Project: WP15

Real Time Quality Control of biogeochemical measurements

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1 Introduction

MyOcean is the implementation project of the GMES Marine Core Service, aiming at deploying the first concerted and integrated pan-European capacity for Ocean Monitoring and Forecasting (http://www.myocean.eu.org). The project objective is to analyze, forecast and observe the oceans at global and regional (European Seas) scales in order to provide a monitoring service for marine environment and security.

Based on the approach on combining space and in-situ observations and their assimilation into 3-D simulation models, the MyOcean Service aims to provide the best information available on the global and regional ocean. These information include temperature, salinity, currents, ice extent, sea level and primary ecosystems. Its target applications are marine safety, marine resources, climate and seasonal forecasting as well as marine and coastal environment.

An important step within the MyOcean project is to harmonize existing Real Time Quality Control (RTQC) and quality assurance procedures of the different nations involved. As the MyOcean service is thought to be available at any time and open to anyone, an agreement in good RTQC methods and procedures is vital to guarantee high data quality distributed to users via international exchange. The agreement on the implementation of uniform RTQC procedures has the severe potential to overcome the non-consistency within the existing datasets actually provided by the international community.

One of the various tasks of the MyOcean project - the Work Package (WP) 15 – deals with the scientific and technical validation of In Situ-TAC (Technical Assembly Centres) products and forms the frame of this document. WP15 aims to perform operational quality control (QC) of global and regional products as well as to lead scientific assessment validation activities with regional responsibilities. Beside global scale products, regional specifications are performed in the Arctic, the Black Sea, the North-western Shelves, the Baltic Sea, the South-western Shelves and the Mediterranean Sea. It follows therewith the EuroGOOS regional approach, with establishing regional alliances.

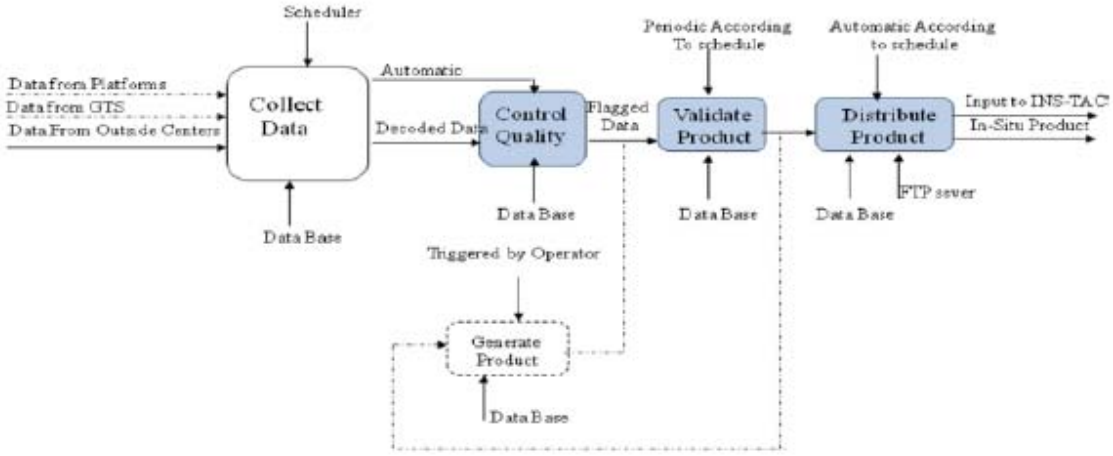

Figure 1: Functions to be implemented by an In-Situ Tac component (meeting report: MYO-INS-MR-2009-03-30)

The different functions to be implemented by the global and regional components of the In-Situ Tac are summarized in Figure 1. This document describes the RTQC to be performed on biogeochemical (BGC) *in-situ* data in the MyOcean project. In MyOcean the quality controlled biogeochemical data will be mainly used for model validation and for satellite ocean colour data assessment. Data will also be made available to users of the marine core service under special agreements.

As recommended at OceanObs09 (Claustre & al 2009), the BGC data compiled within MyOcean are confined to:

- Chlorophyll-a fluorescence
- Oxygen (concentration and saturation)
- Nutrients (e.g. NH_4, NO_3/NO_2, PO_4, Si(OH4))

The main focal point of this document is to describe quality tests recommended to be commonly applied for the BGC data from the various observational platforms. At present the use of nutrient sensors on autonomous platforms is very limited (d'Ortenzio et al 2010). Hence the amount of nutrient data that will be delivered to MyOcean in real time is expected to be very low. The quality tests in this document are therefore defined for chlorophyll-a and oxygen measurements only.

The proposals for RTQC 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 (2007), ECOOP (Tamm and Soetje, 2009), GOSUD (2006), M3A (Basana et al., 2000), Argo (2009) and MyOcean T/S (Schuckmann et al. 2010) QC procedures, as well as in-house expertise from contributors to this report.

