METHOD ARTICLE



REVISED Real-time quality control of optical backscattering data

from Biogeochemical-Argo floats [version 2; peer review: 4

approved]

Giorgio Dall'Olmo ^{[b1,2}, Udaya Bhaskar TVS ^{[b3}, Henry Bittig ^{[b4},

Emmanuel Boss ¹⁵, Jodi Brewster⁶, Hervé Claustre ¹⁷, Matt Donnelly⁸,

Tanya Maurer¹⁰⁹, David Nicholson¹⁰¹⁰, Violetta Paba¹⁰⁸, Josh Plant⁹,

Antoine Poteau⁷, Raphaëlle Sauzède¹⁰⁷, Christina Schallenberg¹¹,

Catherine Schmechtig¹², Claudia Schmid¹³, Xiaogang Xing¹⁴

¹Sezione di Oceanografia, Istituto Nazionale di Oceanografia e di Geofisica Sperimentale - OGS, Borgo Grotta Gigante, Trieste, 34010, Italy

²Plymouth Marine Laboratory, Plymouth, PL1 3DH, UK

³Indian National Centre for Ocean Information Services (INCOIS), Ministry of Earth Sciences (MoES), Ocean Valley, Pragathinagar (BO), Nizampet (SO), Hyderabad, 500090, India

⁴Leibniz Institute for Baltic Sea Research Warnemünde, Rostock-Warnemünde, 18119, Germany

⁵School of Marine Sciences, University of Maine, Orono, ME, 04469-5706, USA

⁶Cooperative Institute for Marine and Atmospheric Studies, University of Miami, Miami, FL, USA

⁷Laboratoire d'Océanographie de Villefranche (LOV), CNRS & Sorbonne University, Villefranche-sur-Mer, 06230, France

⁸British Oceanographic Data Centre (BODC), National Oceanography Centre (NOC), Liverpool, UK

⁹Monterey Bay Aquarium Research Institute (MBARI), Moss Landing, CA, 95039, USA

¹⁰Woods Hole Oceanographic Institution, Woods Hole, MA, 02478, USA

¹¹Institute for Marine and Antarctic Studies, University of Tasmania, Hobart, TAS, Australia

¹²OSU Ecce Terra, CNRS & Sorbonne University, Paris Cedex 05, 75252, France

¹³NOAA/AOML/PHOD, Miami, FL, 33149, USA

¹⁴State Key Laboratory of Satellite Ocean Environment Dynamics, Second Institute of Oceanography, Hangzhou, China

V2 First published: 13 Oct 2022, 2:118 https://doi.org/10.12688/openreseurope.15047.1	Open Peer Review
Latest published: 30 May 2023, 2 :118 https://doi.org/10.12688/openreseurope.15047.2	Approval Status 🗸 🗸 🗸

Abstract

Background: Biogeochemical-Argo floats are collecting an unprecedented number of profiles of optical backscattering measurements in the global ocean. Backscattering (BBP) data are crucial to understanding ocean particle dynamics and the biological carbon pump. Yet, so far, no procedures have been agreed upon to guality control BBP data in real time.

Methods: Here, we present a new suite of real-time quality-control tests and apply them to the current global BBP Argo dataset. The tests were developed by expert BBP users and Argo data managers and have been implemented on a snapshot of the entire Argo dataset. Results: The new tests are able to automatically flag most of the "bad"



BBP profiles from the raw dataset.

Conclusions: The proposed tests have been approved by the Biogeochemical-Argo Data Management Team and will be implemented by the Argo Data Assembly Centres to deliver real-time quality-controlled profiles of optical backscattering. Provided they reach a pressure of about 1000 dbar, these tests could also be applied to BBP profiles collected by other platforms.

Keywords

BGC Argo, BBP, oprical backscattering, particles



This article is included in the Earth and Environmental Sciences gateway.

- 2. Griet Neukermans D, Ghent University, Ghent, Belgium
- 3. Sandy J. Thomalla, CSIR, Rosebank, South Africa
- 4. **Carolina Amadio** (D), Istituto Nazionale di Oceanografia e di Geofisica Sperimentale OGS, Sgonico, Italy

Any reports and responses or comments on the article can be found at the end of the article.



This article is included in the Horizon 2020 gateway.



This article is included in the Biogeochemical Cycles collection.

Corresponding author: Giorgio Dall'Olmo (gdallolmo@ogs.it)

Author roles: Dall'Olmo G: Conceptualization, Data Curation, Formal Analysis, Funding Acquisition, Investigation, Methodology, Project Administration, Resources, Software, Validation, Visualization, Writing – Original Draft Preparation, Writing – Review & Editing; **Bhaskar TVS U**: Conceptualization, Methodology, Writing – Review & Editing; **Bittig H**: Conceptualization, Methodology, Writing – Review & Editing; **Boss E**: Conceptualization, Methodology, Writing – Review & Editing; **Brewster J**: Conceptualization, Methodology, Writing – Review & Editing; **Claustre H**: Conceptualization, Methodology, Writing – Review & Editing; **Donnelly M**: Writing – Review & Editing; **Maurer T**: Conceptualization, Formal Analysis, Investigation, Methodology, Writing – Review & Editing; **Nicholson D**: Conceptualization, Methodology, Writing – Review & Editing; **Paba V**: Conceptualization, Methodology, Writing – Review & Editing; **Plant J**: Conceptualization, Formal Analysis, Methodology, Writing – Review & Editing; **Poteau A**: Conceptualization, Formal Analysis, Methodology, Writing – Review & Editing; **Sauzède R**: Conceptualization, Methodology, Writing – Review & Editing; **Schallenberg C**: Conceptualization, Formal Analysis, Investigation, Methodology, Writing – Review & Editing; **Schallenberg C**: Conceptualization, Formal Analysis, Investigation, Methodology, Writing – Review & Editing; **Schallenberg C**: Conceptualization, Formal Analysis, Investigation, Methodology, Writing – Review & Editing; **Schallenberg C**: Conceptualization, Formal Analysis, Investigation, Methodology, Writing – Review & Editing; **Schallenberg C**: Conceptualization, Methodology, Writing – Review & Editing; **Schallenberg C**: Conceptualization, Methodology, Writing – Review & Editing; **Schallenberg C**: Conceptualization, Methodology, Writing – Review & Editing; **Schmid C**: Conceptualization, Methodology, Writing – Review & Editing; **Xing X**: Conceptualization, Methodology, Writing – Review & Editing

Competing interests: No competing interests were disclosed.

Grant information: The research leading to these results has received funding from the European Union's Horizon 2020 Research and Innovation Programme under grant agreement n. 824131 (Euro-Argo RISE project): see also preliminary results related to this manuscript in the https://www.euro-argo.eu/content/download/157288/file/D4.3_v1.0.pdf}{project report. GDO acknowledges support from the UK National Centre for Earth Observation. DN acknowledges support from U.S. National Science Foundation Awards n. 1946578 and n. 2023080. CS acknowledges grant funding from the Australian Government as part of the Antarctic Science Collaboration Initiative program.

The funders had no role in study design, data collection and analysis, decision to publish, or preparation of the manuscript.

Copyright: © 2023 Dall'Olmo G *et al.* This is an open access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

How to cite this article: Dall'Olmo G, Bhaskar TVS U, Bittig H *et al.* **Real-time quality control of optical backscattering data from Biogeochemical-Argo floats [version 2; peer review: 4 approved]** Open Research Europe 2023, **2**:118 https://doi.org/10.12688/openreseurope.15047.2

First published: 13 Oct 2022, 2:118 https://doi.org/10.12688/openreseurope.15047.1

REVISED Amendments from Version 1

The revised version include all the changes listed in the point-by-point responses to the reviewrers' comments. Major changes include clarifications in the text, new figures that describe the logical flow of each test, as well as improved figures to present the data points flagged by each test.

Any further responses from the reviewers can be found at the end of the article

Introduction

The optical backscattering coefficient quantifies the fraction of incident power that is scattered in the backward direction per unit pathlength, when an infinitesimally small water sample is illuminated by a collimated and monochromatic beam of light (Mobley, 2022). In practice, the total volume scattering function, $\beta(\theta, \lambda)$, i.e., the fraction of incident power that is scattered at a given angle, θ , is measured at a given wavelength in vacuo, λ , and then used to derive the volume scattering function of particles, $\beta_{p}(\theta, \lambda)$, by subtracting the contribution of pure seawater, $\beta_{sw}(\theta, \lambda, T, S, P)$, that also depends on temperature, *T*, salinity, *S*, and (weakly) on pressure, *P* (Hu *et al.*, 2019; Zhang & Hu, 2009; Zhang *et al.*, 2009):

$$\beta_{p}(\theta,\lambda) = \beta(\theta,\lambda) - \beta_{sw}(\theta,\lambda,T,S,P).$$
(1)

Finally, β_p is converted into the particle backscattering coefficient as follows:

$$b_{bp}(\lambda) = 2\pi \chi_p \beta_p(\theta, \lambda), \tag{2}$$

where 2π accounts for the azimuthal integration of the backscattered beam (assumed symmetrical), and χ_p for the conversion between the volume scattering function by particles at a given angle and its integral in the backward direction (Boss & Pegau, 2001; Oishi, 1990). While $b_{bp}(\lambda)$ is the standard symbol used in marine optics to indicate particulate optical backscattering at a given wavelength, the BGC-Argo variable used to indicate this quantity is BBP. We will therefore use BBP in this manuscript that focuses on BGC-Argo data. BBP and b_{bp} are however the same quantity.

BBP measurements and the quantities that can be derived from them are needed to improve our understanding of ocean ecosystems and biogeochemical cycles. BBP is correlated with the concentration of particulate organic carbon (Cetinić *et al.*, 2012; Koestner *et al.*, 2022; Rasse *et al.*, 2017; Stramski *et al.*, 2008) and, near the surface, of phytoplankton carbon (Graff *et al.*, 2015; Martinez-Vicente *et al.*, 2013) and particulate inorganic carbon (Balch *et al.*, 1996; Terrats *et al.*, 2020). Spikes in BBP profiles have also been used to detect large, fast-sinking aggregates (Briggs *et al.*, 2011; Briggs *et al.*, 2020) or animals that may be attracted to the light emitted by the sensor (Haëntjens *et al.*, 2020). Finally, BGC-Argo data provide a means to validate remote-sensing BBP algorithms (Bisson *et al.*, 2019). So far more than 600 BGC-Argo floats have been equipped with optical backscattering sensors, and ~250 of them are currently active. Argo's objective is to sustain 1000 operational six-variable BGC-Argo floats in the global ocean (Claustre *et al.*, 2020; Roemmich *et al.*, 2019). With strong international collaboration and the recent launch of new BGC-Argo float programmes, such as the Global Ocean Biogeochemistry (GO-BGC) array, the value of the global BGC-Argo BBP dataset will continue to expand.

