

Recommendations for enhancement of suspended particles QC Methods

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EXECUTIVE SUMMARY

New tests were developed to quality-control optical backscattering data in the Argo dataset. The tests were developed using a subset of the existing dataset and their results visually inspected by experts. Then the tests were applied to the entire global dataset and statistics generated. A strong emphasis was placed on sharing preliminary results with the Biogeochemical-Argo community, receiving feedback from this community, and facilitating the implementation of the tests at the Argo Data Assembly Centres. Results show that these tests filter as anomalous about 13% of the data present at the Argo Global Data Assembly Centres. Overall these new tests represent the first step towards generating a consistently quality-controlled Argo proxy for suspended particles. Follow up tests to be performed in delayed-mode are also presented together with a methodology to estimate uncertainties in optical backscattering data collected by sensors on BGC-Argo floats.



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1 Introduction

"Suspended particles" is a generic term to indicate the output from optical backscattering sensors mounted on BGC-Argo floats. These sensors determine the light reflected in the backward direction by particles suspended in the water column, which is quantified by the particulate optical backscattering coefficient, BBP. This parameter is important because it is correlated with the concentration of particulate organic carbon, a crucial ocean-ecosystem and biogeochemical variable. Currently (27 September 2021) 614 BGC-Argo floats in the GDAC are equipped with optical backscattering sensors (Fig. 1).



Figure 1. Distribution of BGC-Argo floats equipped with a BBP meter (yellow and grey circles denote active and inactive floats, respectively).



2 Real-Time Quality Control (RTQC)

Currently, BGC Argo have not officially released real-time (RT) or delayed-mode (DM) documents describing quality-control (QC) procedures for BBP. However, a <u>draft manual</u> is available describing some preliminary RT tests. Thus, the operational status of RT QC is still "under discussion", indicating that the methods are still being developed and tested. Any modification to the existing Argo quality-control procedures needs to be approved by the international Argo Data Management Team (ADMT), which meets once a year. It is our intention to officially propose to the ADMT in December 2021 the BBP RTQC tests developed in this project. The ADMT will then decide if they want to accept these tests. Note that several participants in Euro-Argo RISE are members of the ADMT.

Work conducted within Euro-Argo RISE has focused on:

- Assessing current RT QC tests described in the draft manual
- Devising new RT QC tests
- Devising a methodology to quantify the uncertainty in BBP
- Identifying potential DM QC tests

2.1 Assessing current RT QC tests described in the draft manual

A review of the draft manual suggested that the description and presentation of the tests could be improved. The following general structure is recommended to describe tests (both RT and DM), which should allow the reader to better understand the purpose and result of applying the test:

- *Objective*: describing the problem we are trying to deal with.
- *Implementation*: describing what the test is trying to detect and how.
- *Flagging*: describing the Argo QC flag applied to the data when the test fails.
- Pseudo code: presenting the detailed pseudo code needed to implement the test.
- *Example(s)*: presenting a profile, or series of profiles, demonstrating the problem and the result of applying the test.

Assessment of existing RT tests:

- Global range test. The objective of this test is to verify that the estimated BBP values are within a range that is expected to be reasonable. Two ranges are defined, one for BBP measurements collected at 700 nm (covering the great majority of BGC-Argo BBP sensors), i.e. [-0.000025, 0.1] m-1, and one for 532 nm (a smaller subset of BGC-Argo sensors), i.e., [-0.000005, 0.1] m-1. Note that the test allows for negative numbers, which is physically unrealistic, but that could arise because of biases in the dark offset or in the volume scattering function of seawater (see https://archimer.ifremer.fr/doc/00283/39459/56146.pdf). This test was assessed and modified as described below.
- *Bad offset test*. After reading the draft manual, I was unable to understand why this test is needed. Hence it is proposed the recommendations above on how to present tests in the manual.

2.2 Devising new RT QC tests

The main part of the work conducted in this task has been dedicated to devising new RT QC tests for BBP. The driving objective behind these tests was to deliver in real time a quality-controlled BBP dataset that can be used by non-experts (e.g., modellers) interested in retrieving information on

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suspended particles from the BGC-Argo dataset. As a consequence, the new tests presented below should be considered as "conservative". In other words, these tests were tuned specifically to screen most profiles with questionable data, but may also flag as questionable data that are instead of good quality. We therefore anticipate that the DM QC of BBP should start by assessing the results of the RT QC tests for each float (more below on this issue).