While the reduced quality of temperature and salinity data is mainly related to problems with bad geo-localisation, erroneous timing, wrong platform identification, pressure errors and sensor artefacts (introducing spikes, abrupt gradients, stuck values etc.), BGC data is additionally impacted by natural biofouling disturbing the performance of the applied sensors and inadequate drift in sensor calibration. Whatever the carrying platform, specific and accurate calibration of the BGC sensors are required. While the T and S sensors need relatively low frequencies for calibration, i.e. typically in the order of a year, calibration requirements for BGC data are of higher frequency due to higher uncertainty of the stability of the sensors, i.e. typically monthly to weekly (during periods with high biological activity) (see appendix C).

The detection of anomalous values of BGC parameters is challenging due to their inherent high spatial and temporal variability, e.g., Chlorophyll concentration (and fluorescence) can spawn between 2-3 orders of magnitude. Any regional test used to check data quality in sea regions having given characteristics, is therefore a challenge. Historically, the amount of data available for building regional climatologies of BGC parameters is limited. The lack of a common reference database for these parameters makes it difficult to identify anomalies at regional level.

SeaDataNet and EmodNet are ongoing initiatives contributing in the collection of historical biogeochemical data as well as new data in near real time within the European Seas, but with a number of gaps in the comprehensiveness of the datasets. Taking these initiatives as a framework, an effort should therefore be made to extend compiled climatologies, based on additional existing historical datasets. There is also an increasing amount of autonomous platforms collecting BGC data that should be exploited in order to produce the required climatologies. Given the present situation, most quality tests at regional level must be based on expert knowledge, until reliable climatologies are available.

The data qualification tests proposed within this document are threefold:

- Tests that are related to sensor artefacts as adopted from Argo (2009) and Schuckmann et al (2010).
- Tests for quality Control of chlorophyll data as adopted from the PABIM white book (D'Ortenzio et al, 2010).
- Tests needed for BGC data due to calibration and biofouling.

The document is organized as follows. Section 2 will specify Quality control flags. In section 3, automatic RTQC procedures are detailed for different types of measurements. The validation procedure (figure 1) includes the delayed mode quality control of the data and will be specified in another guideline.

2 Quality Control Flags

The in-situ data provided by the MyOcean 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 characterise 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 MyOcean are oriented on the existing standards defined for other observational data sets. Table 1 indicates the flags and their specific meanings. It is important to note that the codes 0, 1, 4 and 9 are mandatory to apply after the RTQC procedure (marked in red).

The minimum requirements for flagging, as defined by MyOcean, are based on a four-level coding, marked in red, in Table 1.

To avoid unnecessary failure in using the data sets, a clear guidance to the user of MyOcean In Situ-TAC data is necessary:
Data with QC flag = 0 are recommended not to be used without a quality control made by the user.
Data with QC flag ≠ 1 on either position or date should not be used without additional control from the user.
If data and position QC flag = 1

- only measurements with QC flag = 1 can be used safely without further analyses
- if QC flag = 2 the data may be good for some applications but the user should verify this eventually by contacting the service manager for more information on the specific data concerned
- if QC flag = 3 the data are not usable but the data centre see potential for correcting the data in the delayed mode
- if 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 1: Quality flag scale. Codes marked in red are mandatory following the RTQC procedure

Code	Meaning
0	No QC was performed
1	Good data
2	Probably good data
3	Bad data that are potentially correctable
4	Bad data
5	Value changed
6	Below detection limit
7	In excess of quoted value
8	Interpolated value
9	Missing value
A	Incomplete information

3 Real Time Quality Control: Automatic Checks

One central part of the functions to be implemented by the In-Situ TAC is the control of incoming decoded measurements (Figure 1). Since at this step data should be available in real time, the QC during that process is limited and automated. An agreement on the RTQC procedure recommendations needs to be achieved in order to guarantee good quality data as well as data consistency throughout the MyOcean in-situ RT database. This is a vital step to be taken before data exchange and scientific analysis can be initiated.

In the following, automated RTQC will be listed for measurements of BGC parameters originating from different platforms, i.e. vertical profiles as well as time series and Ferrybox. The automated QC procedures described here have been developed for the QC for the Argo data management (Argo, 2009) and have been extended for other types of data. Formulations for the QC tests on chlorophyll data have also been adopted from the PABIM white book (D'Ortenzio et al, 2010). To improve the efficiency of some tests, specifications are incorporated into the validation process of regional measurements, depending on local water mass structures, statistics of data anomalies, as well as using regional enhanced bathymetry.

Most of the ARGO QC RT tests are performed to identify problems related to bad geo-localisation, erroneous timing, wrong platform identification, pressure errors etc. For these tests, the ARGO procedure is strictly adopted also for the RTQC on BGC data, although some tests are omitted since they are not relevant or applicable to BGC data. The latter are the digit rollover test, the density inversion test, and the gross sensor drift test.
Other tests are modified to be applicable to BGC data:

- the regional range test,
- the spike test,
- the gradient test,
- the frozen profile test.