The procedure to estimate BBP from different sensors with varying optical designs is standardised in the Argo data system - see here. As with other Argo parameters, BBP data are delivered via two data streams: "Real-Time" (RT) and "Delayed-Mode" (DM), see Argo Data Management Handbook.

Real-Time data should be delivered to users in less than 24 hours of the floats reaching the sea surface. In the Real-Time data stream, only automated quality-control checks can be applied to flag obviously bad data (Bittig *et al.*, 2019). These checks are needed to allow non-experts (e.g., operational modellers) to exploit the Argo BBP data in real time. Delayed-Mode quality control is meant to provide the best-quality data for scientific applications. It is carried out in discrete time intervals of months to years, because it requires operators to implement tests that include comparisons with climatologies or analyses in a multiparameter context.

To deliver these two data streams, the Argo community has been developing common procedures for each of the variables measured. However, presently, the BGC-Argo programme has not officially released any document specific to the BBP parameter describing quality-control procedures (RT or DM). The general Argo Quality Control Manual for Biogeochemical Data version 1.0 lists two tests for BBP (Global-Range and Spike tests) that are now obsolete, given the new tests presented in this work.

The main motivation behind this work is therefore to deliver in real time a quality-controlled BBP dataset that can be used by non-experts interested in retrieving information on suspended particles from the BGC-Argo dataset. The objective of this manuscript is to present a new suite of BBP Real-Time Quality-Control (RTQC) tests, the methodology used to devise them, and the results of implementing them on the entire BGC-Argo BBP dataset. Delayed-Mode Quality-Control procedures are not developed herein, although this document may serve to pave the road for future BBP Delayed-Mode procedures. This work builds on a preliminary set of results from the Euro-Argo Rise project that were presented as a report.

Data and methods

Philosophy behind BBP RTQC tests

All BGC-Argo parameter data are paired with numeric flags that describe their quality (see Table 1 and reference table 3.2 in the Argo user's manual). Given the audience that is expected to use the RTQC BBP dataset (i.e., non experts), the new tests presented in this document should be considered as
 Table 1. Argo quality flags used in this work.
 Argo flags between 5 and 8 are not used in this work (see Argo User's Manual).

QC flag	Meaning
1	"Good data": All real-time QC tests passed
2	"Probably good data": These data are to be used with caution
3	"Probably bad data": Do not use until an expert has checked these data
4	"Bad data": Do not use these data
9	"Missing data"

"conservative". In other words, these tests were tuned specifically to screen most profiles with questionable data, but may also occasionally flag data that are of good quality. To avoid flagging potentially good data as bad, the BBP-RTQC team agreed to use a quality-control flag equal to 3 (i.e., "probably bad" data), which should be interpreted as "do not use these data until an expert has checked them" (Table 1). We therefore anticipate that the "Delayed-Mode Quality Control" of BBP should start by assessing the results of the RTQC tests for each float, following the example of what is done for the core-Argo mission - see here.

The Argo Data Assembly Centres (DACs) have the responsibility of implementing these tests and then submitting the quality-controlled data to the Argo Global Data Assembly Centres (GDACs). To minimise the impact of implementing these tests on the resource-limited DACs 1) tests were kept simple to ease implementation; 2) the number of tests was kept to a minimum; 3) all relevant code was made available; and 4) examples of input and expected output for each test were provided.

Approach

To define the new BBP RTOC tests, we followed an iterative process. Tests were initially applied to a random subset of Argo "B-files" (i.e., containing the raw BBP profiles) extracted from the GDAC dataset (~60 floats from different DACs, covering different ocean regions and different model floats, snapshot from December 2021) and results were visually checked to refine the tests. Visual checks included (i) identifying anomalous profiles based on expert knowledge (e.g., expected range of BBP values at depth and at the surface, expected shape of the profile, negative BBP values) and (ii) verifying that the newly developed tests flagged anomalous values. These preliminary tests were then applied to the entire GDAC dataset (632 floats, snapshot from December 2021) and results assessed by the BGC-Argo community that contributed to the development of the quality control of BBP (i.e., the co-authors of this manuscript). Feedback included a request to minimise the efforts required by DACs to implement these tests and a suggestion to devise fewer and simpler tests. To further limit the overall number of tests to be implemented, an analysis of the overlap between tests was also requested. A revised suite of tests was developed and applied,

and results again shared and discussed by means of a second on-line workshop. The tests were developed for BBP measured at a wavelength in vacuo of 700 nm (i.e., BBP700), but should be applicable to BBP measured at any other wavelength as well.

These interactions with the community allowed us to converge on a final suite of tests that was presented and agreed upon at the 22nd Argo Data Management Team meeting (Dec 2021) and should be implemented by the DACs. All code developed is written in an open programming language (Python) and shared through a dedicated Euro-Argo GitHub repository (the first author is responsible for this repository).

While the interactions with the community were crucial in defining the final test suite, they introduced a certain level of subjectivity in how the tests were selected. This subjectivity, rather than decreasing the value of the resulting tests, incorporates the knowledge of experts in optical backscattering and management of the Argo data stream. We therefore consider this decision step as fundamental in defining the final test suite.

All tests were applied independently of each other (no order was defined) and the statistics computed reflect this choice (i.e., the same data can be flagged by multiple tests). Tests were applied to all data at the GDAC even if profiles had been deemed bad by the DAC operators (i.e., "greylisted", in Argo terminology).

To minimise overlap among tests, the fraction of data points flagged by all pairs of preliminary tests was calculated. Test overlapping was used to both screen the initial set of proposed tests discussed with the BGC-Argo community and to quantify the level of overlap between the final set of tests.

Due to the non-standard missions with which BGC-Argo floats were initially operated, most of the BGC-Argo BBP data collected so far (Argo snapshot of December 2021) have been measured in the upper 1000 dbar of the water column. Our tests therefore were largely based on data at pressures \leq 1000 dbar. Nonetheless, when deeper data were available, the tests and resulting flags were applied to the full profile depth (29% of the analysed profiles had a maximum pressure \geq 1900 dbar). Importantly, this assumes that the profile is collected in deep waters, and far from the bottom near which suspended sediments might invalidate the assumptions of some of the proposed tests (see also discussion on High-Deep-Value test). Pressure values were extracted from the variable "PRES" in the Argo B-files.

To smooth BBP profiles, a median filter with a window size of 11 points was used in some of the proposed tests.

Results

In the following section, we present five new RTQC tests for BBP. The proposed tests were applied to a total of 68,815 profiles from 632 floats, representing all major ocean basins as well as the Mediterranean and Black Seas. The tests, presented in order of decreasing percentage of data points flagged, are: Missing-Data test, High-Deep-Value test, Noisy-Profile test, Negative-BBP test, and Parking-Hook test. This order could be used to define the sequence in which the tests are applied during RTQC. To help the reader interested in directly comparing this manuscript to the corresponding code, in the following text we present the names of specific parameters used in the code using different fonts (e.g., MIN N PERBIN).

Each test is presented with a common structure composed of six parts:

- 1. "Objective", presenting the purpose of the test;
- "Example", a plot of one or more examples of problematic profiles targeted by the test;
- 3. "*Implementation*", explaining how to implement the test (see also related code at the GitHub repository);
- 4. "Flagging", describing what flags are used and how; and

- 5. "*Flow chart*", a figure describing the different steps required to implement the test;
- 6. "*Results*", summarising the results of implementing this test.

Proposed BBP RTQC tests

Missing-Data test. Objective: To detect and flag profiles that have a large fraction of missing data. Missing data could indicate shallow profiles (caused by a specific float mission and/or bathymetry) or incomplete profiles due to a malfunctioning sensor.

Example: See Figure 1.

Implementation: The upper 1000 dbar of the profile are divided into 10 pressure bins with the following lower 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 any of the bins does not contain data points (MIN N PERBIN = 1).

Flagging: Different flags are assigned depending on how many bins are empty. See flow chart in Figure 2.

- (i) If there are bins with missing data, but the number of bins containing data is greater than one (Figure 1a,b), then a QC flag of 3 is assigned to all BBP data in the profile (and the profile can be reviewed further in delayed-mode).
- (ii) If only one bin contains data (Figure 1c), a QC flag of 4 is applied to the entire profile. This condition may indicate a malfunctioning sensor or a problem with how the pressure values were assigned to BBP.

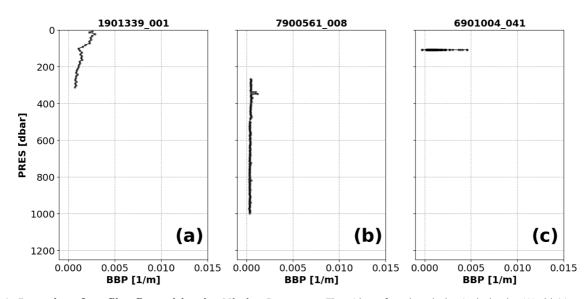


Figure 1. Examples of profiles flagged by the Missing-Data test. The titles of each subplot include the World Meteorological Organisation number of the Argo float and the number of the profile shown.

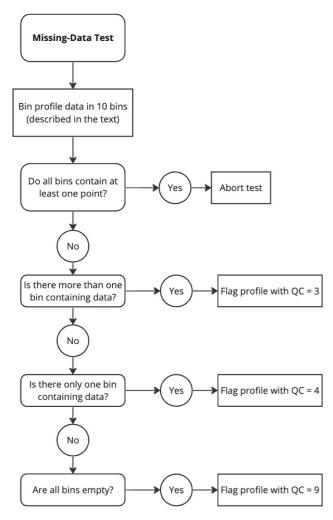


Figure 2. Flow chart for the Missing-Data test.

(iii) If the profile has no data at all, a QC flag of 9 is applied to the entire profile. This condition may indicate a malfunctioning sensor.

Results: This test flagged 10.7% of the analysed data in the GDAC (Figure 3).

High-Deep-Value test. Objective: To flag profiles with anomalously high BBP values at depth. High values at deeper depths could indicate a variety of problems, including biofouling, incorrect calibration coefficients, sensor malfunctioning. Note that high deep BBP values could also be valid data, for example in the case of sediment-resuspension events. A threshold value of 5×10^{-4} m⁻¹ was selected that is half of the value typical for surface BBP in the oligotrophic ocean (Dall'Olmo *et al.*, 2012, e.g.,): median-filtered BBP data at depth are expected to be lower than this threshold value (typically ~ 2.5×10^{-4} m⁻¹) and with a peak-to-peak seasonal variability of $< 1 \times 10^{-4}$ m⁻¹; (Poteau *et al.*, 2017).

Example: See Figure 4.

