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Contents

1 Introduction

The purpose of task 1 in WP7 in AtlantOS project is to harmonize data exchange and data processing procedures for the EOVs that are acquired by multiple networks.

In this framework, the present report [D7.2] establishes recommendations for automatic quality control procedures in Near RT (a few hours to several days) for the core of 7 EOVs (measured by more than one of Networks involved in AtlantOS):

- Physics : temperature (T), Salinity (T), Current for surface and subsurface and Sea level
- Biogeochemistry : Oxygen (O2), Chlorophyll-A, Nitrate (NO3) and Carbon (pCO2) for surface and subsurface

The recommendations have been compiled by experts on those EOVs and validated by the Networks acquiring those EOVs in NRT (link with WP2, WP3 and WP4).

These recommendations will evolve with time under the EuroGOOS DATAMEQ working group umbrella (http://eurogoos.eu/data-management-exchange-quality-working-group-data-meq/) and benefit from scientific progress made by the observing Networks via the Task teams established within EuroGOOS (http://eurogoos.eu/task-teams/)

These recommendations do not address the delayed mode quality control proceeses.

In the rest of the document , whenever "Real Time" or "RT" is used it means "within a few hours or days" and does not refer to processing done within seconds from acquisition as done in operational warning system such as the Tsunami one.

2 Recommendations for temperature (T) and salinity (S)

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2.1 General issues of the parameters (platform independent; sensor dependent)

As for all parameters, the automatic QC objectives for T and S are to provide in real time,or near real-time (i.e. with maximum delay of 7 days), an estimate of whether a particular measurement is possible, based on various definitions of likelihood. Data arrive at different stages of qualification in the real-time data streams. Some of these non-qualified data are subject to errors that make them of no use for any application, whereas in ocean dynamical models, where T and S are fundamental state variables, or in statistical analysis of the ocean variables used to depict a variability of the ocean state, or for other data qualification on the same platform. Some of the errors are related to acquisition or transmission errors, whereas some large errors are caused by instrumental errors, sensor drifts (for example by biofouling for salinity) or instrumental effects on the measurements (for example, influence of internal temperature or lags of flow for the measurements of T and C in cells: the so called response time correction and thermal mass correction). The data might also be misplaced in the vertical, because of pressure measurements errors.

2.2 Specific recommendations (current and future)

There are different documents that summarize recommendations on automatic RT QC (see QARTOD documents at https://ioos.noaa.gov/ioos-in-action/temperature-salinity/ , Coriolis documents endorsed by EuroGOOS http://doi.org/10.13155/36230)

- These documents provide a minimum set of recommendations, that need to be systematically applied at one point of the data stream, and that will be the basis for the current RT data qualification. Notice that there are also recommendations that the data providers apply different corrections in real-time to the data they submit (for example response time and thermal mass corrections) and that they provide sufficient metadata. These recommendations, unfortunately, are currently not often taken into account. Thus, the current data qualification as done by Coriolis (sets of criteria approved by EuroGOOS) may not be sufficient for the real-time users (with the major exception of the Argo data set).

- We should envision in the future the development of a next step in near real time QC, as is done for Argo profile data, which is an automatic comparison of the data to a 'product' (this step is in some way 'Test 5' in the QARTOD document, but is not embodied in the current RT QC list of tests at Coriolis). This 'product' could be a climatology originating from earlier data (monthly or seasonal averages for the last 10 years, for example) or an estimate of the current state variable from other independent products (such as the real-time high resolution SST products; for example, the OSTIA HR SST product at http://ghrsst-pp.metoffice.com/pages/latest_analysis/ostia.html).The statistics of the comparisons to these existing products (with likelihood ranges or standard deviations when the distribution can be expected to be normally distributed) should be used to qualify the individual data points by:

    1. providing a code such as 'likely bad' if exceeding a 99% range, 'probably bad' when exceeding a 95% range, otherwise, probably good (this is an extension of current codes 1,2,3,4, where 4 is 'bad' and '3' probably bad). This could be in addition to the code provided by the current QARTOD/Coriolis based RT QC code, or merging the two.
    2. Providing a deviation range (which would quantify what is the 99% range or the 95% range) of the data with respect to the product, used for estimating the code. Issues there are that there is yet no unanimity on what would be the statistics and the product used for these important

data qualifications. On the other hand, this would be a very important tool for data users from the real time ocean user community.

2.3 Platform-dependent recommendations

- Data can be either delivered in profiles (CTD casts, Argo profiles, sea mammal data, glider data, XBT temperature profiles…), or in point-measurements from fixed depth instruments usually constructing time series (such as on a mooring or on drifting instruments). There are specificities on how the qualification can be done, depending on the platform type, and thus whether data are profiles, individual points or correspond to time series. QARTOD documents approach this issue, in particular for profiles and from point measurements, and some of these tests, for example on vertical gradients, spikes, frozen profile / time series or on sudden changes in time are apparently currently applied, at least for some of the data subsets. For profiles, there is a need to systematically summarize the overall tests for each profile (in particular, the one on deviation from a product, climatology…), for example with a code that would warn if a certain threshold of probably bad data or likely bad data is encountered in the profile.
- When analyzing the time series of profiles from the same platform, that would then give rise to possibly black-listing the data of certain platforms (as is done for Argo floats or for the temperature data of surface drifters). It is more difficult to implement such testing in real time on time series, but that would be also very valuable (but maybe could be done with statistics carried on an appropriately-long previous period of data from the particular platform/instrument: i.e., that time span could be on the order of two weeks either for mooring instruments, ferrybox or other ship TSG from Gosud, surface drifter, wave-gliders…).

