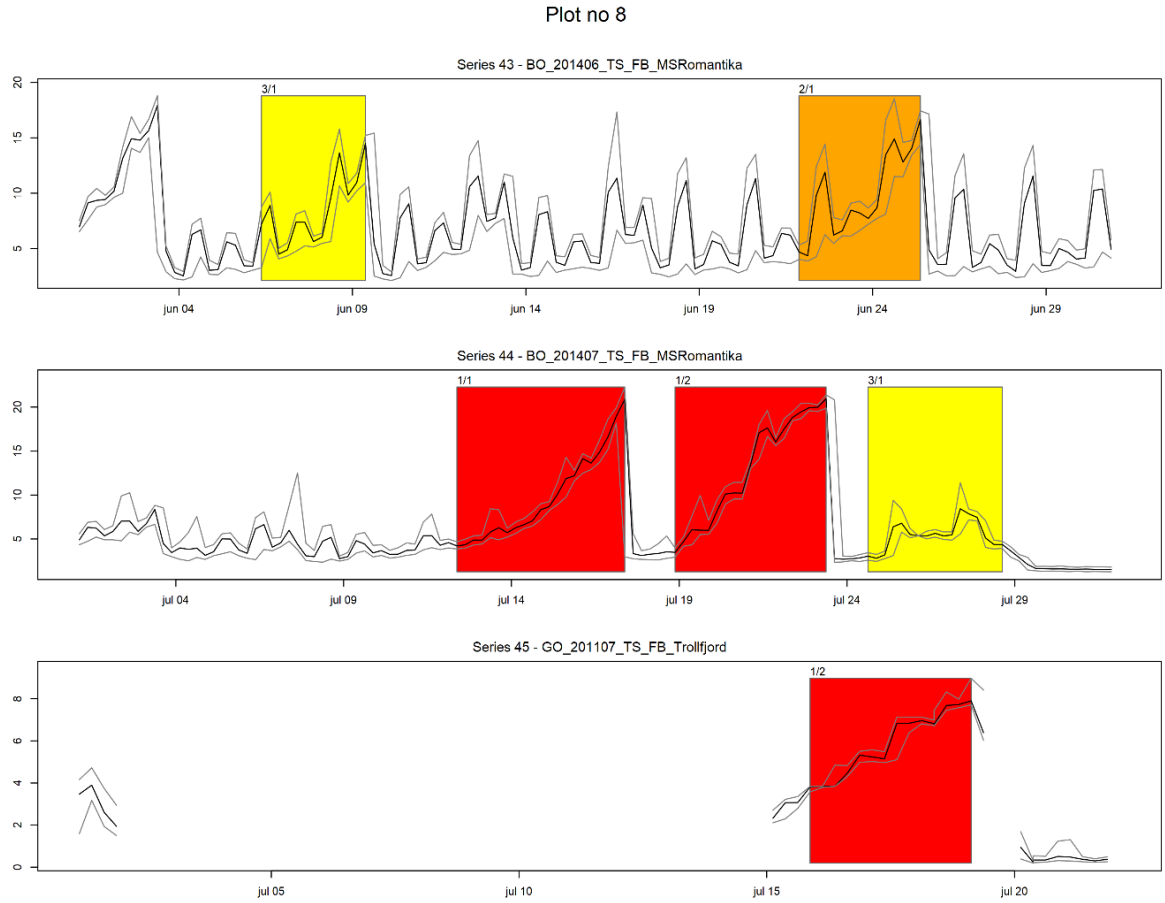

Figure 6 Biofouling indication. The time series shown are 6-hour means of Chl a fluorescence, and the yellow-, orange and red-coloured areas indicate where the mathematical properties of the time series indicate possible fouling. The indication is used together with expert judgement.

5.5.1 Implementation

5.5.1.1 Step 1: Generate 6-hour statistics

Extract slabs of 6-hour duration and calculate the following parameters on these

- $Q_{5,i}$ 5th percentile
- M_i median

The dataset is now described by 4 such parameters a day. They are indexed by *i=1…N* where N is then *4* times the number of days.