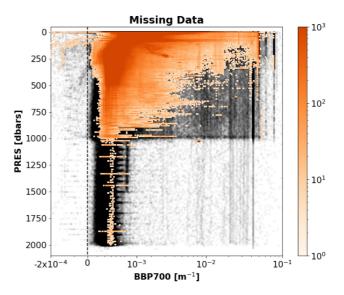


Figure 3. Two-dimensional histogram of the GDAC BBP data flagged by the Missing-Data test (colours represent the number of points in each bin; for clarity, only bins with at least 5 points are visualised). Black/grey points represent the rest of the analysed GDAC BBP data.

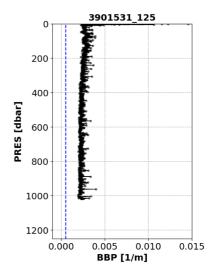


Figure 4. Example of profile flagged by the High-Deep-Value test. The blue dashed line represents the threshold above which the test fails. The title of the subplot includes the World Meteorological Organisation number of the Argo float and the number of the profile shown.

Implementation: This tests fails if there is at least a certain number (C_N_DEEP_POINTS = 5) of points deeper than a threshold depth (C_DEPTH_THRESH = 700 dbar) and if the median of the median-filtered profile below C_DEPTH_THRESH is greater than a predefined threshold (i.e., C DEEP BBP700 THRESH = 0.0005 m^{-1}).

Flagging: If the test fails, a QC flag of 3 is applied to the entire profile. High deep BBP values can result from a variety

of reasons, including natural causes. In the latter case, the quality flag could be set to "good data" during DMQC. See flow chart in Figure 5.

Results: This test flagged 6.2% of the current data in the GDAC (Figure 6).

Noisy-Profile test. Objective: To flag profiles that are affected by noisy data. This noise could indicate sensor malfunctioning, clusters of BBP spikes caused by organisms attracted to the light emitted by the sensor (Haëntjens *et al.*, 2020), or other anomalous conditions.

Example: See Figure 7.

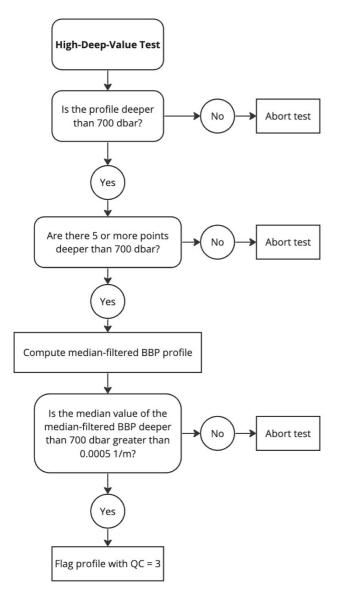
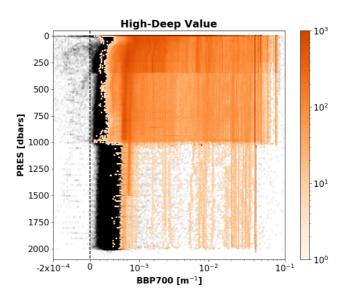


Figure 5. Flow chart for the High-Deep-Value test.





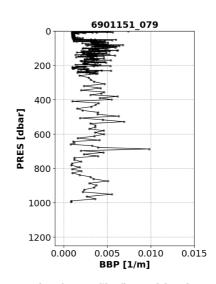


Figure 7. Example of a profile flagged by the Noisy-Profile test. The title of the subplot includes the World Meteorological Organisation number of the Argo float and the number of the profile shown.

The absolute residuals Implementation: 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). Absolute residuals (instead of relative ones) were used to identify signals that are noisy compared to the expected values of BBP in the open ocean. The test fails if residuals with absolute values above a pre-defined threshold (i.e., B RES THRESHOLD = 0.0005 m^{-1}) occur in at least 10% of the profile data (i.e., B FRACTION OF PROFILE THAT IS OUTLIER = 0.10). These threshold values were selected after visual inspection of profiles from a subset of floats.

Flagging: If the test fails, a QC flag of 3 is assigned to the entire profile. See flow chart in Figure 8.

Results: This test flagged 2.8% of the current data in the GDAC (Figure 9).

Negative-BBP test. Objective: To flag negative BBP values due to a variety of reasons including: sensor drift or malfunctioning, inaccurate calibration coefficients, or BBP sensor exposed to air.

Example: See Figure 10.

Implementation: The test is implemented on the unfiltered BBP data.

Flagging: Different flagging is applied depending on whether the negative BBP values occur only near the surface (i.e.,

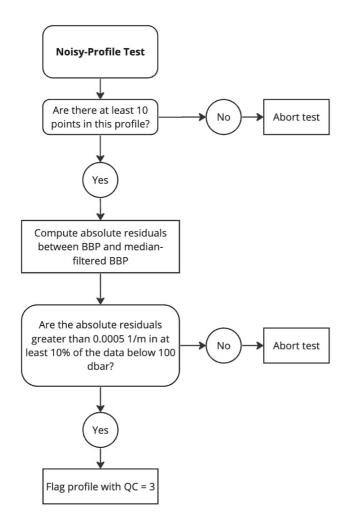


Figure 8. Flow chart for the Noisy-Profile test.

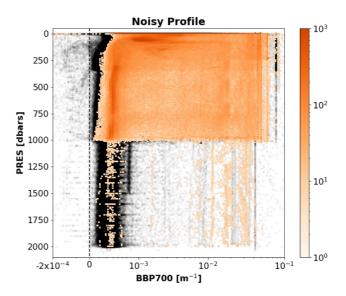


Figure 9. As Figure 3 but for the Noisy-Profile test.

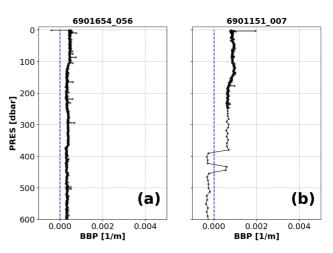


Figure 10. Examples of profiles flagged by the Negative-BBP test. (**a**) Profile with negative BBP values only at pressures shallower than 5 dbar; (**b**) profile with negative BBP values deeper than or at 5 dbar. The blue dashed lines represent the zero threshold beyond which the test fails. The title of the subplot includes the World Meteorological Organisation number of the Argo float and the number of the profile shown.

PRES < 5 dbar) or deeper in the water column (see flow chart in Figure 11):

- (i) A QC flag of 4 is assigned to negative BBP points when these appear at pressures shallower than 5 dbar. This is used to flag negative BBP values near the surface that most likely represent data with a BBP sensor outside of the water.
- (ii) To allow delayed-mode operators to requalify profiles with just a few deep negative points, at pressures greater than 5 dbar the flag is set depending on the fraction of negative BBP values with respect to the

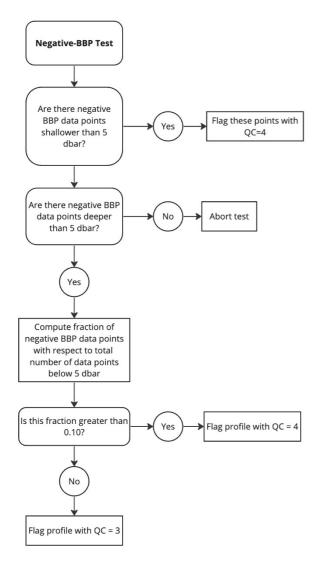


Figure 11. Flow chart for the Negative-BBP test.

number of BBP measurements below 5 dbar. If the fraction of negative BBP values is greater than a pre-defined threshold (i.e., A_MAX_FRACTION_OF_BAD_POINTS = 0.10), then a QC flag of 4 is assigned to the entire profile.

(iii) Otherwise, a QC flag of 3 is assigned to the entire profile. BBP sensors that generate these deep negative BBP values are considered more at risk of malfunctioning and thus the entire profile is flagged.

Results: This test flagged a total of 2.17% of the current data in the GDAC, 2.12% for negative BBP values deeper than or at 5 dbar and 0.05% for BBP values shallower than 5 dbar (Figure 12).

Parking-Hook test. Objective: When a float is drifting with the currents while at its parking pressure (typically 1000 dbar), particles may be depositing on the float and BBP sensor. These accumulated particles are likely released back into the water when the float descends to its maximum pressure (typically 2000 dbar), before starting the ascending profile during which data are collected. However, if the float does not descend to 2000 dbar before starting the BBP measurements, but immediately starts ascending towards the surface and measuring, then the accumulated particles might be measured by the BBP sensor as they are released back into the water. This is the likely cause of an increase in BBP at the start of the profile, when the parking pressure is close to the maximum pressure. The objective of this test is to flag these anomalous BBP points.

Example: See Figure 13.

Implementation: For ascending profiles, we first verify that the nearest BBP measurement above the maximum pressure recorded by the float (maxPRES) is lower than a pre-defined threshold ($G_{DELTAPRES2} = 20$ dbar): if it is not, the

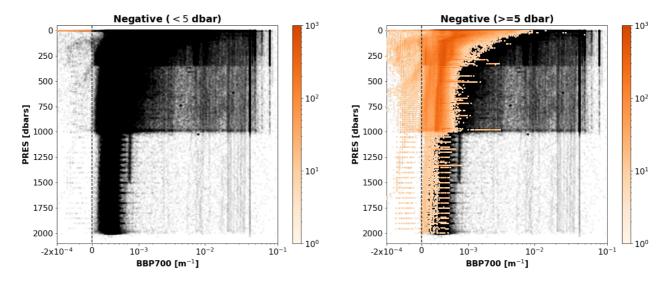


Figure 12. As Figure 3 but for the Negative-BBP test. Left plot: data with negative BBP values only at PRES < 5 dbar. Right plot: data with negative BBP values at PRES >= 5 dbar.

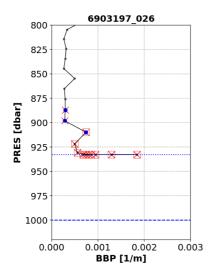


Figure 13. Example of profile flagged by the Parking-Hook test. The dashed and dotted blue lines represent the nominal parking pressure and actual maximum pressure recorded for this profile, respectively. Blue circles represent the points used to compute the baseline. Red crosses are the points to which the test is applied. Red squares are the points that failed the test. The title of the subplot includes the World Meteorological Organisation number of the Argo float and the number of the profile shown.

test cannot be applied to this profile. This is to ensure that the baseline (computed below) is representative of the values of BBP at maxPRES. If the BBP measurement above maxPRES is less than 20 dbar away from it, we check that the profile starts from the parking pressure (parkPRES, extracted from the mission configuration valid for the float cycle under exam) by testing that the absolute difference between the maxPRES and parkPRES is smaller than 100 dbar. If the profile does not start from the parking pressure, the test is aborted. If the profile starts from the parking pressure, a first pressure range is defined (maxPRES - G_DELTAPRES2 > PRES >= maxPRES - G DELTAPRES1, with G DELTAPRES1 = 50 dbar, blue circles in Figure 13) over which a baseline is calculated as the median value of BBP augmented by a threshold value of 0.0002 m-1 (i.e., median (BBP) + G DEV, with G DEV = 0.0002 m-1). The test is then implemented over a second pressure range (i.e., PRES >= maxPRES -G DELTAPRES1). The test fails if BBP within the second pressure range is greater than the baseline.