3 Recommendations for Current

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3.1 General issues of the parameters (platform independent; sensor dependent)

As for all parameters, the automatic QC objectives for Current data in RT are there to identify whether the measurements are likely or not. The RT data are apparently not much used 'directly' in real-time application yet, but are very important as validation data. In situ data originate either from Eulerian instruments (typically, point-current measurements on some moorings, possibly soon from ship-mounted VM-ADCP or moored ADCPs) or from the drifts of floats (typically surface drifters, but also 'integrated' displacements of Argo floats over time). Thus the notion of sensor is strongly related to the type of platform, in particular there is a huge difference in approaches of RT-QC for an Eulerian measurement (a direct measurement of a current) or for a Lagrangian measurement (indirectly derived from a drift). There are no overall sets of recommendation published so far (although there are specific recommendations on ADCP data at https://ioos.noaa.gov/ioos-in-action/currents/ , as well as on other moored data, including from drifters in a Coriolis documents endorsed by EuroGOOS http://doi.org/10.13155/36230).

However, for these different types of data, what will be estimated/transmitted usually represents a time average (and alternatively, a spatial average) of the instantaneous local current.
The ranges of possible data are not well constrained from climatological summaries, in particular in coastal areas or at depth (in coastal areas, and more generally in the surface layers, some hints could be gathered from 'realistic' high resolution ocean models, but there might not be unanimous agreement on what would be realistic ranges of variability from such products).

3.2 Platform-dependent issues

For Lagrangian current estimates, errors originate from position errors, displacements not caused by the current, but by surface waves or when the instrument is towed (for example: fishing gear or platform out of the water on a ship). Errors can also originate when the platform is stuck during part of the time at the bottom. For the drifter data (surface SVP drifters), a quality-control is already in place at Coriolis to estimate whether the drifters have their drogue on or off (see RT-QC document mentioned above). This will need to be a posteriori assessed based on the delayed mode evaluation done at the Global Drifter Program GDAC (AOML, NOAA, Miami, USA) in order to verify the consistency of the criteria applied for this RT validation.
For Eulerian current measurements, the issue is relatively similar to the one in T and S, which is to set whether the values measured are in a reasonable range, either based on the point measurements or on the time series. Typically, in addition to position, time, depth or transmission errors, there is the possibility of erroneous errors resulting from stuck rotors or compass errors, deficient measurements resulting from reflecting objects within the field of measurements (for ADCPs…), or more generally of difficulty of identifying whether a particular acoustic measurement can be trusted or not. For that, the QUARTOD recommendations on ADCP data and the Coriolis recommendations on mooring data provide a large range of tests that should be applied, although the test on overall 'maximum' range in the current is currently not geographically variable (+3 m/s to -3 m/s, except in reginal seas where it is higher).
A possible development would be to use spatially distributed maps of likely range in the currents, and thus use afterwards the same approach as for temperature and salinity (these maps exist for the sea surface currents at 15m from drifters, but that might not be complete enough in some coastal areas inadequately sampled).
The time series or time profile checks proposed in the QARTOD and Coriolis sets of documents are reasonable (to identify stuck instruments or unrealistic profile checks, spikes, unrealistic time or vertical changes) and should be applied.

4 Recommendations for SeaLevel

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4.1 Introduction

4.1.1 General interest

As with the other EOVs, the purpose of NRT QC for sea level data is to determine if an observation is realistic or not. NRT sea level data are used for storm surge and flood warning, to ensure a network is operational, in model calibration and validation, to monitor meteotsunamis (e.g. rissaga and milghuba) and other small scale seiching and also to aid in the navigation of vessels in harbours.

The NRT QC of sea level data is usually performed by the organisation responsible for the collection and distribution of data within a country such as Puertos del Estado in Spain or the Finnish Meteorological Institute, Finland. The Sea Level Station Monitoring Facility, hosted by the Flanders Marine Institute (VLIZ) on behalf of the Intergovernmental Oceanographic Commission of UNESCO, also performs basic NRT QC on data displayed on its portal. The latency of near real time tide gauge data is in the order of less than one hour to a few hours.

4.2 General issues of the parameter

Measurements are made by a sensor which either directly (e.g. a float) or indirectly (pressure sensor) measures the surface of the sea and observations are stored in a data logger from where data are pushed or pulled to a node for quality control and distribution. Errors in the data can arise from mechanical processes e.g. biofouling on the sensors, siltation in stilling wells and pressure problems in bubbler gauges to software errors e.g. corruption in data files and loss of data through transmission issues.

The various different sensor technologies employed in tide gauges are all subject to their own particular biases and sources of error. The Manual on Sea-level Measurements and Interpretation, Volume IV: An update to 2006 (2006) provides a section on the “Summary of the Merits of Different Technologies” e.g. acoustic gauges can suffer from temperature-gradient effects, bubbler gauges may have operational issues in areas with large density ranges and radar gauges will suffer if a reflective surface appears between the gauge and the sea surface i.e. if a boat is moored beneath the gauge.