Some tests not found in the Argo RTQC list or the MyOcean Temperature and Salinity RTQC (Schuckmann et al 2010) are introduced:

- the instrument comparison test,
- the parameter relationship test
- the calibration status test.

3.1 Required Metadata

Detailed Metadata are needed to guideline those involved in the collection, processing, QC and exchange of data. The quality controlled data set requires any data type (profiles, time series, trajectories, etc.) to be accompanied by key background information. A detailed metadata guideline for specific types of data can be found in the document of Eaton et al., 2009. By referring to Eaton et al., 2009, only a short summary of required information is given below:

1. Position of the measurement (latitude, longitude, depth).
2. Date of the measurement (data and time in UTC or clearly specified local time zone).
3. Method of the measurement (instrument type should be specified)
4. Specification of the measurement (platform code should be specified, in addition to e.g. station numbers, cast numbers, name of the data distribution center).
5. PI of the measurement (name and institution of the data originator for traceability reasons).
6. Processing of the measurement (date of last sensor calibration should be given, in addition to e.g. details of processing and calibration already applied, algorithms used to compute derived parameters).
7. Comments on measurement (e.g. problems encountered, comments on data quality, references to applied protocols).

3.2 RTQC for vertical profiles

Automated tests for vertical profiles are presented here, i.e. Chlorophyll-a fluorescence and oxygen measurements from Argo floats profiling systems. The tests are numbered consecutively throughout each subsection. A specific test's number in this document may therefore be different than the numbers given by the Argo RTQC and MyOcean T/S RTQC documents from which most tests have been adopted (Schuckmann et al., 2010).

1. Platform identification: (applies only to GTS data)

Every centre handling GTS data and posting them to the GTS will need to prepare a metadata file for each float and in this is the WMO number that corresponds to each float ptt (platform transmitter terminal). There is no reason why, except because of a mistake, an unknown float ID should appear on the GTS.

Action: If the correspondence between the float ptt cannot be matched to the correct WMO number, none of the data from the profile should be distributed on the GTS.

2. Impossible date test:

The test requires that the observation date and time from the profile data be sensible.

- Year greater than 1997
- Month in range 1 to 12
- Day in range expected for month
- Hour in range 0 to 23
- Minute in range 0 to 59

Action: If any one of the conditions is failed, the date should be flagged as bad data.

3. Impossible location test:

The test requires that the observation latitude and longitude from the profile data be sensible.

- Latitude in range −90 to 90
- Longitude in range −180 to 180

Action: If either latitude or longitude fails, the position should be flagged as bad data.

4. Position on land test:

The test requires that the observation latitude and longitude from the profile measurement be located in an ocean. Use can be made of any file that allows an automatic test to see if data are located on land. We suggest use of at least the 2-minute bathymetry file that is generally available. This is commonly called and can be downloaded from http://www.ngdc.noaa.gov/mgg/global/etopo2.html.

Action: If the data cannot be located in a marine area, the position should be flagged as bad data.

5. Impossible speed test: (applies only to GTS data)

Drift speeds for floats can be generated given the positions and times of the floats when they are at the surface and between profiles. In all cases we would not expect the drift speed to exceed 3 m/s. If it does, it means either a position or time is bad data, or a float is mislabelled. Using the multiple positions that are normally available for a float while at the surface, it is often possible to isolate the one position or time that is in error.

Action: If an acceptable position and time can be used from the available suite, then the data can be distributed. Otherwise, flag the position, the time, or both as bad data.

6. Global range test:

This test applies a gross filter on observed values for chlorophyll and dissolved oxygen. It needs to accommodate all of the expected extremes encountered in the oceans. Partners within MyOcean have reported on observed ranges of values in their respective regions (Appendix A), representing the best expert knowledge. Based on this information we propose to use the following global ranges:

- Chlorophyll in the range -0.1 to 100 *µg/L*
- Dissolved oxygen in the range 0 to 900 mmol/l

Small negative values of chlorophyll could also occur, ascribed mainly to instrumental and electronic “noise” of the fluorescence sensors, e.g. a small drift in fluorometer calibration can cause retrieval of small negative values (-0.1 to 0 *µg/L*) when the real chlorophyll concentration is close to zero.

Action: If a value falls outside the ranges above, it should be flagged as bad data, with the exception that if the chlorophyll concentration is in the range -0.1 to 0.0 µg/L it is flagged as potentially correctable (flag 3).

7. Regional range test:

Biogeochemical parameters are much more variable than temperature and salinity. This variability is observed on the vertical, on the horizontal and on the temporal scales, and it can spawn between 2-3 orders of magnitude. Additionally, there is a general lack of extensive climatology for the BGC parameters. A regional test, which should check the quality of data in sea regions having specific (and identified) characteristics, is therefore challenging.

Any regional range tests on BGC data should therefore be based on expert knowledge, e.g. through careful examination of available historical data (e.g. a ferrybox that has operated in the same waters for several years) that has been thoroughly quality controlled. The expected min/max values may vary throughout the year. For each parameter (especially chlorophyll) several time periods could be specified, thus taking into account expected timing of separate blooming periods.