Flagging: A QC flag of 4 is applied to the points that fail the test. See flow chart in Figure 14.

Results: This test flagged 0.4% of the current data in the GDAC. Although this is a relatively small number of points, these points represent a bias in the dataset that must be flagged. Figure 15 demonstrates that test flagged points near the

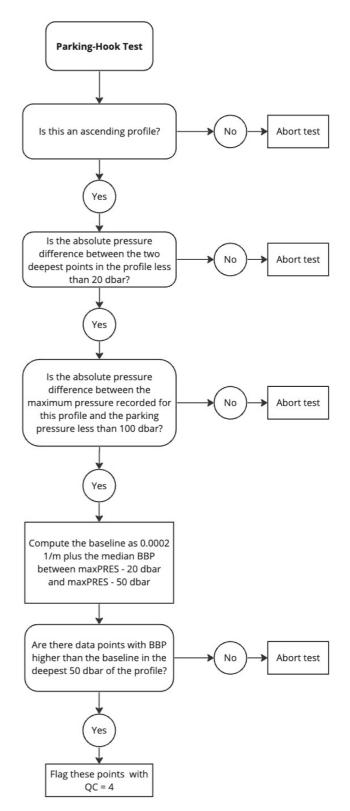


Figure 14. Flow chart for the Parking-Hook test.

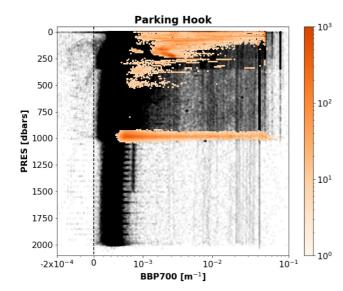


Figure 15. As Figure 3 but for the Parking-Hook test.

standard parking pressure of 1000 dbar, but also several points from floats that were parked at considerably shallower depths.

Test overlap

Figure 16 presents a matrix with the percentage of points from the entire GDAC dataset that were flagged by pairs of tests. Values were computed as the number of points flagged by each pair of tests, divided by the number of points flagged by the test with row label (lower left side of the matrix) or by the test with column label (upper right side of the matrix). To help the reader interpret the values presented in Figure 16, we provide the following example: 2% of the points flagged by the Missing-Data test were also flagged by the Parking-Hook test, while 61% of the points flagged by the Parking-Hook test were also flagged by the Missing-Data test.

Impact of RTQC tests on GDAC BBP data

The new RTQC tests proposed above assigned a QC flag >2 to \sim 19% of the BBP data points analysed and improved the shapes of the remaining profiles relative to expectations (Figure 17). For example, negative values and profiles with consistently high values at depth were removed, and so were high BBP values near parking depths (e.g., 1000 dbar).

Plans for recording the results of the tests

Understanding which BBP-RTQC tests have failed is needed to diagnose the quality of a BBP profile and to implement further DMQC tests. We have therefore started devising a method to record this information in the BGC-Argo files. However, to achieve this while maintaining consistency in file formats across DACs, we first need to find an informal agreement among the Argo DACs and then obtain official approval from the Argo Data Management Team. Therefore, it is impossible at the moment to provide further specifications about how exactly this will be achieved.

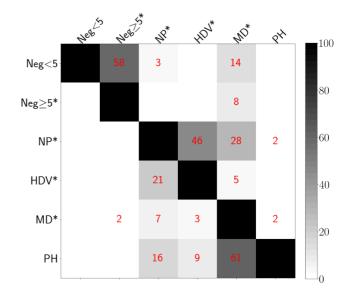


Figure 16. Percent overlap between pairs of different tests. Test labels as follows (* indicates a test that flags the entire profile): Neg<5: Negative BBP only within the upper 5 dbar; Neg≥5*: Negative BBP deeper than 5 dbar; NP*: Noisy Profile; HDV*: High Deep Value; MD*: Missing Data; PH: Parking Hook.

Discussion

Comments on overall results of these BBP RTQC tests The proposed RTQC tests removed most of the anomalous BBP profiles (Figure 17) and improved the overall quality of the BBP dataset, thus making it more suitable to be exploited by users. These tests assigned a QC flag >2 to ~19% of the BBP data points currently present in the GDAC. To ensure that the user can understand the history of the quality control applied to BBP data, pass/fail results of the proposed tests will be stored as a cumulative binary flag in the Argo NetCDF file (specifics will be provided in the Argo BBP quality control manual, when it will become available).

Comments on selected proposed tests

Missing-Data test. The Missing-Data test flagged the largest number of BBP data points because a relatively large fraction of shallow profiles are present in the global data set, due to the initial exploratory phase of the BGC-Argo programme. An additional reason for the large number of flagged data is that this test flags the entire profile, rather than specific points in a profile.

The rationale for defining this rather strict flagging procedure is that the main way in which we can identify faulty BBP values in real time is to inspect values of BBP at depth (with the High-Deep-Value test). Deep values are expected to be relatively small and stable with respect to surface values and can thus be used as a reference to quality control the rest of the profile. If these deep data are not collected, then these important reference values are not available to support the RTQC. Therefore, we decided to assign a QC flag of 3, so

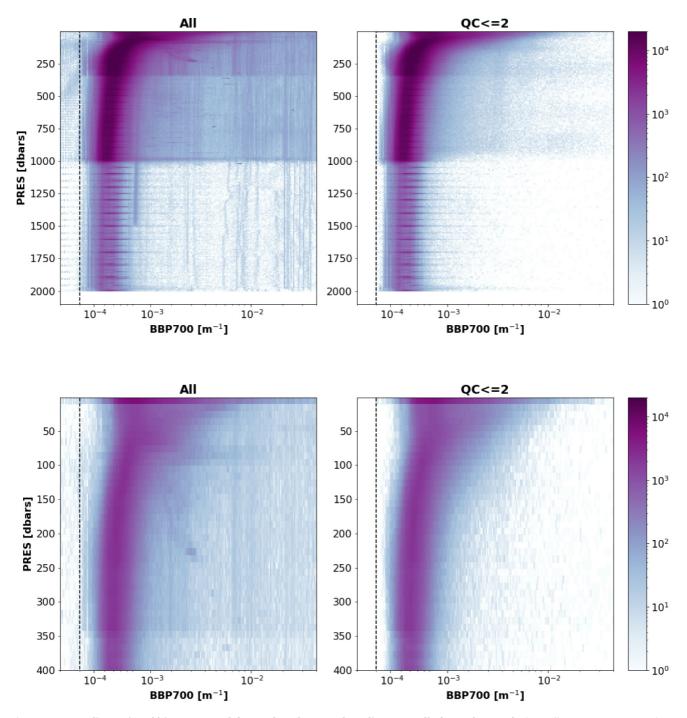


Figure 17. Two-dimensional histograms of the analysed raw and guality-controlled BBP data. Left plots: All current GDAC BBP data. Right plots: Data with QC<=2 resulting from implementing the new RT QC tests. Top and bottom rows present the same data but between 0 and 2000 dbar and 0 and 400 dbar, respectively.

that shallow profiles can be re-assessed more carefully during the DMQC.

A more complex test was initially devised to overcome the above limitation, but feedback from the Argo community suggested that the Missing-Data test should be kept as simple

as possible, in order to avoid overburdening DACs with implementing overly complex tests.

It is envisioned that, during Delayed-Mode Quality Control, shallow profiles could be easily re-qualified as "good data" if floats also collected at least some deep profiles. In other

words, when a float has collected both shallow and deep profiles, the DMQC flags of the deep profiles could be extended (after inspection) to the shallow profiles as well. Alternatively, a delayed-mode operator may have other means to requalify data points that were flagged during the real-time quality control (e.g., comparison to climatologies).

High-Deep-Value test. The High-Deep-Value test is based on the assumption that deep BBP values are low and stable, as it is often the case in the open ocean. As a consequence, this test flags profiles with high values at depth, even if these high values are real. Specific examples include floats that "grounded" (i.e., that touched the sea floor) and floats that sampled high BBP values at depth near continental margins or rivers. A first inspection of the flagged profiles, however, indicates that these specific examples are a relatively small fraction of the profiles flagged by this test.

BBP profiles of grounded floats could be identified in DMQC with the help of bathymetric maps, but again, such operation was deemed too complex for RTQC. Similarly, additional information on bathymetry and rivers could be employed to screen, during DMQC, floats that sampled close to the continental margins. It is thus a test where flags can be reversed in DMQC after careful evaluation of the circumstances (e.g., trajectory and sampling pattern) of the float.

In the future, BBP sensors may also be deployed on Deep-Argo floats (i.e., Argo floats specialised in sampling the entire water column, down to 6000 dbar) to measure sediment resuspension in the bottom boundary layer of the ocean. In this case, the High-Deep-Value test will have to be revisited to only use data in the upper water column (700-2000 dbar). This is not a problem for Argo, yet.

Noisy-Profile test. The Noisy-Profile test was developed and tuned to flag profiles affected by noisy data. Because this test relies on detecting a certain percent of outliers, it could flag profiles containing real spikes (Briggs *et al.*, 2011; Haëntjens *et al.*, 2020). We therefore recommend users interested in implementing spike analyses to use the raw BBP profiles.

Overlapping tests

Some of the tests proposed flagged a significant number of common data (e.g., High-Deep-Value vs. Noisy-Profile and Parking-Hook vs. Missing-Data, Figure 16). Nevertheless, in keeping with our "conservative philosophy" of removing most of the bad data, we have decided to use all five tests proposed. This is because only when applied together were these tests able to generate a satisfactory RTQC BBP dataset.

Potential additional BBP RTQC tests

After implementing the proposed BBP RTQC tests at the DAC level, we envision that additional RTQC tests could be proposed to further improve the quality of the dataset.

One potential future test that could be developed is a Regional-Range test. As the BGC-Argo BBP dataset grows in size, it should become possible to define and tune the parameters of a range test to specific ocean regions and specific seasons of the year. These tuned BBP-range parameters could be used in a Regional-Range test that can deliver better RTQC BBP profiles based on local conditions. It remains to be seen if such a test would be useful.

Another test that could potentially improve the overall quality of the dataset is the Animal-Spike test. Under certain conditions, mesopelagic organisms can be attracted to the light emitted by the optical sensors mounted on BGC-Argo floats, causing large localised spikes in BBP and other optical signals. Haëntjens et al. (2020) developed a detailed procedure to detect these events that could be implemented as a separate BBP RTOC test. As a first step and to avoid increasing the complexity of the proposed tests, we decided not to include this specific test, partly because the Noisy-Profile test already detected some (although not all) profiles affected by animal spikes. Nevertheless, future developments in BBP RTQC could add this test. Animal spikes are real signals that, however, may not be useful to many non-expert users (e.g., focusing on using BBP to estimate particulate carbon concentrations). We have therefore also identified the need to define a specific DMQC flag for this type of data.