The most common errors in data appear as spikes and datum shifts. Some systems still suffer from timing errors but this is less common as modern systems use GNSS time stamps or time allocated by the data logger.

We recommend that the NRT QC for sea level follows the guidance in the EuroGOOS Recommendations for in-situ data Near Real Time Quality Control (2010) report, the QARTOD Manual for Real-Time Quality Control of Water Level Data: A Guide to Quality Control and Quality Assurance of Water Level Observations (2016) and the GLOSS Manual on Quality Control of Sea Level Observations (2011).

The current recommended tests are as follows:

- **Date control/timing/gap test** – check that the timing channel advances chronologically, preferably at a regular time interval and check for gaps.
- **Strange characters detection/syntax test** – Check that the data file conforms to an approved format and that the files is the expected size to ensure the full message has been received.
- **Out-of-range/gross range/climatology test** – This test is particularly difficult for sea level data as expected tidal ranges differ greatly depending on location. The limits must be dependent on the individual station and seasonal limits will also apply.

- **Attenuated signal** – The QARTOD manual provides a recommendation for checking for a series where the signal is not a flat line, but diminishes over a number of cycles. This can be if a well orifice is blocked, or if a compressor fails when using a bubbler gauge.
- **Stability/flat line test** – Ensure that there are not an improbable number of identical consecutive values. The number of same consecutive data points allowed depends on the location of the gauge, the point within the tidal cycle and the sampling interval of the data.
- **Rate of change test** – The QARTOD manual provides a formula for a test that checks that ensures a time series does not exceed a rate of change above a threshold value (assigned for each site).
- **Algorithm for detection of spikes** – Puertos del Estado and the Sea Level Station Monitoring Facility have provided algorithms for the detection of spikes.
- **Position test** – Basic metadata checks could be employed. A position check would ensure that coordinates were valid and could check if the site were on land, though this may be difficult with tide gauges as most are on coastal structures.

The QARTOD manual details two tests that could be developed for the future and we would recommend implementing them in AtlantOS. These are:

- **Multi-Variate Test** – Compare the primary observation with a secondary parameter. This could include comparing the sea level data with atmospheric pressure or wind measurements.
- **Neighbour Test** – Data from a station would be compared with either a second sensor at the same location, or possibly with data from a nearby station to see if events propagate along a coastline.

4.3 References

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Manual on Sea-level Measurements and Interpretation, Volume IV : An update to 2006. Paris, Intergovernmental Oceanographic Commission of UNESCO. 78 pp. (IOC Manuals and Guides No.14, vol. IV ; JCOMM Technical Report No.31; WMO/TD. No. 1339) (English)

5 Recommendations for O2

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5.1 Introduction

5.1.1 General interest

The need for implementing a full-fledged observatory of oxygen in the ocean has been recently recognized by the oceanographic community (Gruber et al, 2010). Indeed, sub-surface oxygen concentrations in the ocean everywhere reflect a balance between supply through circulation and ventilation and consumption by respiratory processes, the absolute amount of oxygen in a given location is therefore very sensitive to changes in either process, more sensitive, perhaps, than other physical and chemical parameters. Oceanic oxygen has therefore been proposed as a bellwether indicator of climate change (Gruber et al, 2010). Dissolved oxygen concentration ([O2]) is also a critical biogeochemical EOV for scientific and operational actions related to marine ecosystem dynamic.

5.1.2 RT relevance and feasibility

The main reason to have [O2] in RT (or NRT) is related to the possibility to develop assimilation schemes (Brasseur et al, 2009) for Operational Biogeochemical Models (OBM).

Generally, [O2] are measured by oxygen sensor mounted on a rosette (CTD-O2 casts). Sensor measurements are calibrated against water samples whose oxygen concentration is determined with the Winkler method demanding chemical facilities. The Winkler analyses are considered providing the “best” evaluation of marine [O2]. The sensors are also mounted on autonomous platforms (moorings, ferrybox, Argo floats, glider), which generalize the acquisition of [O2] data but increases the difficulty to calibrate the data as the opportunity of collecting and analysing water samples during the period of measurements is reduced.

In the general framework of RT or NRT processing discussed here, only sensors mounted on autonomous platforms, moorings and ferry box will be considered in the next.

5.2 General issues of the parameter (platform independent, sensor dependent)

5.2.1 Calibration

Although automatic sensors provide [O2] evaluations without water samples, they still have a low accuracy compared to the classical Winkler method. Moreover, bias on the [O2] evaluations were observed despite a careful pre-deployment calibration as well as trends, in particular during long-term deployments. Consequently, calibration is still a key issue, which is more relevant for platforms like Argo or moorings, which are generally used in long-term deployments, than for the others, which could be calibrated before and after the deployment.

As a general rule, calibrated reference profiles should be systematically acquired at deployment or at the beginning of the mission to check sensors performances, at least for the firsts observations/profiles. Ideally, for profiling platforms, a high vertically resolved profile should be provided, to account for surface and depth observations and to identify errors at gradients.