As a first step towards establishing a set of regional ranges of the BGC parameters a table with relevant ranges for selected regions is collected within the Myocean partners

(Appendix A). The regions are split into Arctic, NorthWest Shelf, Baltic, IBI, Mediterranean, and the Black Sea.

We propose to combine the regional range test, the instrument comparison test and the parameter relationship test. This will reduce the risk of removing good data.

Test: Check if the measured value is within the expected range for the relevant region (see Appendix A for a list of values for each region).

Action: Values that fail the regional range test AND the instrument comparison test AND the parameter relationship test should be flagged as bad

8. Pressure increasing test

This test requires that the profile has pressures that are monotonically increasing (assuming the pressures are ordered from smallest to largest).

Action: If there is a region of constant pressure, all but the first of a consecutive set of constant pressures should be flagged as bad data. If there is a region where pressure reverses, all of the pressures in the reversed part of the profile should be flagged as bad data.

9. Spike test

This test is primarily devoted to the identification of spike, defined as “measurement quite different than adjacent ones” (Argo QC manual, version of February 2009). In this document the Argo spike test is implemented with the adjustments as described for chlorophyll in the PABIM white book (d’Ortenzio et al 2010). The Argo spike test is implemented by computing a “test value” defined as:

$$Test\_Value = |V2 – (V3 + V1)/2| - |(V3 – V1)/2|$$

where V1, V2 and V3 are three consecutive measurements and V2 is the measurement being tested as a spike. Measurements are identified as a spike when Test_Value exceeds a fixed threshold value. In the Argo QC the Test_Value is independent of the depth and of the vertical resolution, though threshold values are different for the two main layers of Argo protocol. The simple adaptation of the Argo Spike test to the chlorophyll-a parameter is complicated by the important differences between T and S and chlorophyll-a vertical distributions:

1. Chlorophyll-a concentration is not uniformly increasing or decreasing with depth;
2. The sub surface chlorophyll-a maxima could be extremely sharp, as chlorophyll concentration values could increase (and decrease) of one or two orders of magnitude in few tens of meters;
3. The vertical distribution of chlorophyll could be highly noisy, especially at depth, where concentrations are (or should be) close to zero.

For the Chlorophyll QC, the functional form of the spike test algorithm is unchanged. However, a threshold value depending of the data is introduced rather than a fixed threshold value. The proposed form for the threshold is:

Threshold_Value = |median(V0,V1,V2,V3,V4)| + |σ(V0,V1,V2,V3,V4)|

Where V0, V1, V2, V3 and V4 are five consecutive measurements where V2 is the measurement being tested as a spike, and σ is the standard deviation operator. This formulation has the advantage to identify as a spike, observations that are locally different of the surrounding data. The use of 5 points for the median and standard deviation computation allow to better account for the high local variability of the chlorophyll-a field, without dramatically change the functional form of the test.

In this document we propose to apply the same formulation of the spike test for chlorophyll and dissolved oxygen.

Action: Values that fail the spike test should be flagged as bad data.

10. Gradient test:

Argo gradient test is introduced to identify data points having difference between vertically adjacent observations too sharp. The objective of this test is to flag points that are really bad, which, for some reasons, have passed the spike test. Similarly to the spike test, it is implemented in the Argo QC, by calculating a test value defined as:

Test_value= |V2 – (V3 + V1)/2|

where V1, V2 and V3 are as in the spike test. Observations with test_value exceeding a fixed threshold value are flagged as bad data. Although most relevant for Temperature and Salinity that change relatively slow with depth, this test is less appropriate for the Chlorophyll-a and oxygen parameters, which could rapidly increase or decrease in few meters.

As for the spike test, the gradient test for chlorophyll and oxygen data has been introduced with the same rationale as described in the PABIM white book. The functional form of the Argo gradient test algorithm is kept with the following proposed threshold values:

Threshold_value (CHL): 3 µg/L
Threshold_value (DO): 90 millimol/m^3

Action: Values that fail the gradient test should be flagged as bad data.

11. Stuck value test:
This test looks for all measurements of a parameter in a profile being identical.

Action: If all measurements of a parameter in a profile are identical, all of the values of the affected variable should be flagged as bad data.

12. Grey list: (Argo only)

This test is implemented to stop the real-time dissemination of measurements from a sensor that is not working correctly. The grey list contains the following 7 items:

- Float Id
- Parameter: name of the grey listed parameter
- Start date: from that date, all measurements for this parameter are flagged as bad and probably bad
- End date: from that date, measurements are not flagged as bad or probably bad
- Flag: value of the flag to be applied to all measurements of the parameter
- Comment: comment from the PI on the problem
- DAC: data assembly center for this float

Each DAC manages a black list, sent to the GDACs. The merged black-list is available from the GDACs. The decision to insert a float parameter in the grey list comes from the PI.