Finally, as the proposed tests are implemented and users begin exploiting the RTQC BBP dataset, we expect that imperfections in the tests will be identified, which will result in further tuning of the test parameters.

Adjusting BBP after RTQC

Argo variables that have been quality-controlled and that have received a correction are typically stored in corresponding "adjusted" variables (e.g., BBP_ADJUSTED). Argo has spent efforts to educate its users to select adjusted variables as the best available Argo data. Although the presented RTQC tests for BBP do not apply corrections to the BBP dataset, following discussions with the Argo community, we decided that DACs should create a BBP_ADJUSTED variable by applying to real-time quality-controlled BBP data a linear equation with OFFSET=0 and SLOPE=1. In other words, BBP and BBP_ADJUSTED variables will be equal. The rationale behind this choice is that non-expert users have been trained to use Argo adjusted variables as the best available Argo data. Our choice therefore aims at delivering a consistent message to the users. Until the delayed-mode quality control of the BBP data has been implemented, we also decided that no error field will be filled for the BBP_ADJUSTED variable.

Conclusions

A new set of real-time quality-control tests for Argo BBP profiles was presented. When implemented, these tests will deliver a BBP dataset that is quality-controlled so that non-experts can use the BBP data in real time. Results of these tests were generated for the entire BBP dataset held at the GDAC and extensively discussed with the interested Argo community. The tests were approved by the BGC-Argo Data Management Team in December 2021. Furthermore, the same tests could also be adopted by or adapted for other measuring networks such as ship-borne or glider measurements.

As discussed, there may be cases where profiles subject to the RTQC tests outlined herein are erroneously flagged. Such profiles could be easily identified with the adopted flagging scheme and then reviewed and potentially recovered by a delayed-mode operator. Additional methods in support of delayed-mode quality control are also currently under development, including semi-annual audits on the global BBP array via comparative analysis against a machine-learning product (Sauzéde et al., 2020).

The final proposed tests resulted from a compromise between i) generating a quality-controlled BBP dataset in real time, ii) assigning flags that help the DM operators, and iii) avoiding burdening DACs with overly complicated tests. The Python code for the tests as well as example inputs and expected outputs for each test have been provided to facilitate implementation at the DAC level.

Ethics and consent

Ethical approval and consent were not required.

Data availability

Underlying data

The original Argo data used in this study (snapshot of December 2021) are freely available in NetCDF format from:

https://www.seanoe.org/data/00311/42182/#90179

This dataset is available under the terms of the Creative Commons Attribution 4.0 International license (CC-BY 4.0).

Software availability

Source code is available from: https://github.com/euroargodev/ BBP_RTQC/releases/tag/BBP_RTQC_v2.0.0

Archived source code at time of publication: https://doi.org/10. 5281/zenodo.7934400

License: MIT

Acknowledgements

These data were collected and made freely available by the International Argo Program and the national programs that contribute to it. (https://argo.ucsd.edu, https://www.ocean-ops. org). The Argo Program is part of the Global Ocean Observing System. Dr. E. Osborne is thanked for comments on an initial draft of this manuscript. We would like to thank the reviewers Dr. G. Neukermans and Dr. G. Volpe for the time they invested providing constructive criticisms and comments to an earlier draft of this manuscript.

References

Balch WM, Kilpatrick KA, Trees CC: The 1991 coccolithophore bloom in the central north atlantic. 1. optical properties and factors affecting their distribution. Limnol Oceanogr. 1996; 41(8): 1669-1683. **Publisher Full Text**

Bisson KM, Boss E, Westberry TK, et al.: Evaluating satellite estimates of particulate backscatter in the global open ocean using autonomous profiling floats. Opt Express. 2019; 27(21): 30191-30203. PubMed Abstract | Publisher Full Text | Free Full Text

Bittig HC, Maurer TL, Plant JN, *et al.*: A BGC-argo guide: Planning, deployment, data handling and usage. *Front Mar Sci.* 2019; 6: 502. **Publisher Full Text**

Boss E, Pegau WS: Relationship of light scattering at an angle in the backward direction to the backscattering coefficient. Appl Opt. 2001; 40(30): 5503-5507

PubMed Abstract | Publisher Full Text

Briggs N, Dall'Olmo G, Claustre H: Major role of particle fragmentation in regulating biological sequestration of CO₂ by the oceans. Science. 2020; 367(6479): 791–793.

PubMed Abstract | Publisher Full Text

Briggs N, Perry M, Cetinic I, et al.: High-resolution observations of aggregate flux during a sub-polar North Atlantic spring bloom. Deep Sea Research Part I: Oceanographic Research Papers. 2011; 58(10): 1031-1039. **Publisher Full Text**

Cetinić I, Perry MJ, Briggs NT, et al.: Particulate organic carbon and inherent optical properties during 2008 North Atlantic Bloom Experiment. J Geophys Res. 2012; 117(C6): C06028. **Publisher Full Text**

Claustre H. Johnson KS. Takeshita Y: Observing the global ocean with Biogeochemical-Argo. Ann Rev Mar Sci. 2020; 12(1): 23-48. PubMed Abstract | Publisher Full Text

Dall'Olmo G, Boss E, Behrenfeld MJ, et al.: Particulate optical scattering coefficients along an Atlantic Meridional Transect. Opt Express. 2012; 20(19): 21532-21551

PubMed Abstract | Publisher Full Text

Graff J, Westberry T, Milligan A, et al.: Analytical phytoplankton carbon measurements spanning diverse ecosystems. Deep Sea Res 1 Oceanogr Res Pap. 2015: 102: 16-25. **Publisher Full Text**

Haëntjens N, Penna AD, Briggs N, et al.: Detecting mesopelagic organisms using Biogeochemical-Argo floats. Geophys Res Lett. 2020; 47(6): e2019GL086088

PubMed Abstract | Publisher Full Text | Free Full Text

Hu L, Zhang X, Perry MJ: Light scattering by pure seawater: Effect of pressure. Deep Sea Res 1 Oceanogr Res Pap. 2019; 146: 103-109. Publisher Full Text

Koestner D, Stramski D, Reynolds RA: A multivariable empirical algorithm for estimating particulate organic carbon concentration in marine environments from optical backscattering and chlorophyll-a measurements. Front Mar Sci. 2022; 9: 941950 **Publisher Full Text**

Martinez-Vicente V, Dall'Olmo G, Tarran G, et al.: Optical backscattering is correlated with phytoplankton carbon across the Atlantic Ocean. Geophys Res Lett. 2013; 40(6): 1154-1158. **Publisher Full Text**

Mobley C: The Oceanic Optics Book. International Ocean Colour Coordinating

Group, IOCCG, 2022. Publisher Full Text

Oishi T: Significant relationship between the backward scattering coefficient of sea water and the scatterance at 120 degrees. Appl Opt. 1990; 29(31): 4658–4665.

PubMed Abstract | Publisher Full Text

Poteau A, Boss E, Claustre H: **Particulate concentration and seasonal dynamics in the mesopelagic ocean based on the backscattering coefficient measured with Biogeochemical-Argo floats.** *Geophys Res Lett.* 2017; 44(13): 6933-6939.

Publisher Full Text

Rasse R, Dall'Olmo G, Graff J, et al.: Evaluating optical proxies of particulate organic carbon across the surface Atlantic Ocean. Front Mar Sci. 2017; 4: 367.

Publisher Full Text

Roemmich D, Alford MH, Claustre H, et al.: On the future of Argo: A global, Publisher Full Text

Sauzéde R, Johnson JE, Claustre H, et al.: Estimation of oceanic particulate

organic carbon with machine learning. ISPRS Annals of the Photogrammetry, Remote Sensing and Spatial Information Sciences. 2020; V-2-2020: 949-956.

Publisher Full Text

Stramski D, Reynolds R, Babin M, *et al.*: **Relationships between the surface concentration of particulate organic carbon and optical properties in the eastern South Pacific and eastern Atlantic Oceans.** *Biogeosciences.* 2008; 5(1): 171-201.

Publisher Full Text

Terrats L, Claustre H, Cornec M, et al.: Detection of coccolithophore blooms with biogeochemical-argo floats. Geophys Res Lett. 2020; 47(23): e2020GL090559.

PubMed Abstract | Publisher Full Text | Free Full Text

Zhang X, Hu L: Estimating scattering of pure water from density fluctuation of the refractive index. *Opt Express*. 2009; **17**(3): 1671–1678. PubMed Abstract | Publisher Full Text

Zhang X, Hu L, He MX: Scattering by pure seawater: Effect of salinity. Opt Express. 2009; **17**(7): 5698–5710. PubMed Abstract | Publisher Full Text

Open Peer Review

Current Peer Review Status:

Version 2

Reviewer Report 12 September 2023

https://doi.org/10.21956/openreseurope.17363.r32322

© **2023 Volpe G.** This is an open access peer review report distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

/ / / /



Gianluca Volpe 问

Consiglio Nazionale delle Ricerche, Istituto di Scienze Marine (CNR-ISMAR), Rome, Italy

I have no other issues to rise; I am satisfied with the quality of the revised work for which I recommend indexing.

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Optical oceanography

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Reviewer Report 05 September 2023

https://doi.org/10.21956/openreseurope.17363.r34187

© **2023 Amadio C.** This is an open access peer review report distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.



Carolina Amadio ២

Istituto Nazionale di Oceanografia e di Geofisica Sperimentale OGS, Sgonico, Italy

Editorial Note from F1000Research – 6th September 2023: It has come to our attention that Carolina Amadio shares an affiliation with Giorgio Dall'Olmo. This was a result of honest error, and the conflict of interest statement has been updated to reflect this.

The paper introduces a new quality control procedure for optical backscattering data measured by BGC-Argo. Five tests are chosen to obtain the "best available Argo data" in real time, labeled as

Adjusted Mode (AM). The document can be particularly useful for both the Argo community and non-expert users, as it is clear and well structured.

General comments:

• I appreciate the choice to present QC tests using a common structure (objective, example, implementation, flagging, flow_chart, results).

However, I would expect to receive similar information for all tests in each of the sections. For example, in the "High-Deep-Value test" the choice of a threshold is explained in the "Objective" section, while in the other tests the thresholds are explained in the "Implementation" section. In the section "Implementation" of the "Negative-BBP-test", I would expect to find the information that the test is performed at 2 depths/layers (as for the other tests).