Because of those calibration issues, oxygen data transmitted in NRT is of limited use for many applications related to [O2] observations (water mass tracers, air-sea fluxes estimates) because high accuracies are required. However, the optode-based oxygen sensor technology has reached what is probably the highest maturity among all oxygen sensors. During recent years nearly all relevant characteristics of oxygen optodes have been studied intensively in view of their readiness for float applications (Bittig *et al*., 2012, 2014, 2015, D’Asaro and McNeil, 2013; Bittig and Körtzinger, 2015, Bittig et al, 2016a). All these studies provided the insight into the possibilities and limitations to achieve highest data quality that is needed to develop protocols and best practices recommendations. Recently, the functioning and utility of in-air oxygen measurements as a means of *in situ* calibration and drift correction of oxygen optodes on Argo floats has been demonstrated (Bittig and Körtzinger, 2015; Johnson *et al*., 2015) and the SCOR WG 142 on *Quality Control Procedures for Oxygen and Other Biogeochemical Sensors on Floats and Gliders* recommends to implement in-air-measurements in routine on Argo floats (Bittig et al., 2016b). If the in-air correction can be implemented in real-time, the usefulness of RT [O2] data will be significantly increased.

5.2.2 Coastal waters

RTQC procedures for [O2] observations acuqired in coastal waters are described in the Quartod Manual for Real-Time Quality Control of Dissolved Oxygen Observations (2015). They will not be discussed further.

5.3 Platform dependent recommendations for deep waters

This section concerns RTQC procedure for [O2] observations acquired in deep waters. Section “Argo” summarizes the RTQC for [O2] of the existing procedures for Argo. In the others sections, only platform specific suggestions are indicated because in general, post-deployment calibration and trend removal associated with sensor drift and other delayed-mode QC practices cannot be applied in near real time.

5.3.1 Argo

A RTQC procedure has been agreed at international level (Wong et al, 2014) and implemented in each Argo data assembly center. The four RTQC tests are a global range test, a spike test, a gradient test and a stuck value test.
See Argo documentation available at http://www.argodatamgt.org/Documentation/Bio-Argo-Oxygen-data-management-by-DACs
The RTQC procedure is described in the Argo Quality Control Manuals dedicated to biogeochemical data acquired by Argo floats (Schmechtig et al, 2016, Thierry et al., 2016).

5.3.2 Gliders

The RTQC for Argo is totally applicable to gliders equipped with [O2] sensors.
No RTQC procedures are implemented yet on gliders Dissolved Oxygen data, but the Argo procedures will be applied soon, once the official release of the Argo Quality Control Manual dedicated to biogeochemical data is available.

5.3.3 Profiling automatic device on rosette

Although the RTQC for Argo is totally applicable to ship based [O2] sensors, the transmission of ship based [O2] data in real-time is not done. The SBE43 sensor, which is the oxygen sensor mounted on a rosette, needs to be calibrated against water samples because the sensor is generally biased, because the sensor is subject to a hysteresis effect at high pressure and because of a possible sensor drift even during the period of the cruise. As a calibration of ship based [O2] data is necessary, those data will only be available in delayed-mode.

5.3.4 Moorings

For mooring equipped with profiling systems, the NRT QC for Argo is totally applicable.
For mooring having [O2] sensors at fixed depths, post-deployment calibration is necessary. The data will only be available in delayed-mode.

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6 Recommendations for Chla

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6.1 Introduction

6.1.1 General interest of the parameter

Chlorophyll *a* is the main pigment involved in photosynthesis and found in all phototrophic organisms. The concentration of chlorophyll *a* (Chla) is the most widely used proxy for phytoplankton biomass and thus a critical biogeochemical/biological EOV.

6.1.2 RT relevance and feasibility

High Performance Liquid Chromatography determination – Since the JGOFS program in the 1990's, High Performance Liquid Chromatography (HPLC) has been considered as the standard reference technique for determining Chla in addition to other phytoplankton pigments (JGOFS 1994). HPLC determination of Chla requires seawater collection using a CTD-rosette equipped with Niskin bottles, filtration, storage of filters in liquid nitrogen until analysis in the laboratory, and interpretation of the chromatograms in terms of pigment concentrations.

Because seawater sample collection and final interpretation in terms of Chla are typically a few days to a few months apart, HPLC-determined Chla data are not distributed in real time (RT). In the context of AtlantOS, however, HPLC determinations conducted by some of the networks (e.g. WP2 ship-based networks) are useful for fluorescence calibration in delayed mode (DM) applications (see Sect. 2.1).

In vitro determination of chlorophyll a fluorescence – An alternative way of estimating Chla is to use a benchtop fluorometer and to measure the fluorescence of chlorophyll *a* after chemical extraction from a seawater sample (Holm-Hansen et al. 1965). Then the fluorescence signal (counts) has to be converted into Chla equivalent using a calibration curve established in the laboratory (sensor-dependent). This technique has been commonly used, primarily because of its relatively low cost and ease of implementation. Seawater sampling and Chla determination are usually a few hours apart so, theoretically, *in vitro* fluorometric determinations could be considered near RT. In practice, though, they are typically not transmitted RT.

In vivo determination of chlorophyll a fluorescence – A third way of estimating Chla is to use an in situ fluorometer (Lorenzen 1966) and to convert the in situ fluorescence signal into Chla equivalent. This task is a lot more complex than the *in vitro* determination because the fluorescence-to-Chla ratio does not only depend on the sensor characteristics but also varies with multiple environmental factors.