5.5.1.2 Step 2: Normalize over a 6-day period

In order to evaluate possible biofouling for a given point in time, i.e., 6-hour period number *i*, we group these parameters over a 6-day period, starting 5 days before the time in question and ending 1 day

after. So for 6-hour period *i*, we used the 24 6-hour means from *i*-19 to *i*+3. We then normalize $Q_{5,i}$ and M_i, so the resulting normalized parameters $q_{5,i}$ and m_i fill the range 0 to 100 inclusive. For the 5th percentile values:

$$\begin{aligned} Q_{\min} &= \min(Q_{5,i}, Q_{95,i}) \\ Q_{\max} &= \max(Q_{5,i}, Q_{95,i}) \\ q_{j,i} &= \frac{Q_{j,i} - Q_{\min}}{Q_{\max} - Q_{\min}} \quad j = 5,95 \end{aligned}$$

And the same is performed for the median values

$$\begin{aligned} M_{\min} &= \min(M_i) \\ M_{\max} &= \max(M_i) \\ m_i &= \frac{M_i - M_{\min}}{M_{\max} - M_{\min}} \end{aligned}$$

5.5.1.3 Step 3: Calculate features of each 5-day period

Based on the numbers of the previous step, we calculated the following two numbers for each 5-day period:

1) *Rsq*Q5$_i$ = R^2 value for the linear regression of the 20 normalized 5th percentiles ($q_{5,i}$) from i-19 to i as a function of time

2) MedianDiff $_i$ = min(m_{i-4}, m_{i-3}, m_{i-2}, m_{i-1}) – max(m_i, m_{i+1}, m_{i+2}, m_{i+3})

5.5.1.4 Step 4: Define the end point of the possible biofouling periods

Based on the features defined in the previous step , we calculated the following value

$P_{biofoul,i} = e^{A(i)}$

A(i) = 0.05648 + 0.3771* $RsqQ5_{,i}$ + 0.006733*MedianDiff $_i$

If $P_{biofoul,i}$ exceeded 0.35, we considered it to be the end point of a possible biofouling period. This value was calculated for all 6-hour periods, giving a list of end points. The coefficients used were developed using statistical analysis of a test set of data.

5.5.1.5 Step 5: Define the start point of the possible biofouling periods

For each end point, we found the median (M_i) and the 5th percentile ($Q_{5,i}$) fluorescence value 12 hours later, which we denoted M_{crit} and $Q_{5,crit}$, respectively. We then went back in time and found

1) The last 6-hour period before the end point where M_i / M_{crit} < 1.5

2) The last 6-hour period before the end point where $Q_{5,i}$ / $Q_{5,crit}$ < 1.5

The start point of the possible biofouling period was then defined as the first of those two (i.e., lowest *i*).

5.5.1.6 Step 6: Categorize the possible biofouling periods

The colour of the possible biofouling period (yellow, orange and red in Fig. 5) was defined by the value of $P_{biofoul,i}$ of the end point of the period:

$0.35 < P_{biofoul,i} \leq 0.45$: yellow

$0.45 < P_{biofoul,i} \leq 0.60$: orange

$0.60 < P_{biofoul,i}$: red

6 DOXY

6.1 Data Selection

Tests in this section can be applied on variables satisfying

1. The variable name is DOXY and
2. the unit is mmol m^{-3} or an equivalent

6.2 Global Range Tests

Table 11 Global range thresholds for DOXY

	Min	Max
DOXY (µM)	0	500

6.3 Local Range Tests

Table 12 Local range thresholds for DOXY

	Month		Longitude		Latitude		Depth		DOXY (µM)	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Global	1	12	-180	180	-90	90	0	200	-0,1	500
Global	1	12	-180	180	-90	90	0	200	-0,1	300
Arctic	1	12					0	200	-0,1	500
Arctic	1	12					200	10000	-0,1	300
North Sea	1	12					0	200	-0,1	500
North Sea	1	12					200	10000	-0,1	300
Baltic	1	12					0	200	-0,1	500
Baltic	1	12					200	10000	-0,1	300
Celtic Sea	1	12					0	200	-0,1	300
Celtic Sea	1	12					200	10000	-0,1	250
Mediterranean	1	12					0	200	-0,1	350
Mediterranean	1	12					200	10000	-0,1	250
Bay of Biscay	1	12					0	200	-0,1	350
Bay of Biscay	1	12					200	10000	-0,1	250
Black Sea	1	12					0	200	-0,1	500
Black Sea	1	12					200	10000	-0,1	300

6.4 Frozen Profile Test

The thresholds to be used for data from variable DOXY are

$$\overline{\Delta P} < 0.6\mu M$$
$$\overline{\Delta P}_{\min} < 0.03\mu M$$
$$\overline{\Delta P}_{\max} < 9\mu M$$

7 DOX1

7.1 Data Selection

Tests in this section can be applied on variables satisfying

3. The variable name is DOX1 and
4. the unit is ml l^{-1} or an equivalent

7.2 Global Range Tests

Table 13 Global thresholds for DOX1

	Min	Max
DOX1 (ml/l)	0	20

7.3 Local Range Tests

Table 14 Local range thresholds for DOX1

	Month		Longitude		Latitude		Depth		Range test	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Global	1	12	-180	180	-90	90	0	200	-0,1	15
Global	1	12	-180	180	-90	90	0	200	-0,1	12
Arctic	1	12					0	200	-0,1	15
Arctic	1	12					200	10000	-0,1	12
North Sea	1	12					0	200	-0,1	15
North Sea	1	12					200	10000	-0,1	12
Baltic	1	12					0	200	-0,1	20
Baltic	1	12					200	10000	-0,1	12
Celtic Sea	1	12					0	200	-0,1	13
Celtic Sea	1	12					200	10000	-0,1	8
Mediterranean	1	12					0	200	-0,1	10
Mediterranean	1	12					200	10000	-0,1	8
Bay of Biscay	1	12					0	200	-0,1	13
Bay of Biscay	1	12					200	10000	-0,1	8
Black Sea	1	12					0	200	-0,1	10
Black Sea	1	12					200	10000	-0,1	8

7.4 Frozen Profile Test

The thresholds to be used for data from variable DOX1 are

$$\overline{\Delta P} < ml/l$$
$$\overline{\Delta P}_{\min} < ml/l$$
$$\overline{\Delta P}_{\max} < ml/l$$

8 DOX2

8.1 Data Selection

Tests in this section can be applied on variables satisfying

5. The variable name is DOX2 and
6. the unit is µmol kg^{-1} or an equivalent

8.2 Global Range Tests

Table 15 Global range thresholds for DOX2

	Min	Max
DOX2 (µmol kg^{-1})	0	600

8.3 Local Range Tests

Table 16 Local range thresholds for DOX2

	Month		Longitude		Latitude		Depth		Range test	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Global	1	12	-180	180	-90	90	0	200	-0,1	400
Global	1	12	-180	180	-90	90	0	200	-0,1	400
Arctic	1	12					0	200	-0,1	400
Arctic	1	12					200	10000	-0,1	600
North Sea	1	12					0	200	-0,1	400
North Sea	1	12					200	10000	-0,1	300
Baltic	1	12					0	200	-0,1	400
Baltic	1	12					200	10000	-0,1	300
Celtic Sea	1	12					0	200	-0,1	400
Celtic Sea	1	12					200	10000	-0,1	300
Mediterranean	1	12					0	200	-0,1	300
Mediterranean	1	12					200	10000	-0,1	250
Bay of Biscay	1	12					0	200	-0,1	300
Bay of Biscay	1	12					200	10000	-0,1	300
Black Sea	1	12					0	200	-0,1	400
Black Sea	1	12					200	10000	-0,1	300