The proposed new RT QC tests were applied and results visually checked on a subset of the GDAC dataset (~60 floats from different DACs). The tests were then applied to the entire dataset (614 floats) and statistics derived. All tests were applied independently of each other (no order has been defined) and the statistics below reflect this choice (i.e., the same data can be flagged by multiple tests).

New preliminary tests were presented during ADMT21 to the BGC-Argo community and a workshop was organized (14 Dec 2020) to discuss in depth each test. Results from this community consultation included specific actions on each test that were implemented in the version presented here.

Following the consultation above, new tests were also implemented. A new workshop to discuss the status of the newly proposed RTQC tests was organized with the interested BGC-Argo community before ADMT22. The aim of this new meeting was to finalize at least some of the tests so that these can be officially proposed at ADMT22 and implemented by the DACs.

All code developed is open and shared through the Euro-Argo GitHub repository: https://github.com/euroargodev/BBP_RTQC

To support DACs with implementing the tests, Python code for each test was shared, but also we created examples for each test with inputs and expected output. These examples should allow DACs to implement tests in their preferred programming language, while ensuring consistency across DACs. In addition, the shared Python code can be used as a template to implement tests in other languages. Finally, the examples can be (and are) used to ensure that if the code is modified, it still delivers the results it is expected to deliver.

In the next pages, we present the different proposed RT QC tests for BBP. Note that a QC flag of 3 (i.e., "probably bad" data) is used to flag data that would need to be inspected by an expert during the DMQC. The tests are presented in order of decreasing percentage of the current GDAC data points flagged. This order may be used to define the order in which the tests are applied during RTQC.

In the tests below, the variable pressure is often used. This pressure is the pressure corresponding to the BBP profile and extracted using the Argo N_PROF variable.



3 High-Deep-Value test

3.1 Objective

To flag profiles that have anomalously high values at depth. These high values at depth could indicate a variety of problems, including biofouling, incorrect calibration coefficients, sensor malfunctioning, etc. A threshold value of 0.0005 m-1 was selected, that is half of the value typical for surface BBP in the oligotrophic ocean: median-filtered BBP data at depth are expected to be considerably lower than this threshold value.

3.2 Implementation

To flag profiles that have anomalously high values at depth. These high values at depth could indicate a variety of problems, including biofouling, incorrect calibration coefficients, sensor malfunctioning, etc. A threshold value of 0.0005 m-1 was selected, that is half of the value typical for surface BBP in the oligotrophic ocean: median-filtered BBP data at depth are expected to be considerably lower than this threshold value.

3.3 Flagging

If the test fails, a QC flag of 3 is applied to the entire profile.

3.4 Results

If the test fails, a QC flag of 3 is applied to the entire profile.

3.5 Proposed follow up during DMQC

None.



Figure 2. All profiles currently present in the GDAC and flagged by the High-Deep-Value test (red). Blue points represent the rest of the current GDAC BBP data. For clarity, only every other 100th point is plotted.



4 Missing-Data test

4.1 Objective

To detect and flag profiles that have a large fraction of missing data. This test can also detect profiles that are too shallow. Missing data could indicate shallow or incomplete profiles.

4.2 Implementation

The upper 1000 dbar of the profile are divided into 10 pressure bins with the following upper boundaries (all in dbar): 50, 156, 261, 367, 472, 578, 683, 789, 894, 1000. For example, the first bin covers the pressure range [0, 50), the second [50, 156), etc. The test fails if in any of the bins there are fewer data points than MIN_N_PERBIN = 1.

4.3 Flagging

Different flags are assigned depending on which bins are empty.