In the context of AtlantOS, fluorometric determinations of Chla apply to both ship-based (WP2) and autonomous platform-based (WP3) networks. For ship-based networks, Chla is determined with an in situ fluorometer attached to a CTD-rosette system, or using an on-board benchtop fluorometer. Autonomous platform-based networks (WP3), which include profiling floats, gliders and moorings, rely on in situ fluorescence sensors. Here we consider only in situ fluorescence determinations of Chla for RT QC recommendations.

6.2 General issues of the EOV (platform independent / sensor dependent)

6.2.1 Calibration

Calibrating the in vivo fluorescence signal into Chla equivalent is a complex issue because the fluorescence-to-Chla ratio is highly variable (Falkowski and Kiefer 1985). It depends on multiple factors including the sensor characteristics (e.g. excitation and emission wavelengths), environmental conditions (light, nutrients), and biological factors (phytoplankton physiological status, size and taxonomic composition) (e.g. Cunningham 1996; Proctor and Roesler 2010 and references therein).

6.2.2 Non-photochemical quenching

Non-photochemical quenching (NPQ) is a physiological process responsible for large variations in the fluorescence-to-Chla ratio and affects daytime *in situ* fluorescence measurements. NPQ is a mechanism by which phytoplankton cells protect their photosystems from damage by dissipating excessive light energy as heat (Kolber and Falkowski 1993; Muller 2001). This mechanism results in a reduction of the chlorophyll fluorescence with no concomitant decrease in Chla and, if not accounted for, leads to an underestimation of the Chla. NPQ typically occurs in relatively shallow mixed layers of stratified environments under high light stress.

6.2.3 Biofouling

Biofouling is a common issue for *in situ* marine sensors and its impact is particularly detrimental for optical instrumentation. *In situ* fluorometers are open instruments, with optical windows exposed to surrounding waters and are thus highly subject to biofouling. Biofouling is more critical for optical sensors installed on surface moorings or buoys because of superior exposure to light and associated biological activity compared, for example, to Bio-Argo profiling floats that spend most of their lifetime at depth. Sensors deployed in productive (as opposed to oligotrophic) systems are also more subject to biofouling because of stronger biological activity in these environments.

Biofouling affects measurements accuracy and reduces deployment longevity (Manov et al. 2004). A broad variety of techniques have been proposed to stopp or reduce algal growth, thereby preventing biofouling, e.g. toxic chemicals, copper plates and rings, automatic scrubbing devices (Manov et al. 2004). Nevertheless manual cleaning of optical windows on a frequent basis has proven to be a most efficient anti-fouling strategy (e.g. Antoine et al. 2006).

Finally, it should be stressed that the particular operation of Bio-Argo profiling floats (regular drift in deep waters with high pressure, low temperature and dark conditions) seems to be the most efficient way to prevent sensors from biofouling. Return of experience shows that floats/sensors operated on the Argo mode (one profile every 10 days) do not present any sign of biofouling after two years of autonomous observations.

6.3 Platform-dependent recommendations

NB: Sect. 6.3.1 summarizes the RT QC protocol for the EOV Chla from the existing Argo procedure. In the other sections, only platform-specific recommendations are proposed.

6.3.1 Argo

The implementation of chlorophyll fluorescence sensors on Argo floats is relatively recent (Boss et al. 2008; Claustre et al. 2010). Today Chla is one of the core parameters of the Bio-Argo network and most of the newly deployed Bio-Argo floats carry a chlorophyll fluorometer. Therefore the international community has rapidly identified a critical need for developing a standard RT QC procedure (D’Ortenzio et al. 2010; IOCCG 2011).

The Bio-Argo RT QC procedure includes a general calibration followed by a sequence of quality control tests (Schmechtig et al. 2014):

1- <u>General calibration</u>

In this first step, Chla is calculated as:

Chla = (fluorescence_Chla – Dark_Chla) * Scale_Chla

where fluorescence_Chla is the measured fluorescence signal; Dark_Chla is the dark value (measured in a pool with black tape on the sensors during the preparation of the float prior to deployment); and Scale_Chla is the calibration factor provided by the manufacturer.

First, we note that the Dark_Chla value can be adjusted further in the NRT QC protocol when it is not reliable. Second, the factor Scale_Chla can be improved, but not as part of the NRT QC (in DM only).

2- <u>Adjustment at depth</u>

When Dark_Chla is not reliable, a correction is applied. In non-mixed water column conditions, Chla is assumed to be null at depth. The profile is thus adjusted to zero at depth and this offset is propagated up to the surface to the entire profile.

3- *Sensor failure*
The offset observed at depth is used to detect any drift in the sensor. If the offset is not within 20% of the dark factor provided by the manufacturer (Dark_Chla) then the signal is considered to be drifting.

4- *Range and spikes*
The range test checks that the Chla falls between a reasonable minimum and maximum values. The considered acceptable range is -0.1–50 1mg m^{-3}.
Spikes are defined as data points departing from adjacent (above and below) values beyond a predetermined threshold (based on a median filter). Fluorescence spikes may contain biological information (see Briggs et al. 2011) and do not necessarily point to a sensor failure. Therefore the spike test aims to discriminate positive spikes and flag the negative ones as bad data.