- Regarding the use of the thresholds, it is understandable that they are based on visual inspection and/or expert assessment. It would be helpful to better explain the choice of the thresholds used (e.g. like it is done for the "High-Deep-Value test"). Furthermore, did you evaluate the impact of using different thresholds? Have you considered to statistically define the thresholds?
- It might be useful to summarize the information and the results of the tests in a table. Here is an example:

in rows the 5 tests, in columns:

Depth/layer (m) || Threshold (m-1) || Nr. of points || QC(s)* || % discarded *QS --> specifying whether a label refers to the entire profile or to single points

 If I understand correctly, the Missing Data-test assigns QC=3 to all profiles shallower than 895-1000 dbar (the last bin). Does this mean that no real-time data are available in areas of the ocean where bathymetry is < 895 dbar (e.g., regional seas)?

If the answer is yes:

(i) I suggest specifying this problem as a test limitation for shallow basin/areas(ii) in the High-Deep-Value test the condition "is the profile deeper than 700 dbar" becomes useless.

(iii) in the Noisy-BBP test the condition "Are there at least 10 points in this profile?" become useless

If the answer is no:

(i) Highlight what happens in cases of shallow bathymetry.

- Test overlap: The main purpose for which you decided to implement the test is not completely clear from the text. On the one hand, the overlap test can be useful to confirm the presence of anomalous profiles, demonstrating the robustness of your tests choice. On the other hand, however, it could be used as an indicator of test redundancy. If I understand correctly, which of the two aspects (confirm the test/avoid redundancy) do you consider more relevant?
- The RTQC uses 4 different values of QC (1, 3, 4, 9). It can probably be

useful to list them at the beginning of the "Results" Section, also explaining why QC=2 is never used (since QC=2 appears in the table 1 and figure 17)

Detailed comments (minor):

Introduction:

- Add bbp unit of measurements at the beginning of the introduction .
- "Argo's objective is to sustain 1000 operational six-variable BGC-Argo floats in the global ocean" list variables or remove sentence. "So far more than 600 BGC-Argo floats have been equipped with optical backscattering sensors, and ~250 of them are currently active." I suggest reversing the order of the two sentences.
- "now obsolete, given the new tests presented in this work" Why are the tests obsolete? I suggest to explain better or remove the sentence.

Results:

- "Objective, presenting the purpose of the test" I suggest adding "presenting the purpose of the test and the BGC-Argo target problem(s) to be addressed" (e.g. malfunctioning of sensor etc.).
- High-Deep-Value test: I suggest moving the explanation of the threshold value to the "Implementation" section.

Furthermore, I find a slight discrepancy between the order of magnitude of the threshold value (10-4 m-1) and the x-axis label (10-2) in Figure 4. It can be solved by making explicit in the text "the blue line in Figure 4" when introducing the threshold value or by changing the x-axis label in Figure 4.

• Parking-Hook test: I suggest rephrasing the "Implementation" part, reducing the information. For example: "The test is applied to all ascending profiles when the distance (LAYER1) between the last 2 points of a profiles is less than 20 meters (G_DELTAPRES2) and the distance (LAYER2) between the parking pressure and the maximum depth (maxPRES) is less than 100dbar. The median between BBP at LAYER1 and LAYER2 is added to a threshold (G_DEV = 0.0002 m-1). The test fails whenever data in LAYER2 are higher than the computed baseline.

Discussion:

"Finally, as the proposed tests are implemented and users begin exploiting the RTQC BBP dataset, we expect that imperfections in the tests will be identified, which will result in further tuning of the test parameters." By using "further" in the previous sentence, I understand that you have tuned the parameters, but I do not see any reference to this in the "Results Section".

Is the rationale for developing the new method (or application) clearly explained?

Yes

Is the description of the method technically sound?

Yes

Are sufficient details provided to allow replication of the method development and its use by others?

Yes

If any results are presented, are all the source data underlying the results available to ensure full reproducibility?

Yes

Are the conclusions about the method and its performance adequately supported by the findings presented in the article?

Yes

Competing Interests: 1. Giorgio Dall'Olmo and I share the same OGS affiliation and the same Section (Oceanography Section). Despite this, we work/are involved in: - different groups (Amadio works in the Dynamics of Ecosystems and Computational Oceanography group, while Dall'Olmo in the Physical Oceanography group) see https://www.ogs.it/en/section-oceanography for OGS group's organisation; - different projects (Amadio is mainly involved in Copernicus Marine Service as BGC modeller while Dall'Olmo is involved in some BGC-ARGO projects); - different Departments (Amadio's office is located in Via Beirut, 34151 Grignano TS while Dall'Olmo office is located in Borgo Grotta Gigante, 42/c, 34010 Sgonico TS). Furthermore, I work mainly at home (I'm a postdoc), and in another city (Bologna). 2. I have never contacted Dall'Olmo directly by phone, email or social media (but of course we receive the same communications by email from OGS and/or OGS sections/groups/subgroups). Furthermore, I have only met Dall'Olmo at the OGS (internal/eternal) seminars/meetings (maximum 4 in 2 years). 3. Dall'Olmo attended my seminar at OGS on January 2022 "NEW DEVELOPMENTS ON THE OXYGEN DATA QUALITY CHECK ASSESSMENT" 4. Up to now, we never collaborate for common projects. 5. The article I am reviewing was never discussed between us. In the light of what has been listed and stated above, I believe I am in a position to evaluate this article impartially.

Reviewer Expertise: BGC-Argo dataset and BGC-Argo data assimilation in operational models

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Reviewer Report 10 August 2023

https://doi.org/10.21956/openreseurope.17363.r33065

© **2023 Thomalla S.** This is an open access peer review report distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

\checkmark

Sandy J. Thomalla

Southern Ocean Carbon and Climate Observatory (SOCCO), CSIR, Rosebank, South Africa

Review: Real-time quality control of optical backscattering data from Biogeochemical-Argo

floats

Sandy Thomalla

This manuscript presents a suite of 5 real-time quality control tests for application to optical backscattering profiles in the BGC-Argo data set. The paper is well written and clearly explains the structure of the tests, why they are needed, how they are implemented and the impact that their implementation has on the data set. I particularly liked the flow charts which I found especially clear (and indeed in some cases easier to follow than the "Implementation" text). These methods are needed by the growing user community that is interested in carbon flows, in particular those wanting access to real time data that is appropriately quality controlled to exclude bad or suspect data.

I find this manuscript suitable for publication with only minor comments listed below. Without line numbers it was challenging to identify their specific reference, so in addition I have included all comments on the attached .pdf with the location of their relevance highlighted in green. I have chosen to sign my review as I am an advocate for transparency and accountability of review.

Introduction.

It is maybe worth highlighting that the typical bbp wavelength of the BGC argo data base is 700nm? And why? And what alternate wavelengths are typically implemented?

I think that it is worth adding that in particular bbp can be used as an alternate proxy for phytoplankton biomass that is not impacted by quenching. I would suggest highlight that optical observations such as backscatter are better correlated to carbon than chlorophyll and that they can provide independent measures of phytoplankton biomass in open ocean waters (away from regions with highly scattering inorganic material). Unlike chlorophyll, bbp is more likely to be insensitive to changes in the intracellular concentration of pigments. In addition, the ratios between chlorophyll and bbp can be used to correct for quenching and in addition, chl:bbp ratios can be used to infer and elucidate on possible physiological adjustments to environmental stressors and community structure (i.e. i would recommend providing additional motivation for why the variable bbp is useful to the community).

Add parenthesis (RT) and (DM) to the first use of Real Time and Delayed Mode.

I am curious as to why you highlight non-experts per se (here and elsewhere). I appreciate that so called experts would be more inclined to examine the data and post-process it allowing for corrections to be applied where appropriate (e.g. a revised dark count to prevent negative offset etc.). But to me the key user here is anyone who needs to access near real-time data (regardless of their level of expertise). You provide one example of a non-expert user as an operational modeller, could you possibly elaborate on this further? Specifically, are you able to highlight the benefits to operational modellers of having access to real time data instead of delayed mode data (especially considering that delayed mode data are generally considered "better" having undergone the QC scrutiny in addition to the application of corrections where possible).

Are the two tests listed for bbp in the Argo Quality control manual currently being implemented to the ARGO data set? i.e. is some level of QC being implemented and data being flagged, albeit that

these 5 tests are considerably better?

Can you possibly elaborate on the obsolete global rage and spike tests please? I appreciate that the ensemble of tests being presented here is better, but I think that it is worth elaborating on why the current tests are inadequate (how do they work?/ why don't they work well?). If those obsolete tests are being ineffectually implemented you could also compare the % of flagged data from the implementation of the current 2 tests versus your suite of 5 (to highlight how much suspect data was passing QC). A slight elaboration on this would provide additional motivation and rationale for the relevance of the tests being proposed in this manuscript and the requirement for them to be implemented as standard procedure.

Data and Methods

Hyphenate non-experts (as per other references)

The reason for number 4) of minimising impact to the DAC's is not clear to me (i.e. providing input and expected output for each test). Is this for comparison to your application to ensure that it is being applied correctly? Maybe this point could be made clearer, or elaborated or even possibly excluded?

Approach

Can you please clarify that to define the new BBP RTQC tests, you followed an iterative process of community engagement. When I first read this sentence I thought it was referring to the iterative application process of one QC step after the other (which is not I think what you meant in this instance).

The 'in vacuo' in this instance is confusing me. Since the 5 RTQC tests were actually developed for the bbp measurements made in situ by BGC-Argo at 700nm (i.e. not in a vacuum)? Albeit that θ , is measured at a given wavelength in vacuo.

Can you elaborate on how many other BGC-Argo floats there are with bbp at a wavelength other than 700? if so what is it typically? Also, why not test and show/confirm that the RTQC does apply to different wavelengths and works just as well at 700nm (as with any other wavelength)?

Consider altering this sentence structure to read as follows (less negative). "Interactions with the community were crucial in defining the final test suite. Although this approach introduced a certain level of subjectivity in how the tests were selected, it incorporated the knowledge of experts in optical backscattering and management of the Argo data stream providing fundamental input towards critically determining the final ensemble of test definitions."

Please clarify the statement regarding "even if profiles had been deemed bad by the DAC operators"? How were bbp profiles deemed bad by the DAC given that no real time QC on bbp was being implemented? Or were they deemed bad by the two obsolete QC steps mentioned earlier?

Your first step to minimise overlap is not clear to me. To me, determining the fraction of data points flagged by all pairs of tests does not minimise overlap. Especially if "All tests were applied independently of each other (no order was defined) and the statistics computed reflect this choice (i.e., the same data can be flagged by multiple tests)." Surely overlap would only be minimised if

you instead applied the tests in series (and not in parallel) i.e. if a profile was deemed bad by the first test in the series it did not undergo the other 4 tests.

Results

"This order could be used to define the sequence in which the tests are applied during RTQC". Indeed, were that approach taken it would understandably minimise implementation overlap by the DAC.