- If there are data in only one bin or no data at all, a QC flag of 4 is applied to the entire profile. This condition may indicate a malfunctioning sensor or a profile that is so shallow that it is too difficult to quality control in real time.
- If bins are empty only at the bottom of the profile, then we check if this was because the float measured BBP over fewer pressure bins than it was programmed to do. This is achieved by verifying that the deepest bin containing data also contains the maximum pressure measured by the float. If it does not, a QC flag of 3 is assigned to the entire profile. These conditions indicate a "shallow profile" due to missing data and may be due to a malfunctioning sensor.
- Alternatively, if bins are empty only at the bottom of the profile, but the deepest bin containing data also contains the maximum pressure measured by the float, additional checks are implemented. A pressure threshold (E_PRESTHRESH = 200 dbar) is used to check if the profile is deep enough to implement a "shallow-profile deep-value test".
 - If the profile is shallower than E_PRESTHRESH, then a QC flag of 3 is assigned to the entire profile. These conditions indicate a profile that is so shallow that we cannot apply even a modified High-Deep-Value test and could be anomalously high. The profile will need to be checked during DMQC.
 - If the profile is deeper than E_PRESTHRESH, then the median value of the points below E_PRESTHRESH is computed. If this median value is less than E_DEEP_BBP700_THRESH = 0.0005 m-1, a QC flag of 2 is assigned to the entire profile. These conditions indicate shallow profiles that do not appear to be anomalously high. However, because the pressure used to check for anomalous values is rather shallow, then these profiles should probably be checked during DMQC.
 - If the median value of the points below E_PRESTHRESH is larger than E_DEEP_BBP700_THRESH, then a QC flag of 3 is applied to the entire profile. These conditions indicate a shallow profile that appears to be anomalously high. However, because the pressure used to check for anomalous values is shallow, then these profiles should be checked during DMQC
- If some of the bins are missing data, but not consecutively from the bottom, then a QC flag of 3 is assigned to the entire profile. This condition may indicate a malfunctioning sensor.

4.4 Results

This test flagged 4.2% of the current data in the GDAC.



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4.5 Proposed follow up during DMQC

See above comments regarding need for additional tests during DMQC.



Figure 3. All profiles currently present in the GDAC and flagged by the Missing-Data test (red). Blue points represent the rest of the current GDAC BBP data. For clarity, only every other 100th point is plotted.



5 Global-Range test

5.1 Objective

To flag data points or profiles outside an expected range. The expected range is defined by two extrema: A_MIN_BBP700 = 0 m-1 and A_MAX_BBP700 = 0.01 m-1. A_MIN_BBP700 is defined to flag negative values, while A_MAX_BBP700 is a conservative estimate of the maximum BBP to be expected in the open ocean, based on statistics of satellite and BGC-Argo data (Bisson et al., 2019).

5.2 Implementation

The test is implemented on data that have been median filtered (to remove spikes) using an adaptive filter (proposed by C. Shallemberg for CHLA) with a window size (w) that depends on the vertical resolution (Δ PRES) of the data: w = 11 if Δ PRES < 1 dbar, w = 7 if 1 ≤ Δ PRES ≤ 3 dbar, and w = 5 if Δ PRES > 3 dbar. This adaptive median filter is applied also to other tests based on median filtered data.

5.3 Flagging

A QC flag of 3 is assigned to data points that fall above A_MAX_BBP700, while the entire profile is flagged with QC = 3 if any data point falls below A_MIN_BBP700 (this is to reflect the more serious condition of having negative median filtered data in a profile).

5.4 Results

This test flagged a total of 3% of the current data in the GDAC, 2.0% for medfilt(BBP700) > A_MAX_BBP700 and 1.0% for medfilt(BBP700) < A_MIN_BBP700 .

5.5 Proposed follow up during DMQC

Investigate if negative values are due to incorrect calibration parameters for BBP (e.g., by comparing the calibration parameters used for this sensor with statistics for calibration parameters for the same sensor).



Figure 4. All data points currently present in the GDAC and flagged by the Global-Range test (red). Blue points represent the rest of the current GDAC BBP data. Left plot: positive flagged data. Right plot: negative flagged data. For clarity, only every other 100th point is plotted.



6 Noisy-Profile test

6.1 Objective

To flag profiles that are affected by noisy data. This noise could indicate sensor malfunctioning, some animal spikes, or other anomalous conditions.

6.2 Implementation

The absolute residuals between the median filtered BBP and the raw BBP values are computed below a pressure threshold B_PRES_THRESH = 100 dbar (this is to avoid surface data, where spikes are more common and generate false positives). The test fails if residuals with values above B_RES_THRESHOLD = 0.0005 m-1 occur in at least B_FRACTION_OF_PROFILE_THAT_IS_OUTLIER = 10% of the profile.