5- *Non-photochemical quenching*
Several methods were proposed for correcting autonomous platform data from NPQ (Xing et al. 2012; Biermann et al. 2015). The method used for corrected NPQ in the Bio-Argo protocol is based on that of Xing et al. (2012). Essentially, the depth within the mixed layer corresponding to the maximum daytime chlorophyll fluorescence (ZMaxFluo) is used as a proxy to estimate the thickness of the layer potentially affected by NPQ (depthNPQ). Then the maximum Chla value is extrapolated throughout the layer comprised between the surface and depthNPQ. We note that this test requires concurrent temperature and salinity profiles to be available for estimating the depth of the mixed layer.
Chlorophyll fluorescence measurements from Bio-Argo floats are not critically affected by biofouling because, in the standard Bio-Argo cycling strategy, floats spend most of their lifetime (~90%) drifting in the darkness at a parking depth of 1000 m.
Many of the recommendations and tests developed for Bio-Argo chlorophyll fluorescence measurements are also recommended in the QUARTOD manual for RT QC of optical measurements from various types of platforms (see QUARTOD 2015).
As a consequence of the many technical, environmental and biological factors driving variations in the fluorescence-to-Chla ratio, the calibration coefficient provided by fluorescence sensor manufacturers is often inappropriate. Hence, several methods have been proposed for improving the calibration of fluorescence profiles from Bio-Argo floats. Those include calibration against concurrent HPLC determinations of Chla (Lavigne et al. 2012), merging with matched-up satellite Chla (Boss et al. 2008; Lavigne et al. 2012), retrieval based on a concurrent use of float fluorescence and irradiance profiles (Xing et al. 2011), or retrieval based on the shape of the float fluorescence profile (Mignot et al. 2011; Sauzède et al. 2015). Nevertheless, we note that such methods are not relevant to RT QC and can only be applied in the context of DM studies.

6.3.2 Gliders
The RT QC procedure developed for Bio-Argo Chla data will be adapted to bio-glider data in a near future (see GROOM 2014). Interestingly, gliders perform measurements at depth, thus permitting the step “2) Adjustment at depth” to be applied. Except in the case of very long missions (~3 months) where the glider is operating in the 0–200m layer, fluorescence sensors implemented on gliders are not critically subject to biofouling. In addition, a significant advantage of gliders is that they are recovered after each mission, which enables the sensor to be cleaned and the performances to be checked.

6.3.3 Profiling automatic device on rosette
The Bio-Argo RT QC procedure is fully applicable to ship-based chlorophyll fluorescence measurements collected by *in situ* sensors attached to the CTD-rosette system of the ship (not to measurements obtained from a benchtop fluorometer).

6.3.4 Moorings
The Bio-Argo RT QC procedure is fully applicable to fluorescence measurements from mooring equipped with profiling systems provided that temperature/salinity measurements are also available (which is usually the case).

For moorings with fluorescence sensors at fixed depths, we recommend applying the following Bio-Argo steps: 1) General calibration and 4) Range and spike test. Here, however, the spike test can be applied by comparing adjacent data points from a short time series. The Bio-Argo NPQ correction cannot be applied here because the corresponding mixed layer depth may be unavailable (or may be available but at very low vertical resolution). An alternative is to discard all the daytime measurements as they are potentially affected by NPQ.
For such systems (both profiling and at fixed depths) particular attention should be paid to biofouling effects and, if possible, frequent cleaning is recommended (see Sect. 2.2).

6.3.5 Continuous surface monitoring

Measurements from fluorescence sensor directly connected to the continuous surface pumping system of the ship may be treated in a similar manner as those from moorings at fixed depths, i.e. by applying the Bio-Argo 1) General calibration and 4) Range and spike test. Again, an option for correcting measurements from NPQ is to discard all the daytime measurements. In cases where seawater samples for HPLC determination are collected along the ship's track, fluorescence-based Chla data can be further corrected in DM (not as part of the RT QC).
Critical attention should be paid to biofouling of the tubing of the surface flow-through system of the ship and accumulation of particles onto the system's inlet filter. Those should be cleaned frequently.
Measurements from seawater samples collected from the ship's surface pumping system and analysed with a benchtop fluorometer are not considered RT.

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7 Recommendations for Nitrate

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7.1 Introduction

7.1.1 General interest

Nitrate (NO3) represents one of the most relevant chemical components in the oceans, as it is the principal nutrient and limiting factor for marine phytoplankton productivity. Nitrate concentration ([NO3]) is consequently considered one of the most critical biogeochemical EOV, in particular for scientific and operational actions related to marine ecosystem dynamic.

7.1.2 RT relevance and feasibility

The main reason to have [NO3] in RT (or NRT) is related to the possibility to develop assimilation schemes (Brasseur *et al.*, 2009) for Operational Biogeochemical Models (OBM). Existing OBMs are mainly based on NO3, and, consequently, [NO3] EOV is one of the most obvious candidates to provide in-situ data in the assimilation OBM schemes (Fontana *et al.*, 2013).

Generally, [NO3] is evaluated by ship-based observations (i.e. water samples), with colourimetric methods (Wood *et al.*, 1967) demanding chemical facilities and usually carried out on land. These colourimetric analyses are considered providing the "best" evaluation of ocean [NO3] and they will be considered in the following as the reference for any other kind of [NO3] estimations. However, although Near RT strategies are attempted in the past with water samples based data (for example by carrying out chemical analysis directly on board of R/Vs after sampling), [NO3] NRT feasibility was difficult in the past. Only recently, sensors measuring [NO3] without any water sample have been developed, opening the possibility to obtain [NO3] in a RT (or Near RT) context. The most important autonomous platforms were equipped with [NO3] sensors: Argo, gliders, moorings, ferry box. The new sensors were also interfaced with CTDs, providing complementary [NO3] estimation on R/Vs.