8.4 Frozen Profile Test

The thresholds to be used for data from variable DOX2 are

$$\overline{\Delta P} < 0.6\mu\text{mol/kg}$$
$$\overline{\Delta P}_{\min} < 0.03\mu\text{mol/kg}$$
$$\overline{\Delta P}_{\max} < 9\mu\text{mol/kg}$$

9 SCIENTIFIC BACKGROUND

9.1 Chlorophyll *a*

As described below, conditions affecting in vivo or *in situ* Chl a fluorescence emission are:

- Light regime (t/day, day length)
- Self-shading and dense blooms
- Different species and groups
- Regional variability
- Nutrient status

When eukaryotic algae absorb light (Photosynthetically Active Radiation (PAR, 400-700 nm)), 1-5 % of this light will be re-emitted as fluorescence. Many pigments (light absorbing molecules) are involved in the light harvesting (Figure 6), but the fluorescence is mainly (95 %) emitted from the pigment Chl a in the reaction center II (RC II) of the photosynthesis light reactions in photosystem II (PSII).

Pigments in the phytoplankton cells form antenna like structures for an effective harvesting of the spectral light. The absorption happens when an electron of the pigment is excited into a higher energy state. This energy is sent down the antennae of pigments to the reaction center (RC) Chl a (Figure 6). When the RC Chl a is excited, the excitation energy can be released mainly by three competing de-excitation pathways; heat, photochemistry and fluorescence. The amount of fluorescence from the absorbed light is the yield of fluorescence (ϕF), which increases from 0 in total darkness to 3-5% in saturating light intensities. If the cells are extracted, e.g. in methanol, the connection from RC to photosynthesis is broken and fluorescence can reach 30 % (Krause and Weis, 1991, Owens, 1991, Govindje, 1995, Falkowski and Raven, 1997, Huot and Babin, 2010, Johnsen et al., 2011).

The ratio of in vivo Chl *a* fluorescence against extracted Chl a concentration may vary remarkably (Figure 7). This is a result of physiological processes in algae such as photosystem regulation,

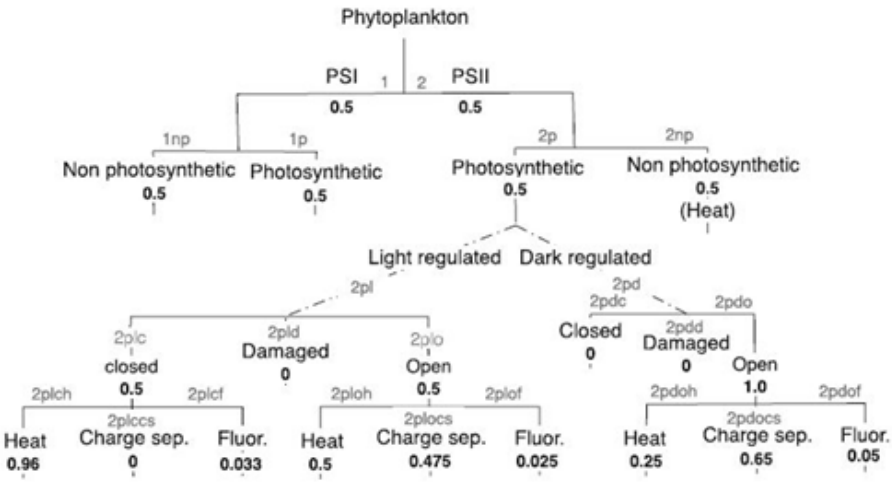

Figure 7 Fates of absorbed photons in phytoplankton as originally shown in Huot and Babin, 2010. RC's can either be closed (excited) or open (not exited) and is dependent on light acclimation status.

acclimation to environmental conditions (e.g. low light, nutrient stress etc.), or adaptation to different environmental pressures conditions in order to optimize their evolutionary fitness (Raven and Geider, 2003). One example from the Ferrybox system in Norway (Figure 7) shows that the Chl a fluorescence often appears too high at low Chl *a* concentrations and too low at high Chl *a* concentrations, using a calibration of the sensor based on cultures (Figure 6). This figure does not leave out any outliers, which i.e. could be caused by patchiness in the distribution of algae, leading to inconsistency between sensor and sampling, and thus it also shows how a validation and calibration procedure can be biased by inaccurate sampling (Johnsen et al., 2011).