6.3 Flagging

If the test fails, a QC flag of 3 is assigned to the entire profile.

6.4 Results

This test flagged 1.7% of the current data in the GDAC.

6.5 Proposed follow up during DMQC

None.



Figure 5. All data points currently present in the GDAC and flagged by the Noisy-Profile test (red). Blue points represent the rest of the current GDAC BBP data. For clarity, only every other 100th point is plotted.



7 Negative Non-Surface test

7.1 Objective

To flag negative data points below the surface in raw profiles. A specific test was developed for negative surface values (Surface-Hook test). This could indicate sensor malfunctioning or incorrectly entered calibration coefficients. Note: this test is in addition to the Global-Range test, because the latter is applied to median-filtered data.

7.2 Implementation

This test fails if for data deeper than D_ISURF = 5 dbar, BBP is less than D_MIN_BBP700 = 0 m-1.

7.3 Flagging

A QC flag of 3 is applied to the data points that fail the test.

7.4 Results

This test flagged 0.5% of the current data in the GDAC. the test fails, a QC flag of 3 is applied to the entire profile.

7.5 Proposed follow up during DMQC

Inspect these negative values and determine if the data points or the entire profile need to be flagged with QC = 4.



Figure 6. All data points currently present in the GDAC and flagged by the Negative Non-Surface test (red). Blue points represent the rest of the current GDAC BBP data. For clarity, only every other 100th point is plotted.



Parking-Hook test 8

8.1 Objective

To flag data points near the parking pressure with anomalously high values, when the parking pressure corresponds to the maximum pressure of the profile. This could indicate that particles have accumulated on the sensor or the float.

8.2 Implementation

First the parking pressure (PARK PRES) is extracted from the metadata file. Then, we verify that the vertical resolution of the data near PARK-PRES is greater than G DELTAPRES2 = 20 dbar: if it is not, the test cannot be applied to this profile. If the vertical resolution is sufficient, we verify that the maximum pressure of the profile is less than 100 dbar different from PARK_PRES (i.e., that PARK_PRES ~= max(PRES)), i.e., that the profile starts from the parking pressure. If it is, a pressure range iPRESmed (max(PRES) - G DELTAPRES2 > PRES >= max(PRES) - G DELTAPRES1, with G DELTAPRES1 = 50 dbar) is defined over which the baseline for the test will be calculated. This baseline is computed as the median + G_DEV = 0.0002 m-1. The test is implemented in the pressure range iPREStest (where PRES>= maxPRES - G_DELTAPRES1). The test fails if BBP within iPREStest is greater than the baseline.

8.3 Flagging

A QC flag of 4 is applied to the points that fail the test..

8.4 Results

This test flagged 0.3% of the current data in the GDAC.

8.5 Proposed follow up during DMQC None.



Figure 7. All data points currently present in the GDAC and flagged by the Parking-Hook test (red). Blue points represent the rest of the current GDAC BBP data. For clarity, only every other 100th point is plotted.



9 Surface-Hook test

9.1 Objective

To flag data points that are negative near the surface. This might be due to uncertainties in the pressure sensor. The rational for differentiating this test from the Negative Non-Surface test is that in this case the reason for negative surface values may be different from those causing the deeper negative values and possibly specific to uncertainties in the pressure sensor.

9.2 Implementation

This test fails if $BBP < D_MIN_BBP700 = 0 \text{ m-1}$ in the top $D_ISURF = 5$ dbar of the profile.

9.3 Flagging

A QC flag of 3 is applied to the points in the profile that fail the test.

9.4 Results

This test flagged 0.04% of the current data in the GDAC.

9.5 Proposed follow up during DMQC

Investigate reasons for these negative surface values (if these are the only ones negative in the profile and possibly verify if there is a trend towards these negative values in the part of the profile deeper than D_ISURF.



Figure 8. All data points currently present in the GDAC and flagged by the Surface-Hook test (red). Blue points represent the rest of the current GDAC BBP data. For clarity, only every other 100th point is plotted.



10 Impact of new RTQC tests on GDAC BBP data

The new RT QC tests proposed above assign a QC flag >2 to about 13% of the BBP data points currently present in the GDAC.