The following comment is true for all Implementation text regarding the use of words, code and units. I think it is appropriate that the code be included in parenthesis (but that it should exclude the units) but not that the thresholds are excluded from the text, which I think should be clear in the text and include the units. I would suggest that all "Implementation" sections be edited as per this example for the HIgh-Deep-Value test:

Implementation: This test first determines s fails if there are is at least 5 points a certain number (C_N_DEEP_POINTS = 5) of points deeper than a threshold depth of 700 dbar (C_DEPTH_THRESH = 700 dbar) and it fails if the median of the median-filtered profile below 700 dbar C_DEPTH_THRESH is greater than a predefined threshold of 0.0005 m-1 (i.e., C_DEEP_BBP700_THRESH = 0.0005 m-1).

Consider including a possible reason for deep bbp values being an incorrect dark count (i.e. if underestimated). Which I believe can be quite common and easily rectified in DMQC. Add a space: to "good"

Put (B_PRES_THRESH = 100) in brackets like the other code examples.

Please adjust as follows: The test fails if residuals with absolute values above a threshold value of 0.0005 m - 1 (i.e., B_RES_THRESHOLD = 0.0005) occur in at least 10% of the profile data below the 100 dbar threshold.

Negative-BBP test could similarly occur if darkcount is too high, which is easily accounted for in DM processing to recover profiles.

Pressure limit is missing from the code in brackets for second depth range test: "The test is then implemented over a second pressure range (i.e., PRES >= maxPRES - G_DELTAPRES1 = 20)."

Figure 13: I was wondering if there is a way to identify the points that fall into both the 20mn and 50m depth ranges? Shouldn't all dots in the bottom 50m of the profile be blue? (only three looking blue to me?). The two depth ranges that are compared to each other (via the mean) is not clear (to me) in the figure.

Discussion

By users ... add "that access to require real time data"

The second two sentences of the Discussion are repetitive (and just recently covered in the previous sections).

Adjusting BBP to RTQC. For what it is worth (and this is just my personal opinion here) I would have to disagree with the Argo community on this. If a non-expert user is after real time bbp data and there is none in bbp_ adjusted then they will by default fall back on using the unadjusted BBP data, which will have undergone RTQC and will have flags associated with it. As such, they will know that it has passed quality control measures but that it has NOT been adjusted in any way. I strongly feel that data should only be labelled as adjusted if it has indeed been adjusted e.g. by subtracting a revised dark count based on a percentile of deep data to compensate for incorrect dark values (as is applied for the chlorophyll in delayed mode processing).

Is the rationale for developing the new method (or application) clearly explained? $\ensuremath{\mathsf{Partlv}}$

Is the description of the method technically sound?

Yes

Are sufficient details provided to allow replication of the method development and its use by others?

Yes

If any results are presented, are all the source data underlying the results available to ensure full reproducibility?

Yes

Are the conclusions about the method and its performance adequately supported by the findings presented in the article?

Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Biogeochemistry, phytoplankton photophysiology, biological carbon pump, Southern Ocean, primary production, carbon export.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Reviewer Report 20 June 2023

https://doi.org/10.21956/openreseurope.17363.r32321

© **2023 Neukermans G.** This is an open access peer review report distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.



Griet Neukermans 问

Biology Department, MarSens Research Group, Ghent University, Ghent, Belgium

I have no further comments. Griet

Is the rationale for developing the new method (or application) clearly explained? $\ensuremath{\mathsf{Yes}}$

Is the description of the method technically sound?

Yes

Are sufficient details provided to allow replication of the method development and its use by others?

Yes

If any results are presented, are all the source data underlying the results available to ensure full reproducibility?

Yes

Are the conclusions about the method and its performance adequately supported by the findings presented in the article?

Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Particle backscattering, BGC-Argo data, biogeochemistry

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Version 1

Reviewer Report 30 January 2023

https://doi.org/10.21956/openreseurope.16269.r30309

© **2023 Neukermans G.** This is an open access peer review report distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

? Griet Neukermans 匝

Biology Department, MarSens Research Group, Ghent University, Ghent, Belgium

This paper clearly describes five real-time quality control tests applied to optical backscattering data from BGC-Argo floats. This paper is timely, given the rapidly growing non-expert user base of BGC-Argo bbp data and will be very useful to the BGC-Argo community and its users. The paper is well written and well structured, the data and results are of good quality, and the discussion is

thorough. I recommend indexing of this work, but I have a few minor comments that may help improve the paper. I have provided my comments in comment boxes on the pdf paper which can be found here. I have listed them below for completeness and transparency:

Minor comments:

- replace reflected by scattered. Reflection is only a part of light scattering. Please carefully check the definitions of backscattering and the VSF.
- remove "backward"
- wavelength in vacuo or in water?
- VSF by particles at a given angle
- and PIC see Balch *et al.* (1996) and Terrats et al. (2020) papers.^{1,2}
- Do QC flags values between 5 and 8 have any meaning? If yes, please specify
- replace with e.g.? the BGC-Argo community interested in the quality control of BBP is probably wider than the list of co-authors of this paper.
- Wavelength in vacuo
- Correct: this repository if the the first author
- new, with respect to what?
- I suggest to add a figure with a decision tree for each of the QC tests for quick and easy visualization of the tests and QC flags.
- what is the rationale for defining these bins?
- please give range for "considerably lower"
- because of the high overlap between flagged data and non-flagged data it may be better to use density plots for the entire dataset, showing the number density of points with and without flags. Same comment to Fig 2, 4, 6, 8, and 10.
- Perhaps useful to say how these spikes differ from spikes associated with large particles that are not large organisms
- do you mean absolute values? as the residuals can be negative because of the medianfiltering
- is there an explanation for these two vertical lines?
- useful to specify which expectations you mean
- but see seasonality in Poteau et al. 2017.³
- meaning of "grounded"? Touched the seafloor?
- also add Haentjens ref
- Again, all data can be plotted using density plots showing the number density of observations but data in the BBP adjusted variable are only BBP data with QC flag <2?
 Perhaps worth being explicit about what BBP_ADJUSTED i

References

 Balch W, Kilpatrick K, Trees C: The 1991 coccolithophore bloom in the central North Atlantic. 1. Optical properties and factors affecting their distribution. *Limnology and Oceanography*. 1996; **41** (8): 1669-1683 Publisher Full Text

2. Terrats L, Claustre H, Cornec M, Mangin A, et al.: Detection of Coccolithophore Blooms With BioGeoChemical-Argo Floats.*Geophys Res Lett.* 2020; **47** (23): e2020GL090559 PubMed Abstract |

Publisher Full Text

3. Poteau A, Boss E, Claustre H: Particulate concentration and seasonal dynamics in the mesopelagic ocean based on the backscattering coefficient measured with Biogeochemical-Argo floats. *Geophysical Research Letters*. 2017; **44** (13): 6933-6939 Publisher Full Text

Is the rationale for developing the new method (or application) clearly explained? Yes

Is the description of the method technically sound?

Yes

Are sufficient details provided to allow replication of the method development and its use by others?

Yes

If any results are presented, are all the source data underlying the results available to ensure full reproducibility?

Yes

Are the conclusions about the method and its performance adequately supported by the findings presented in the article?

Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: particle backscattering, BGC-Argo data, biogeochemistry

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 10 May 2023

Giorgio Dall'Olmo

Griet Neukermans, Biology Department, MarSens Research Group, Ghent University, Ghent, Belgium

This paper clearly describes five real-time quality control tests applied to optical backscattering data from BGC-Argo floats. This paper is timely, given the rapidly growing non-expert user base of BGC-Argo bbp data and will be very useful to the BGC-Argo community and its users. The paper is well written and well structured, the data and results are of good quality, and the discussion is thorough. I recommend indexing of this work, but I have a few minor comments that may help improve the paper. I have provided my comments in comment boxes on the pdf paper which can be found here. I have listed them below for completeness and transparency:

OUR ANSWER: We thank very much the reviewer for the time they invested in reading and providing suggestions to our manuscript. Below we provide a point-by-point response to each of the reviewer's comments.

Minor comments:

Annotation Page Our response/action: replace reflected by scattered.

Reflection is only a part of light scattering We agree, done.

Same comment We agree, done.

Remove "backward" We agree, done.

in vacuo

We agree, done.

VSF by particles at a given angle

We agree, done.

and PIC see Balch and Terrats papers

We agree, done.

Do QC flags values between 5 and 8 have any meaning? If yes, please specify

These Argo QC flags are not used in this manuscript, therefore are not described here. We've added a link to the Argo User's Manual, where all Argo flags are described.

replace with e.g.? the BGC-Argo community interested in the quality control of BBP is probably wider than the list of co-authors of this paper.

We have now specified "the community that contributed to the development of the quality control...". feedback

Corrected

Importantly, this assumes that the profile is collected in deep waters far from the bottom near which suspended sediments might invalidate the assumptions of some of the proposed tests (see also discussion on High-Deep-Value test). We have modified the sentence to make it clearer.

in vacuo

Done

Therefore to smooth BBP profiles, an adaptive median filter is used in some of the proposed tests with a window size (w) that varies depending on the vertical resolution (\triangle PRES) of the data: w = 11 if \triangle PRES < 1 dbar, w = 7 if $1 \le \triangle$ PRES \le 3 dbar, and w = 5 if \triangle PRES > 3 dbar.

Corrected.

please correct

Corrected.

if the the first

Corrected.

new, with respect to what?

With respect to the existing tests we mentioned in the introduction.

I suggest to add a figure with a decision tree for each of the QC tests for quick and easy visualization of the tests and QC flags.

This is a good idea: we have now added a flowchart to explain each test

what is the rationale for defining these bins?

The rationale is to avoid "round numbered" depths that are typically selected to acquire measurements (e.g., 150, 200, 250, 350, etc.)

please give range for "considerably lower"

We agree, done.

because of the high overlap between flagged data and non-flagged data it may be better to use density plots for the entire dataset, showing the number density of points with and without flags. Same comment to Fig 2, 4, 6, 8, and 10.

Done.

Perhaps useful to say how these spikes differ from spikes associated with large particles that are not large organisms

We have now specified that these "animal spikes" appear in clusters.

do you mean absolute values? as the residuals can be negative because of the medianfiltering

Yes, thank you: corrected.

is there an explanation for these two vertical lines?

The "vertical lines" are profiles of BBP values where the sensor had saturated (likely because of intense biofouling)

useful to specify which expectations you mean

We agree: done.

but see seasonality in Poteau et al. 2017

Indeed Poteau et al (2017) observed a seasonality in the BBP signal at 900 dbar, but the maximum observed peak-to-peak variability was on the order of <0.00001 1/m. We have now specified that this seasonal variability is considerably lower than the threshold value used.

meaning of "grounded"? Touched the seafloor?

Yes, we have now added this specification.

also add Haentjens ref

Done.

Again, all data can be plotted using density plots showing the number density of observations

Done.

but data in the BBP adjusted variable are only BBP data with QC flag <2? Perhaps worth being explicit about what BBP_ADJUSTED is.