This high variation in fluorescence is a result of varying light conditions (irradiance, spectral composition and day length) and different algae groups and species (described below). In low light conditions, light harvesting pigments (LHP's) efficiently transfer the light energy to the reaction centers (RC) of photosynthesis, and chloroplasts are distributed to give maximum light harvesting. The efficiency is reduced in high light conditions, because photo-protecting carotenoids (PPC's) increase in amount and thereby reduce the flux of photons to the reaction centers. In addition, high light conditions can cause a reduction in the amount of Chl a within each cell as well as the number, size and distribution of the chloroplasts (Johnsen et al., 2011, Brunet et al., 2011).

Different groups/species of phytoplankton contain different additional pigments (LHC's and PPC's), and different xanthophyll cycles, i.e in diatoms (diadinoxanthin to diatoxanthin) or green algae (violaxanthin to zeaxanthin) which are processes related to light stress (Brunet et al., 2011). Some algae (green and phycobiliprotein-containing) have state transitions between light harvesting complexes related to RCII and RCI.

The processes described above all reflect in in vivo fluorescence measurements, because, as mentioned before, the absorbed light energy (photons) can be released mainly by three competing de-excitation pathways; heat, photochemistry and fluorescence as was schematically shown in Huot and Babin, 2010 (Figure 6).

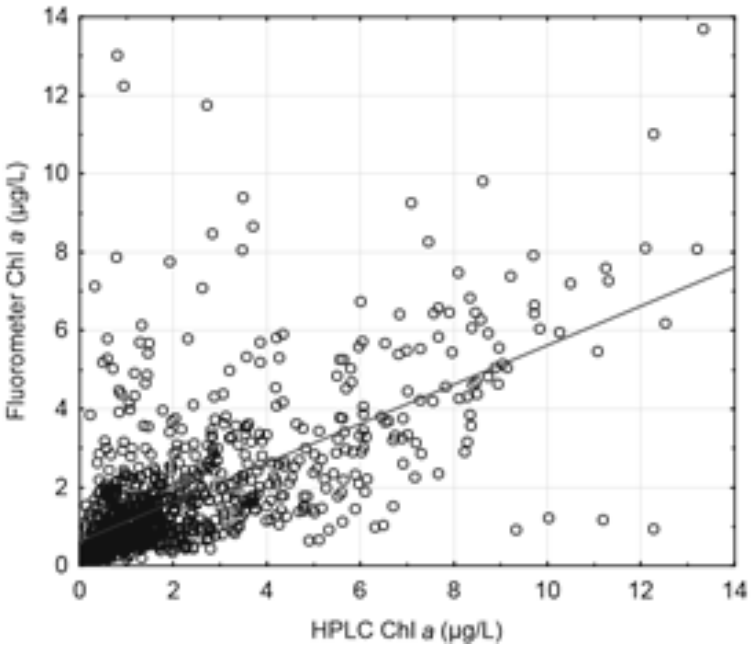

Figure 8 Regression plot between Fluorometer Chl a and HPLC Chl a concentration (from Ferrybox data during the years 2003-2008), r2= 0.3909.