Figure 9. Left plot: All current GDAC BBP data. Right plot: Data with QC<=2 resulting from implementing the new RT QC tests. For clarity, only every other 100th point is plotted.



11 Methodology for quantifying uncertainties in BBP

A methodology has been proposed to the BGC-Argo community (at the International BGC-Argo steering team meeting held before the Argo Steering Team meeting 21) on how to estimate uncertainties in BBP values estimated by BGC-Argo floats. Uncertainties in BBP values are important to quantify the reliability of the measurement and are also needed by the data-assimilation community.

The proposed method is based on the Standard Law of Propagation of uncertainty ("Evaluation of measurement data - Guide to the expression of uncertainty in measurement", Joint Committee for Guides in Metrology, 2008.)

The method is based on the measurement equation, i.e., the relationship that links the output of the calculation (BBP700) to all the variables and parameters used as input for the calculation of the output. For BBP700, the measurement equation is:

BBP700 = $2^{\pi} \chi^{*}$ [(BETA_BBP700 - DK_BBP700)*SC_BBP700 - BETASW700],

and the input variables and parameters are χ , BETA_BBP700, DK_BBP700, SC_BBP700, and BETASW700.

The first step is to quantify or estimate the uncertainties associated with each of the input variables. These uncertainties can be either directly quantified, in which case they are known as "Type A" uncertainties, or derived from the literature, in which case they are known as "Type B" uncertainties). A proposal for quantifying these uncertainties in the input variables and parameters is presented in Figure 10:

x ,	u(x,) [units of x,]	Туре	Ref
x	χ*0.0292	в	Sullivan and Twardowski, 2009
BETA_BBP700	Uncertainty in BBP counts	A	Estimated as robust std of residual from medfilt1 of profile
DK_BBP700	2.5	в	Estimated (likely larger). We could estimate it by comparing darks from factory to darks measured by operators.
SC_BBP700	SC_BBP700*0.08	в	Based on the 8% (when one does NOT use 0.1-um NIST certified beads, as is the case for BGC-Argo sensors) from Sulfivan et al. 2012 Light scattering review vol. 7 (see also Dall'Olmo et al., 2012)
BETASW700	BETASW700*0.0224	в	betaw_zhanghu09 is within 2% of MoreIs measurements and the salinity correction is within 1% (on average)

Figure 10. Input variables and parameters and proposed associated uncertainties.

Then the uncertainties in Table 1 can be propagated through the measurements equation by using the standard law of propagation of uncertainties (assuming uncorrelated variables):

$$u_{c}^{2}(y) = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_{i}}\right)^{2} u^{2}(x_{i})$$

In this general formula y is BBP700, x_i are the input variables and parameters listed in Table 1, $u_c^2(y)$ is the estimated combined variance of BBP700, $u^2(x_i)$ are the uncertainties in the input variables and



parameters, and the partial derivatives are the partial derivatives of BBP700 to each of the input variables and parameters, which is computed using the measurement equation.



Figure 11. Left plot: Example of BBP profile. Right plot: Estimated relative uncertainty in BBP.

Figure 11 presents an example of a BBP700 profile and the derived relative uncertainty. We also devised an approximate technique to estimate u(BBP700), but discussion with the data management team indicated that it may not be needed at the DAC level. Future work will include testing the uncertainty calculation at the DAC level to understand the impact of the computing time, agreeing with the BGC-Argo community on the uncertainties in Table 1, and finally working towards implementing the computation at the DAC level.



12 DM QC – R&D

DM QC tests for BBP are still in their infancy. Work conducted within Euro-Argo RISE has focused on devising new RM QC, but some potential DM QC tests are presented below. At this time, we have only employed the tests on a limited number of floats. Thus, we still have not investigated the impact of these tests on the BGC-Argo dataset.

12.1 Proposed new DM QC tests

12.1.1 RT Follow-Up tests

As mentioned in the RTQC-test section, we propose a follow up examination of profiles flagged by some of the RTQC tests. This is because, during RTQC we assumed that only single profiles can be examined. However, temporal patterns that have emerged in the data during the float lifetime can be used in DM to implement additional quality-control tests.