In the general framework of RT or NRT processing discussed here, only autonomous sensors will be considered in the following.

7.2 General issues of the parameter (platform independent, sensor dependent)

7.2.1 Calibration

Although automatic sensors provide [NO3] without water samples, they still have a low accuracy compared to classical colourimetric estimations. Moreover, bias or trends on the [NO3] values from automatic device were observed, in particular during long-term deployments (although this effect is considered as a consequence of the biofouling, see next point). Accordingly, calibration and post-prcessing are still a key issue, which is more relevant for platforms like Argo or moorings (which are generally used in long-term deployments) than for the others (which could be calibrated before and after the deployment).

As a general rule, colourimetric estimations at deployment or at the beginning of the mission should be systematically provided to check sensors performances, at least for the first observations/profiles. Ideally, for profiling platforms (as Argo or gliders), a high vertically resolved profile should be provided, to account for surface and depth observations and to identify errors at gradients. Colourimetric [NO3] values should then be used to (re)calibrate the autonomous estimations and to provide correction factors for the whole mission/deployment. Note, however, that to use colourimetric estimations in the NRT QC procedure, the analysis should be performed rapidly, which is, for most of the cases, simply not possible.

Salinity and temperature also impact the [NO3] estimations obtained by automatic sensors. Methods of correction of temperature and salinity effects are generally required and developed (Sakamoto *et al.*, 2009).

It is strongly recommended to also have as much as possible concomitant measures of O2, which could be used for the scientific relevance of the [NO3] parameter.

Finally, although the [NO3] data shows a large spatial-temporal variability in the ocean, some common features could help to identify calibration issues. From a climatological point of view (Garcia *et al.*, 2006), [NO3] vertical distribution is characterized by high values at depth (the deep reservoir), a (step) gradient towards lower values close to surface, and by a surface layer where [NO3] is generally lower than at depth (and in most of the oceanic regions and for most of the time close to zero). Deep values are widely stable (i.e. weakly variable with time), at least at seasonal and annual scales (note, however, that intense mixing could modify this deep reservoir of [NO3], by homogenizing the water column). Ancillary data at depth (for example estimated by existing climatologies of colourimetric observations, as World Ocean Atlas, https://www.nodc.noaa.gov/OC5/indprod.html) or at surface (for example in ultra-oligtrophic environments, where surface [NO3] are permanently zero) could be then used to check the calibration and the processing of the automatic sensors and, if required, to correct the observations (Johnson *et al.*, 2013).

7.2.2 Bio-Fouling

Biofouling is a common issue for all marine sensors, although its impact is particularly relevant for optical instruments (as the most widely used [NO3] sensors). The most important effect of biofuling on the existing [NO3] sensors is a progressive degradation of the [NO3] accuracy, which was already identified on Argo (D'Ortenzio *et al.*, 2014) and on moorings (Johnson *et al.*, 2006). Without a regular cleaning of the instruments, the biofuling could strongly decrease the sensor performance.
As a general rule, [NO3] automatic sensors should be deployed using strategies keeping them far from natural light sources, which, if stimulating biological activity, are the first cause of biofouling. An efficient cleaning of the sensor and of the platform should be performed, as frequently as possible.
Hardware solutions are also possible, for example by using repellent varnishes, copper elements or electrical charges. These solutions have, however, limited effects, in particular in the case of long deployments/missions.

7.3 Platform dependent recommendations

NB: Section “Argo” summarizes the RTQC of [NO3] for the existing procedures for Argo. In the other sections, only platform specific suggestions are indicated.

7.3.1 Argo

The use of [NO3] sensors on Argo is relatively recent, although the number of Argo floats equipped with [NO3] instruments is continuously increasing. By consequence, a first RTQC procedure has been implemented by the international data center, although it is still under evaluation by the Argo Data Management Team. Most of the scientific and theoretical background of RTQC for [NO3] sensors on Argo are published on rang A journals (Ascani *et al.*, 2013; D'Ortenzio *et al.*, 2014; Johnson *et al.*, 2006; Johnson *et al.*, 2007). Note, also, that the [NO3] sensors on Argo are all based on optical estimations.
Based on UV absorption, [NO3] is estimated by deconvolution of the measured absorption spectrum in the range 214-270 nm (Johnson and Coletti, 2002). Corrections to account for other components absorbing in the UV range (i.e. bromide and other salt components), and based on the temperature and salinity, are then applied on the observed spectrum (Sakamoto *et al.*, 2009).
Altough [NO3] computation is performed on board, the whole measured spectrum is transmitted on land to allow also a complete reprocessing of the data, if better algorithms are developed in the future.
After the [NO3] computation, a NRT QC procedure is applied, and the profiles are modified (if required) and then stored as “Adjusted”. To the “Adjusted” profiles, a second set of QC tests is performed, to assess the level of quality of the profile.
A first NRT test (the “range” test) identifies aberrant values on the computed [NO3] values.
Two others tests are applied on the spectral absorbance values (“absorbance tests”): a first test controls that the measured 240nm absorbance (i.e. the peak of absorbance of [NO3]) is not aberrant; a second test evaluates the residual error of the deconvolution algorithms.
Pressure effects (which could be identified at very low values of [NO3]) are evaluated with a specific test (“Pressure test”), and eventually corrected.
Altough not still implemented, another test is in discussion at international level. The difference at depth between the [NO3] profile from float and from existing climatologies (as WOA) at the same geographical