13. Frozen profile test:

This test can detect an instrument that reproduces the same profile (with very small deviations) over and over again. This test has been introduced for temperature and salinity data (e.g. Schuckmann et al 2010). However, it should be equally applicable to BGC data.

A. For each parameter derive profiles by averaging the original profiles to get mean values for each profile in 50 dbar slabs (CHLprof, CHL_previous_prof and OXYprof, OXY_previous_prof). This is necessary because the instruments do not sample at the same level for each profile.

B. Subtract the two resulting profiles for chlorophyll (CHL) and oxygen (OXY) to get absolute difference profiles:

- deltaCHL = abs(CHLprof − CHL_previous_prof)
- deltaOXY = abs(OXYprof − OXY_previous_prof)

C. Derive the maximum, minimum and mean of the absolute differences for chlorophyll and oxygen:

- mean(deltaCHL), max(deltaCHL), min(deltaCHL)
- mean(deltaOXY), max(deltaOXY), min(deltaOXY)

D. To fail the test, require that:

- max(deltaCHL) < 0.3
- min(deltaCHL) < 0.001
- mean(deltaCHL) < 0.02
- max(deltaOXY) < 9
- min(deltaOXY) < 0.03

- mean(deltaOXY) < 0.6

Note: Threshold values above are selected as a first approach. The values should be investigated and new values may be proposed in the future.

Action: if a profile fails this test, all measurements for this profile are flagged as bad data (flag '4'). If the float fails the test on 5 consecutive cycles, it is inserted in the grey-list.

14. Deepest pressure test (Argo only):
This test requires that the profile has pressures that are not higher than DEEPEST_PRESSURE plus 10%. DEEPEST_PRESSURE value comes from the meta-data file of the instrument.

Action: If there is a region of incorrect pressures, all pressures and corresponding measurements should be flagged as bad data.

15. Instrument comparison test
This test is applied if the same platform is hosting two or more sensors for the same parameter. If two different sensors measure the same parameter, the difference between two simultaneous measurements should not be greater than a fixed limit.

Test_value: $|V_{s1} - V_{s2}|$

where s1= sensor1 and s2 = sensor2. We propose to set the following fixed threshold values:

Threshold_value (CHL): 1µg/L
Threshold_value (DO): 10millimol/m^3

Note: Threshold values above are selected as a first approach. The values should be investigated and new values may be proposed in the future.

We propose to combine the regional range test (test 7), the instrument comparison test (test 15, if applied) and the parameter relationship test (test 16, if applied). This will reduce the risk of removing good data.

Action: Values that fail the regional range test AND the instrument comparison test AND the parameter relationship test should be flagged as bad

16. Parameter relationship test
The value of different BGC parameters has often a causal relationship. An example of that is the decreased oxygen saturation in the existence of a phytoplankton bloom that is indicated by increased chl-a values. It is therefore recommended to implement a test taking into account such relationships

If high Chl-a and low oxygen saturation is observed during daytime, both parameters should be flagged.

The test is failed if VCHL > Threshold_CHL AND VOXY< Threshold_OXY,

The thresholds should ideally be selected at a regional level. However, as a first approach we propose to apply the Threshold_CHL = 5µg/L, and Threshold_OXY = 90%. Note that for this test the oxygen saturation (not concentration) is used.

Action: Values that fail the regional range test AND the instrument comparison test AND the parameter relationship test should be flagged as bad

17. Calibration status test

This test will check the status of the calibration compared to the recommended maximum interval *tcal_interval* for calibration of the sensor. Recommended values of *tcal_interval* for different sensors have been collected within MyOcean and are summarized in a look-up table (Appendix C). The approach requires that the time of the last performed calibration is given in the metadata for each sensor. Furthermore the recommended maximum time interval is platform dependent, as for example for Argo floats there are no calibration after deployment and the instruments spend most of their time at depth that are much more stable then on platforms that are always in the upper part of the water column

The test fails if $t_V - t_C > t_{cal\_interval}$ where t_v is the time of measurement, t_c is the time of last performed calibration and $t_{cal\_interval}$ is the recommended maximum time interval for calibration of the sensor (Appendix C).

Action: The test result should be written to the calibration field in the netcdf format. It can be used to flag data as 2 (probably good).

3.3 RTQC for vertical profiles: Gliders and AUVs

Automated tests for vertical profiles as measured by Gliders are presented here and automatic QC should be applied as listed below. Specifications are given if tests differ from those already described in section 3.2.

1. Platform identification: (Slocum Gliders)
2. Impossible date test:
3. Impossible location test:

4. Position on land test:
Since glider deployments are also performed on the shelf and Autonomous underwater vehicles (AUV) work in shallow waters, we suggest using the high resolution 30" second bathymetry file that is generally available. This is commonly called STRM30+ and can be downloaded from http://topex.ucsd.edu/WWW_html/srtm30_plus.html.