In some regions cyanobacteria can dominate the phytoplankton biomass. Cyanobacteria are considered to be the most primitive organisms and they have prokaryotic cell structure. They have a different allocation of energy regarding the photosystems. In cyanobacteria the most of Chl a is located in the non-fluorescing photosystem I. However this Chl a is included in the extracted Chl a yield. On the other hand, phycobilin pigments such as phycocyanin (specific for filamentous cyanobacteria) provide strong in vivo fluorescence. Consequently during abundant cyanobacteria blooms occurring annually in the Baltic Sea, the phycocyanin fluorescence should be used as auxiliary parameter to correct the ratio of in vivo Chl a fluorescence against extracted Chl a concentration (Seppälä et al., 2007).Moreover, the ratio between in vivo Chl a fluorescence measurements and in vitro HPLC or spectrophotometric Chl a concentration is not constant and may vary significantly with a factor 3-4 depending on various conditions. Thus, when using real-time measurements of Chl a fluorescence as a proxy for Chl a concentration, the users should be aware of the natural variation in Chl a fluorescence relative to Chl a concentration. Subsequently, there is a need to make clearly distinctions between bad Chl a fluorescence data caused by sensor failure, or a bad calibration, and "uncertain" estimates of Chl a concentration caused by inherent natural variations in the Chl a fluorescence.

This is clearly observed in Figure 8where one year of Chl a measurements using both fluorescence sensor from a Ferrybox and HPLC analysis from water samples are compared. The signal from fluorescence is higher during the night. The difference between day and night is even higher during blooming periods. This difference is also depending on whether the HPLC analysis is using samples taken during day or night.

Similarly, Figure 9 shows the difference one will measure with the same fluorescence sensor in water masses containing different algae species. This introduces typically uncertainties on measurements from moving platforms travelling through different water masses.

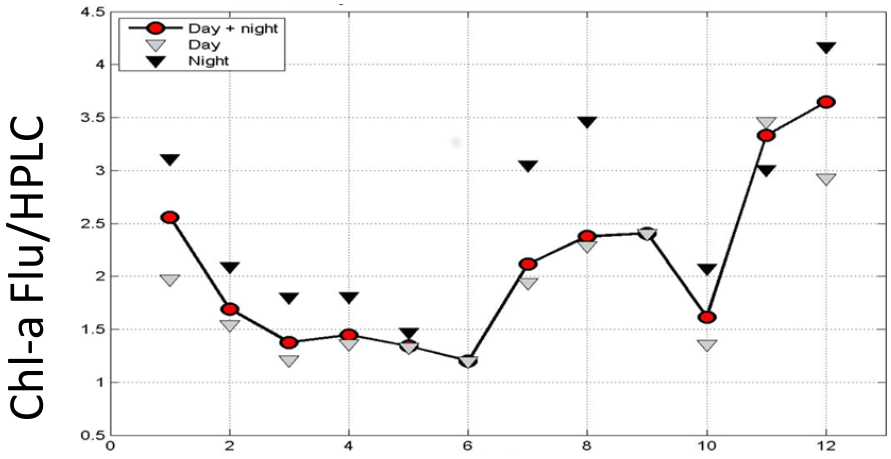

Figure 9 Study of measurements for Chl a from fluorescence sensor and HPLC analysis during one year of Ferrybox data.