location could be calculated. The obtained offset (i.e. "deep offset") could be then systematically applied to all the profiles of that float (as for example in Pasqueron de Fommervault et al. 2015).
See Argo documentation: "Bio-Argo quality control Manual for biogeochemical data", the latest version is available at http://dx.doi.org/10.13155/40879 , and also "Processing Bio-Argo nitrate concentration at the DAC Level", available here http://dx.doi.org/10.13155/46121.

7.3.2 Gliders

The NRT QC for Argo is totally applicable to gliders equipped with [NO3] sensors.
In addition, the possibility to have in situ colorimetric estimations at the deployment and at the recovery of the platform could strongly ameliorate the computation of the "deep offset" (Note, however, that colorimetric estimations should be available rapidly to be considered in the NRT QC). Moreover, except under specific case (i.e. long endurance missions), gliders are relatively weakly affected by biofuling.
See GROOM deliverable:
http://www.groom-fp7.eu/lib/exe/fetch.php?media=public:deliverables:groom_d_3_05_upmc.pdf

7.3.3 Profiling automatic device on rosette

The NRT QC for Argo is totally applicable to ship based [NO3] bio-optical sensors.
Instead of using climatology data, the "deep offset" could be calculated by using in situ colorimetric data performed on board, if available in NRT (see suggestions in "Gliders" section).

7.3.4 Moorings

For moorings equipped with profiling systems, the NRT QC for Argo is totally applicable.
For moorings having [NO3] bio-optical sensors at fixed depths, only the "absorbance tests" could be applied. For these systems, particular attention should be paid to biofueling effect. At our knowledge, despite of locating sensors at depth (i.e. far from sun light) and/or frequently cleaning the sensors by maintenance ships, the issue is without solution (at least at data level).

7.3.5 Continuous surface monitoring

The NRT QC for Argo is partially applicable to the continuous surface monitoring of [NO3].
For bio-optical sensors, the "absorbance tests" could be pertinent, whereas, the "range" test could be applied to all the existing sensors. Method of "deep offset" (see Argo paragraph 7.3.1) is not pertinent for these platforms. However, as for gliders, the possibility to collect in situ samples to colorimetric analysis before, after and during the deployment could provide ancillary data to verify the [NO3] osbervations obtained by automatic sensors.

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8 Recommendations for Carbon

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8.1 Introduction

In Europe NRT data streams for carbon dioxide (pCO2) are handled thought the ICOS Ocean Thematic Centre and the capacity for NRT data handling is currently implemented and will be finalized in late 2017/early 2018. It will receive data from a number of platforms, including instruments deployed on voluntary observing ships (VOS lines), fixed buoys, and repeat sections carried out at extended intervals. 18 stations have registered to participate in the ICOS project1, all of which are VOS lines or fixed buoys measuring surface CO2; repeat sections will be registered as they are organised during the project.

8.1.1 Platforms and instrumentation

The instruments in use are deployed in hostile environments: on buoys they are exposed to the elements, and VOS instruments are typically installed in the ship's engine room, with extreme temperatures and vibration. The combination of specialist application and small research budgets prevents the market from producing off-the-shelf products with the desired resilience. Indeed, many of these instruments are hand-built by the scientists themselves from basic components. Maintenance windows are typically small, with buoys being visited at sea, and ship access limited to a few hours during port visits. Failures are commonplace.

8.1.2 Data transmission

While satellite transmission of data is possible, budget constraints mean that this is rarely used. Data retrieval is therefore limited to routine maintenance visits every few weeks. After this, the data must be processed to convert the raw measurements into the required CO2 values (calibration, temperature and moisture adjustments, etc.). Extensive quality control must be performed to ensure that all sensors are working correctly (the small signals being measured makes this is non-trivial). Much of the code for this work was developed by individual scientists leading to inconsistencies in processing methods. While expert manual quality control is still required, many simple checks (range checking, outliers etc.) could be automated to reduce the workload.

The lack of perceived need for fast access to this data historically meant that many months could pass before it was made public. Recent demands from a variety of stakeholders have brought all these shortcomings into focus, and created the need to expedite the entire process.

8.1.3 NRT data and data processing

The ICOS OTC is developing tools to expedite the process of turning raw data into fully processed, quality controlled ocean surface CO2 data. The core of this effort will be QuinCe, a web-based tool that will automate the processing of measurements and the basic quality control. Raw data from the instruments will be uploaded and converted to a common format. This will be processed according to the internationally approved methods e.g. Pierrot et al. [2009]., ensuring consistency across all stations in the network and reducing the likelihood of unnoticed bugs.

Next, a selection of automatic quality control routines (GPS validation, range checking, spike detection etc.) will identify and flag possible problems. These routines will be based on those used in the SOCAT project to maintain consistency with the wider global surface ocean carbon community. These reduced and automatically quality controlled measurements will constitute NRT data

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