12.1.2 Deep-Initial-Drift test

Objective: to check if the BBP sensor drifted at the start of the deployment, and, if so, to correct for this drift. Drifts of this type have been detected by Wojtasiewicz et al. (2018, 10.1175/JTECH-D-18-0027.1) and Rasse and Dall'Olmo (2019, 10.1029/2019GB006305).

Implementation: Visual inspection of time series of deep data (e.g., <900 dbar), which are assumed to be relatively stable. Fit deep data using a nonlinear function (e.g., negative exponential with background) and test if coefficients of fit indicate that a drift is present. An initial inspection of (very) few floats indicates that the fit should be applied to the first ~1000 days of data. This temporal window will need to be verified using a larger number of floats. Remove drift and leave background values.

Flagging: not defined yet.

Pseudo code: not defined yet.

Example(s): An example of this correction is presented in Rasse and Dall'Olmo (2019, 10.1029/2019GB006305). Figure 12 shows a time series of deep BBP700 data that presents a relatively pronounced initial drift; the correct (i.e., de-biased) time series is also shown.



Figure 12: Top plot: Time series of BBP700 data (averaged between 900 dbar and the bottom of each profile) demonstrating an initial drift of the BBP sensor and the fit that is used to correct the data. Bottom plot: time series of BBP700 from which the initial drift was removed using the fitted equation but excluding the offset.



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12.1.3 Deep-Biofouling test

Objective: to check if the BBP sensor is affected by biofouling (first we need to exclude grounded profiles, which may show high BBP values at depth due to re-suspended sediments). Deep BBP values that are affected by biofouling are typically much higher than expected and often show an exponential increase with time.

Implementation: Visual inspection of the entire time series of deep data (e.g., <900 dbar), which are assumed to be relatively stable. Define max value of bbp expected at this depth (maxBBP700GT900). Check if median-filtered (i.e de-spiked) BBP values at >900 dbar are higher than maxBBP700GT900. Set the QC=4 (Bad data).

Flagging: proposed QC=4.

Pseudo code:

set a max expected value of BBP at >900 dbar maxBBP700GT900 = 0.001; # [1/m] # if the de-spiked bbp(pres>900dbar) is above maxBBP700GT900 # then set QC flag to "bad data that are potentially correctable)" IF any(medfilt1(bbp700(pres>900dbar),w_size=5)>=maxBBP700GT900) QC flag = 4 Example(s): not available yet.

12.1.4 Deep-Step-Change test

Objective: to check if there are step changes in the deep BBP values indicating a potential change in instrument performance. Faults of this type have been detected in at least two publications: Wojtasiewicz et al. (2018, 10.1175/JTECH-D-18-0027.1) and Rasse and Dall'Olmo (2019, 10.1029/2019GB006305).

Implementation: Visual inspection of the entire time series of deep data (e.g., <900 dbar) after removing initial drift, which is expected to be relatively stable. For each profile, check if median of BBP deeper than 900 dbar is greater or smaller than a factor 2(proposed) from the median of the previous profile (BBP700_DEEP0). If it is, then flag data.

Flagging: proposed QC=3.

Pseudo code: IF median(BBP700(pres>900dbar)) >= 2*BBP700_DEEP0 OR median(BBP700(pres>900dbar)) <= 1/2* BBP700_DEEP0 THEN QC FLAG = 3 Example(s): not available yet.



13 Conclusions

A new set of tests to quality control BBP data in real time was developed and applied to the entire BGC-Argo dataset hosted at the GDAC. A subset of these tests has now been presented and accepted by the Biogeochemical Argo Data Management Team as the official RTQC procedure for BBP. These tests will allow non-expert users (e.g., operational modellers) to have access to an unprecedented dataset that can be used as a proxy of the concentration of suspended particles in the open ocean. The next step to achieve this is to update the official Argo documentation related to the RTQC of BBP so that the DACs can implement these tests.

We have also presented some ideas to develop the delayed-mode (DM) quality control of the BBP data. However, given that reliable RTQC tests were not available before the start of Euro-Argo RISE, the great majority of the work conducted within this task was dedicated to fill this gap. Future investment is needed to develop DMQC tests for BBP.

finally, we have proposed a methodology to estimate the uncertainty associated with BBP data measured from BGC-Argo floats. Such uncertainties and related uncertainty budgets are crucial not only when assimilating these data into operational models, but also for better understanding the limitations and potential routes for improvement of these measurements.