5. Impossible speed test:
Gliders usually work in upper layers and have their own speed (~0.4 m/s) and thus remain in areas where currents are strong. Drift speeds for gliders can be generated given the positions and times of the glider. In all cases we would not expect the drift speed to exceed 3.5 m/s plus the maximum platform speed of the glider or the propelled AUVs. If it does, it means either a position or time is bad data.

Action: If an acceptable position and time can be used from the available suite, then the data can be distributed. Otherwise, flag the position, the time, or both as bad data.

6. Global range test:
7. Regional range test:
8. Spike test
9. Gradient test:
10. Stuck value test:
11. Frozen profile test:
12. Deepest pressure test:
13. Instrument comparison test
14. Parameter relationship test
15. Calibration status test

3.4 RTQC for time series (Argo, moorings)

Automated tests for time series are presented here. Recommended tests for time series have been chosen based on RTQC of Argo data and RTQC of the M3A mooring site (Basana et al., 2000). Specifications are given if tests differ from those already described in section 4.1.

1. Impossible date test
2. Impossible location test
3. Global range test
4. Regional range test
5. Pressure increasing test
6. Spike test
7. Frozen Profile test
8. Rate of change in time:

The aim of the check is to verify the rate of the change in time. It is based on the difference between the current value with the previous and next ones. Failure of a rate of the change test is ascribed to the current data point of the set.

Action: Temperature and salinity values are flagged if

$|V_i - V_{i-1}| + |V_i - V_{i+1}| \leq 2*(2*\sigma_V)$,

where V_i is the current value of the parameter, V_{i-1} is the previous and V_{i+1} the next one. σ_V is the standard deviation of the examined parameter. If the one parameter is missing, the relative part of the formula is omitted and the comparison term reduces to $2* \sigma_V$. The standard deviation is calculated from the first month of significant data of the time series.

9. Instrument comparison test

10. Parameter relationship test

11. Calibration status test

3.5 RTQC for Ferryboxes

Automated tests for ferrybox measurements are presented here. Recommended tests are based on RTQC for time series (see section 3.4), but somehow modified due to the geospatial coverage of measurements. Specifications are given if tests differ from those already described in section 3.2.

1. Impossible date test
2. Impossible location test
3. Frozen date/location/speed test

This tests checks whether the navigation system is updating. It should be performed on all measured parameters.

4. Speed range test

This test includes both a test for maximum speed and another one for minimum speed (some ferrybox systems are turned off at lower ship speed in order to avoid pumping of particles in harbours). Threshold values will depend on the ship capabilities and the area of navigation. This test replaces the impossible speed test.

5. Pump/ flow rate test

A test checking the state of the pump should be performed. If the Ferrybox is equipped with a flow rate meter (should be specified in metadata), threshold values should be applied for flagging of data

6. Pump history test

Pump should be working during a minimal period after it has been stopped in order to make sure water in the system has been renewed and stability has been achieved The correct threshold value will depend on the pump capacity and system design. Note: NIVA applies a threshold of 10min for a system pumping appr. 2L/min

7. Global range test
8. Regional range test
9. Spike test
10. Gradient test

Note: Horizontal spike and gradient tests must take into account the distance between adjacent measurements. This will depend on ship speed and data logging frequency. Moreover, only adjacent data measured at expected interval should be taken into account in the test. This test includes testing of spikes. Threshold values are likely to depend very much on regional specifications. However, as a first approach the same formulations and threshold values as for vertical profiles can be applied.

11. Stuck value test

12. Instrument comparison test

13. Parameter relationship test

NB! The test 12 and 13 and the regional range test (test no. 8) are combined, so that data are flagged as bad only if all tests fail. This will reduce the risk of removing good data

14. Calibration status test

15. Subsequent trip test

The test is applied to Ferrybox Chl data only and aims to detect biofouling. Ferrybox systems are generally cleaned at regular intervals, but biofouling does still occur. The signal offset caused by the biofouling will increase with time as a result of increased amount of biofouling. Most Ferrybox systems operate along fixed routes with a revisit frequency ranging from hours to several days. If the measured values of Chl-a fluorescence on one trip exceed the values from the previous trip along the entire (or most parts of the) transect, this indicates possible biofouling. This information can then be used to flag the data. The time step between two consecutive trips (or revisit time at specific locations) should also be taken into account. The test requires that the ferrybox is expected to pass different water masses (in order to reduce the risk of erroneous flagging of data during the start of a bloom event) and that it has a short revisiting time (max. 2-3 days).

Approach:

- The ferrybox transect is divided into 0.1x0.1 degree Lat/Lon boxes
- For trip number N the mean of Chl values are calculated for each box and compared with values from the previous trip (N-1).
- The test fails and data are flagged as bad data if $CHL_N > CHL_{N-1}$ for more than n % of the boxes. We propose to apply $n = 75$

Action: Values that fail the subsequent trip test should be flagged as Bad data that are potentially correctable.