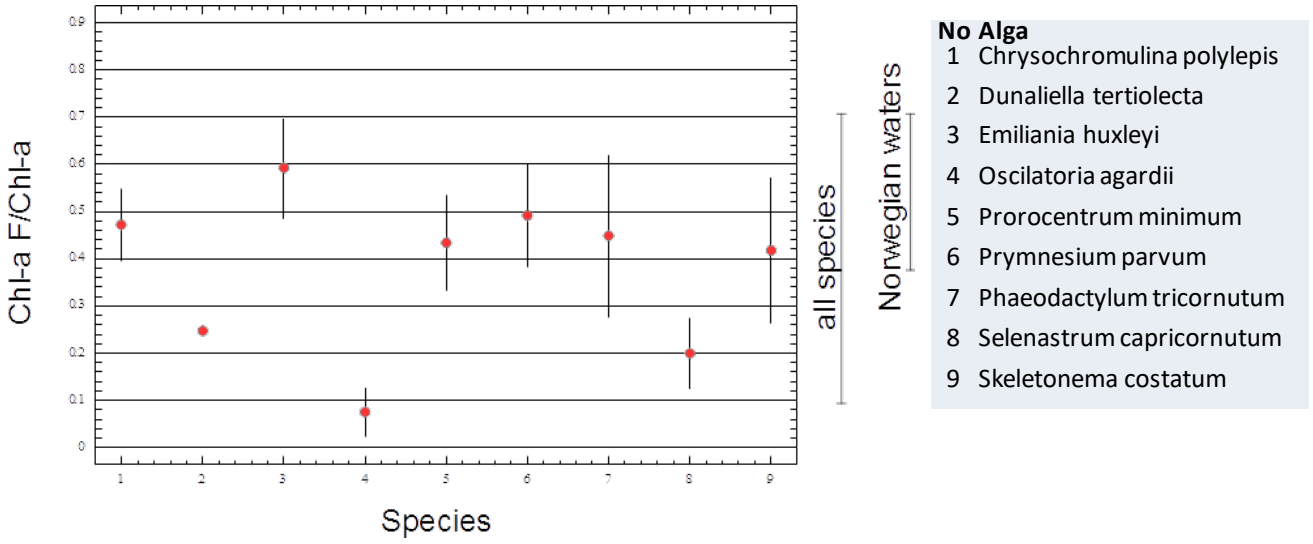

Figure 10 Study of measurements for Chl *a* from fluorescence sensor and HPLC analysis for different algae species. The list of algae species on the x-axis is on the right side of the figure.

Phytoplankton growth, chlorophyll content and fluorescence response are strongly related with nutrient status (Kruskopf & Flynn 2006). Nutrient stress cause increased chlorophyll a fluorescence. Consequently, when the phytoplankton spring bloom collapses after the dissolved nitrogen is exhausted, the increased chlorophyll fluorescence in comparison to chlorophyll a content is observed.

9.2 Oxygen Concentration

Most biological and chemical processes are influenced by dissolved oxygen concentrations. The standard measurement of oxygen includes fixation and precipitation followed by titration and is known as the Winkler titration (Winkler, 1888).

For high temporal and spatial resolution data this method is not suitable. For direct measurements of oxygen, optodes may be more suitable (Tengberg et al., 2006). Optodes are based on excitation of ruthenium-complexes and measurements of the red luminescence. Oxygen measurement is made by phase shift detection of the returning, oxygen quenched red luminescence. This phase shift is a function of the O2 partial pressure and hereby dissolved oxygen concentration.

Calibration of optodes is usually performed using water solution with 0% and 100% saturation. Temperature and salinity are used to calculate the concentration. For the AADI optode, the first parameter is provided by an internal sensor while salinity is a constant with a factory default set to zero psu.

Typically, an error of 1°C will lead to an error of about 4µM oxygen concentration. For salinity, an error of 2ppm yields a difference close to 3µM on oxygen concentration. Therefore, measurements must be corrected with the most accurate temperature, salinity and pressure values available. If this is not performed prior to data distribution, meta information for the correction should be at least provided.

9.3 Concluding Remarks

Using a fluorescence sensor to measure Chl a concentration can only provide a proxy for the real chlorophyll -a concentration. Results will depend on incident irradiance, self-shading, physiological states, community composition etc. light conditions and algae species the sensor was used during calibration. The sensor will provide a measurement close to reality for the conditions closest to those applied during calibration. For measurements performed in the field, different light conditions and water masses should lead to a relative uncertainty of anything up to 50% or more.

If dissolved oxygen is obtained from a signal proportional to saturation, the oxygen concentration is not provided by a direct measurement but by a conversion involving auxiliary data. These do not necessary provide a satisfying accuracy or configuration level. Consequently, the converted oxygen concentrations should be either converted before distribution or provide meta data about auxiliary values.

10 REFERENCES

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