4 References

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5 Appendix A: Regional Ranges of BGC parameters

Table of regional ranges of BGC parameters as reported by MyOcean partners. Note that only Chlorophyll-a and Oxygen data ranges are applied for the regional range tests defined in this document

Chlorophyll-a (µg/L)	Min	Max	Time period
Arctic	0	10	Jan-Dec
NWS	0.01	95	Jan-Dec
Bay of Biscay	0	100	Jan-Dec
IBI -Cantabric Sea	0.01	5	Jan-Dec
Baltic/Western Gulf of Finland (59.45-60.3N, 23.22-30.2E)	0.5	25	Oct-Feb
Baltic/Western Gulf of Finland (59.45-60.3N, 23.22-30.2E)	1.5	77.6	Mar-May
Baltic/Western Gulf of Finland (59.45-60.3N, 23.22-30.2E)	0.5	36.8	Jun-Sep
Northern Baltic Proper (58.36-59.62N, 19.88-23.21E)	0.5	6	Oct-Feb
Northern Baltic Proper (58.36-59.62N, 19.88-23.21E)	1.5	31	Mar-May
Northern Baltic Proper (58.36-59.62N, 19.88-23.21E)	0.5	13	Jun-Sep
Southern Baltic Proper (54.52-56.2N, 12.27-17.09E)	0.5	7.6	Oct-Feb
Southern Baltic Proper (54.52-56.2N, 12.27-17.09E)	1.5	27.3	Mar-May
Southern Baltic Proper (54.52-56.2N, 12.27-17.09E)	0.5	20.5	Jun-Sep
Oxygen (mmol/m^3)	Min	Max	
Arctic	130	425	
NWS[2]	0.3	720	
IBI-Cantabric Sea[1]	220	300	
IBI-Iberia[1]	0	310	
Bay of Biscay[1]	0	625	
Nitrate (NO-3, µmol/L**)**	Min	Max	
Arctic	0	14	
NWS	0	450	
IBI-Cantabric Sea	0.01	5	
BayofBiscay	0	1000	
Baltic/Western Gulf of Finland (59.45-60.3N, 23.22-30.2E)	0	33.5	
Northern Baltic Proper (58.36-59.62N, 19.88-23.21E)	0	8.7	
Southern Baltic Proper (54.52-56.2N, 12.27-17.09E)	0	17.1	
Phosphate (µmol/L)	Min	Max	
Arctic	0	1	
NWS	0	30	
IBI-Cantabric Sea	0.01	0.6	
BayofBiscay	0	100	
Baltic/Western Gulf of Finland (59.45-60.3N, 23.22-30.2E)	0	5	
Northern Baltic Proper (58.36-59.62N, 19.88-23.21E)	0	1.1	
Southern Baltic Proper (54.52-56.2N, 12.27-17.09E)	0	1.4	
Silicate (µmol/L)	Min	Max	
Arctic	0	8	
NWS	0	210	
IBI-Cantabric Sea	0.01	6	
BayofBiscay	0	1000	
Baltic/Western Gulf of Finland (59.45-60.3N, 23.22-30.2E)	0.3	41	
Northern Baltic Proper (58.36-59.62N, 19.88-23.21E)	2.3	16.6	

Southern Baltic Proper (54.52-56.2N, 12.27-17.09E)	1.7	56.2	
NH4 (µmol/L)	Min	Max	
BayofBiscay	0	1000	
NO2 (µmol/L)	Min	Max	
BayofBiscay	0	100	

1 Values converted from originally reported units in mg/L
2 Values converted from originally reported units 0.01-16ml/L

6 Appendix B: User Guide Measurements and Maintenance

Automatic Chlorophyll-a sensors use the fluorescence properties of the chlorophyll pigment as a proxy for the Chl-a concentration. The chlorophyll-a fluorescence sensor must therefore be calibrated against Chl-a concentration accurately measured in the laboratory, e.g. by using a standard algae cell culture that is representative for a given water mass and/or by using water samples that are collected in-situ and coinciding with the operation of the sensor. The relationship between in-situ Chl-a fluorescence and concentration may vary between night and daytime (due to light adaptation of the phytoplankton), between different growth stages of the phytoplankton population, and with the phytoplankton species assemblage. Therefore, the conversion rate between fluorescence values measured by the sensors and the determined Chl-a concentration cannot be assumed to be fixed for all conditions.

The sensors which are exposed to sea water for several days or weeks without manual maintenance (e.g. ferryboxes) are subject to accumulation of microorganisms, algae and/or animals, also called biofouling. Biofouling may affect significantly the accuracy of measurement sensors and especially optical sensors (e.g. chlorophyll-a, oxygen). Thus the systems have to be cleaned regularly. Automatic chemical or mechanical (pressure air, wipers or brushing) cleaning or washing is recommended. The EC supported project BRIMOM has undertaken large efforts to develop antifouling methods, in order to enlarge the period between necessary maintenance/cleaning intervals. Since that is still an open issue and the antifouling methods are still under development, the degree of biofouling on the sensors has to be checked frequently and optical systems have to be manually cleaned when necessary. A recommendation for the frequency of maintenance/cleaning intervals for a number of popular sensors is given in Appendix C. In contrast to the physical parameters like temperature and salinity, the biofouling more often lead to decreased quality of BGC data.

The cleaning procedures and methods for subsequent assessment of the magnitude of biofouling and correction or flagging of data will differ between sensors. Taking fluorometers as an example, the cuvette should be filled with distilled water for recording the contaminated blank record. Then the cuvette is removed and the optical lens is cleaned with cleaning tissue for optics using appropriate detergent. After cleaning, the cuvette is filled with distilled water and blank value is recorded. The records before and after cleaning are used to audit the biofouling. The difference between the blank values from previous cleaning procedure (after cleaning) with the current blank value before cleaning should be used to correct the drift of blank values for the record period. However, this method for detection of sensor drift caused by biofouling cannot be applied in real-time due to the requirement for manual operation. Alternative methods should therefore be sought to detect biofouling in real-time and to perform subsequent flagging of suspicious data.

7 Appendix C: Recommended maintenance/cleaning intervals

Table 3: Recommended maintenance/cleaning intervals for sensors applied within MyOcean InSituTAC. The sensor type should be given in the metadata of the in situ data delivered to MyOcean. The list of sensors can therefore be updated and completed when the exact list of applied sensors within MyOcean is known.

Parameter	Measurement principle	Sensor	Manufacturer	Unit	Detection range	Accuracy	Resolution	Typical obs. range (min. - max.)	Maintenance procedure	Maintenance interval	Calibration frequencyQuality assessment and other remarks
chlorophyll-a	Chlorophyll-a Fluorescence	Scufa II	Turner design (USA)	µg/l	0 – 200		0.01	0.5 – 55	cleaning, calibration check	weekly	Validation against laboratory measurements of water samples stored by the FerryBox system; analysis done within 24h, if stored longer storage below – 18 oC; comparison with laboratory analyses..
automatic water sampler	phytoplankton nutrients chl-a-analysis		ISCO (USA)						cleaning	Weekly or when samples taken	Temperature volume control.
chlorophyll-a	Fluorescence	Chlorophyll-a fluoro-meter	SeaPoint Sensor Inc	µg/l	0 – 25	< 2%	0.02	0 – 25	cleaning	weekly	
dissolved oxygen	Clark electrode	COS4-2		mg/l	0 – 20	0.2% F.S.	0.2 % F.S.	8 – 15	cleaning, calibration check	monthly	Calibration outside of the flow through system.

nitrate	UV detection	UV-NO3 Analyser	Trios (Germany)	µmol/l	0.5	50	0.1		cleaning, calibration check	monthly	Comparison with filtrated samples; first tests.
nitrate	Photometric	automatic pump photometer (APP)	ME (Germany)	µmol/l	0.5 – 300	15%	0.01	0 – 250	cleaning, change of chemicals, calibration check	fortnightly	Inter-calibration with monthly taken samples.
ammonia	Fluorometric	automatic pump photometer (APP modified)	ME (Germany)	µmol/l	0.1 – 20	15%	0.01	0 – 7	cleaning, change of chemicals, calibration check	fortnightly	Instrument modified for fluorescence measurements (OPA reagent).
o-phosphate	Photometric	automatic pump photometer (APP)	ME (Germany)	µmol/l	0.05 – 10	15%	0.05	0 – 3	cleaning, change of chemicals, calibration check	fortnightly	
silicate	Photometric	automatic pump photometer (APP)	ME (Germany)	µmol/l	0.2 – 100	15%	0.01	0 – 70	cleaning, change of chemicals, calibration check	fortnightly	
fluorescence (flow-through)	Fluorescence		Seapoint	10^{-6} g/l	00 – 150	10%	0.02	0 – 50	cleaning, calibration check	monthly	Inter-calibration with laboratory measurements; flow-through system.
chlorophyll-a	Fluorescence blue LED (470 ± 30 nm)	CTG Mini-Tracka II	Chelsea Instruments	V / µg/l	0.03 – 100 µg/l		0.01 µg/l	not yet established		Fortnightly	
chlorophyll-a	fluorescence excitation	CTG MiniPack	CTG	µg/l	0.03 – 100		0.01	0 – 20	weekly cleaning, Weekly calibration 2004 weekly drift check	Yearly	Inter-calibration with acetone extracted chlorophyll-a Solid block state test

oxygen	dynamic luminescence quenching	Oxygen Optode 3830	Aanderaa	micro-Moles/l	0 - 500	<8uM or 5%	<1% or 0.4 %	200-400	weekly cleaning monthly calibration check	Yearly	New 2005 Better than specification. Little drift
Algae groups (chlorophyll-a)	fluorescence (excitation at different wavelengths)	Chlorophyll-sensor	bbe-moldaenke (Germany)		1 – 200 0.1	0.5	depends on algae group			.	Inter-calibration with HPLC measurements and cell counting (2-monthly); test phase