We have now modified the related text to clarify this.

Competing Interests: No competing interests were disclosed.

Reviewer Report 27 January 2023

https://doi.org/10.21956/openreseurope.16269.r30306

© **2023 Volpe G.** This is an open access peer review report distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

了 🛛 Gianluca Volpe 匝

Consiglio Nazionale delle Ricerche, Istituto di Scienze Marine (CNR-ISMAR), Rome, Italy

This is the revision of the paper "Real-time quality control of optical backscattering data from Biogeochemical-Argo floats" by Giorgio Dall'Olmo and co-authors. The manuscript describes five tests for the real-time quality assessment of automatically-acquired backscattering profiles from BGC-Argo platforms. The work is relevant not only for the Argo community but also for BGC-Argo users for which provides a valid background, as such it surely deserves publication in Open Research Europe. There are however a few remarks that I encourage the authors to take into consideration.

A general comment is that the whole work looks too descriptive reading more like a meeting report (often highlighting the points of agreement) than a scientific paper. The five tests rely on thresholds whose definition is apparently based on subjective judgement, which for as intuitive and reasonable they can be they are still not supported by any scientific evidence or statistical analysis. This points to the question not explicitly addressed in the manuscript on whether DMQC is only applied to profiles initially flagged as 3 or to all profiles, independently of the RTQC. If all profiles do undergo DMQC independently of RTQC then the importance of RTQC is only relevant to applications needing real-time data (e.g., operational modelers). On the contrary, if DMQC is only applied to suspicious profiles determined by the RTQC, then it is important to determine the various thresholds in a more rigorous manner. To give the readers the flavor from one side of the importance of the expert review and on the other of the robustness of the general approach described in the manuscript, I would suggest the authors to color (or simply to provide percent numbers) the profiles shown in the various examples that effectively changed their status: for example, how many profiles were originally flagged as 2 or 1 and then turned 3 or 4 after expert judgement? And similarly how many profiles that were originally flagged as 3 or 4 actually turned 2 or 1 after expert judgement?

Moreover, I understand that a quasi-binary (e.g., good vs no good data) flagging system is much easier to handle than a more complex system like the one adopted by the satellite data processing in which the flags surely provide a better means to quality assess the data. In this context, I do not see any reason for keeping things easier but rather to help users be more confident in data usage. One drawback of the proposed flagging system is that it does not allow users to discriminate data according to the various tests. This could also give useful feedbacks to the test developers.

Going through the manuscript, I found curious and a bit frustrating as well that at the end of "Data and methods" it was still unclear what the tests are about and what are they aimed at. I would suggest the authors to reshape a bit the way the information is conveyed and in case to compact the relevant information about the five RTQC tests (e.g., thresholds, filtering application etc ...) into a table that could be referred to.

Information on the general Argo data handling approach could provide a context for non-expert users or for the non-community members and help them understanding what is behind the choice of simplicity or . For example, how frequent are the RTQC and DMQC testing? How many profiles the single DAC has to handle in terms of both testing (RTQC and DMQC)? How many DACs are involved?

Here below more detailed comments on the various sections.

The **abstract** is schematic and effective.

Introduction

Since the Argo variable used to represent b_{bp} is BBP, we will use the latter in this manuscript. – Nonexpert readers may surely benefit from the addition of one sentence that explains the difference between the two bbps if indeed it exists. The way it is presented this sentence may create confusion, please rephrase it.

Data and methods

Approach section is not entirely clear and I personally find it a bit confusing. It refers to a series of details that surely provide the context in which the manuscript has developed but probably do not add any significant science to the paper. A better place where mentioning this kind of details would probably be the introduction. I would expect Data and methods to cover aspects that help the reader discriminating whether the tests are useful, scientifically sound and operationally feasible.

Other things that I found confusing/not clear in this section are:

- 1. the tests that are often mentioned are not yet defined nor there is a link to any table/figure or section that the reader can promptly refer to: this is also mentioned in the general comments.
- 2. the authors refer to themselves as the community and this is done in a way as if the consensus reached among the coauthors of the manuscript should per se be a proof of the validity of the approach.
- 3. *These interactions with the community allowed us ...* this sentence does not add any particular or relevant information: that the coauthors/community of a work do interact among them is pretty obvious as it is obvious that they eventually reach an agreement.
- 4. It is not clear why the overlap among tests should be minimized. Having more than one test telling that the profile is not the best you might have measured is probably better, especially if the goal is to worn non-expert users on their usage. I suggest here to add a sentence to better explain why it is advisable that the tests do not overlap, if that is the case.
- 5. The link between the different sampling rate and the vertical resolution of the various sensors and missions with the need of smoothing the data with a median filter is not entirely straightforward. I can understand that for the sake of QC tests the application of a median filter to smooth the profile could be useful, advisable and foreseeable, but this should be properly justified.

Probably a better title for this section could be "background".

Results

Very often, to explain the various tests, English is substituted by a sort of programming language notation: although most of the times the meaning is intuitive it still distracts and one often has to

go back and forth reading the same sentence to make sure the meaning is appropriately taken. I recommend the authors to use English and where necessary or helpful to add the "programming language" notation. I found this particularly true in correspondence of the implementation of the parking-hook test.

Missing-Data test

Since the 10 bins are quite large (50 to 100 m), I would expect data abundance per bin to be higher, so perhaps MIN_N_PERBIN should be set larger than 1 according with the rate of acquisition and the float vertical velocity.

High-deep-value test

My understanding is that the rationale for the high-deep-value test is to spot profiles affected by any kind of sensor issues. In this view, it would probably make sense, once a profile is flagged, to also look at the temporal variability of the closest profiles acquired with the same float. Similarly, the overall shape of the profile should somehow suggest whether the profile should be flagged as 2 or 4, thus removing the need of the expensive expert judgement.

Right out of my curiosity (other readers could find it interesting as well), how would the profile of Figure 3 be flagged by an expert? At a very first sight the profile looks absolutely reasonable but probably affected by a bias depending whether or not it was acquired in a high productive area.

Noisy-Profile test

Why is this test based on the absolute residuals and not over a percent or relative units threshold? The percent threshold is probably easier to implement especially if the test is meant to be applied to all sensors deployed globally.

Parking-Hook test

The implementation part should be rewritten. Many times the authors refer to variables that have not previously defined making the reading heavier than necessary. Similarly, as already mentioned, the authors should write in proper English avoiding coding language where possible. The addition of equations could go in the right direction.

Test overlap

Before reading about the example provided by the authors to interpret figure 11, I understood that the test overlap was computed over single measurements (points). Then I wonder, how can a data point fail both the missing data test and the parking hook test, especially because the missing data test is applied over a depth range totally different than the parking-hook test? I am confused perhaps because I still don't understand the point of considering the test overlap. One consideration is that perhaps there should be two different flagging systems: one for the profile and the other for the single measurement. Moreover, the authors may want to consider the additive flagging system method used, for example, in the Level-1 to Level-2 satellite data processing. The advantage of this method is that each test has its own value which can then be added to the others and independently of the others; the result is that pixel (data point in this case) can be flagged with and thus sorted according to any of the applied tests.

Discussion

Comments on selected proposed tests

One important remark is about the authors' choice (driven by the Argo community feedback) of

keeping the various tests as simple as possible even if more complex and likely more robust tests can be envisaged also in real-time. These tests should be as robust and reliable as possible with the general aim of minimizing as much as possible the expensive human intervention. Given the general simplicity of the shown tests, it is hard to see how a "more complex" test could overburden DACs. The point here is to operationally run the RTQC procedure (i.e., a python script?) to assign a specific value to the profile or to each of its data points. This has little or nothing to do with the complexity of the test which could also take account of the local bathymetry or climatology, which could and actually should be generated at GDAC level and disseminated to local DACs. Lack of ancillary data at the time of RTQC appears a much solid reason for not running the test, not simplicity.

Missing-Data test.

An additional reason for ... - this is connected to one of my previous comments on the need of either splitting the QC flagging system into two (profile and single data record) or to adopt an approach similar to satellite data processing.

High-Deep-Value test

I do not see any inconvenience nor complexity in using the bathymetry also in real-time quality testing.

Is the rationale for developing the new method (or application) clearly explained? V_{AS}

Yes

Is the description of the method technically sound?

Yes

Are sufficient details provided to allow replication of the method development and its use by others?

Yes

If any results are presented, are all the source data underlying the results available to ensure full reproducibility?

Yes

Are the conclusions about the method and its performance adequately supported by the findings presented in the article?

Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: optical oceanography

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 10 May 2023

Giorgio Dall'Olmo

Gianluca Volpe, Consiglio Nazionale delle Ricerche, Istituto di Scienze Marine (CNR-ISMAR), Rome, Italy This is the revision of the paper "Real-time quality control of optical backscattering data from Biogeochemical-Argo floats" by Giorgio Dall'Olmo and co-authors. The manuscript describes five tests for the real-time quality assessment of automaticallyacquired backscattering profiles from BGC-Argo platforms. The work is relevant not only for the Argo community but also for BGC-Argo users for which provides a valid background, as such it surely deserves publication in Open Research Europe. There are however a few remarks that I encourage the authors to take into consideration.

1) OUR ANSWER: We thank the reviewer very much for the time they invested in reading and providing suggestions to our manuscript. Below we provide a point-by-point response to each of the reviewer's comments. In general we found that several of this reviewer's comments might have arisen from a lack of understanding of how the Argo Data Management system works. Other publications have described how the system works and we cannot repeat this here. However, to benefit the reviewer and readers, we have provided brief explanations and added citations to the main text and inside our responses.

A general comment is that the whole work looks too descriptive reading more like a meeting report (often highlighting the points of agreement) than a scientific paper.

2) OUR ANSWER: This is a "Method Article" in which we describe the method we have devised to quality control BBP data in real time, i.e., the RTQC tests. By its nature, it is a descriptive piece of text, and there is no scientific breakthrough. Moreover, we think it is important to highlight the points of agreement, because these have required important efforts to balance flagging accuracy and test simplicity.

The five tests rely on thresholds whose definition is apparently based on subjective judgement, which for as intuitive and reasonable they can be they are still not supported by any scientific evidence or statistical analysis.

3) OUR ANSWER: Indeed we have used subjective judgement to define many of the tests. This judgement is based on our experience with open-ocean BBP data collected in-situ and estimated from space during the last 15 years. Of course, there are likely to be flaws in our global and general tests (for example they may flag good data as "bad"), but this is the best we can do at the moment. We envisage that as the dataset grows and DACs start implementing the tests, we will need to revise them accordingly (see Discussion section). Supporting these tests using "scientific evidence or statistical analysis" would require to have an independent dataset against which we can compare the QC BBP data. Unfortunately, as the reviewer certainly knows, at the moment there are no other data that can be used for this purpose, especially in the deep open ocean, where most of the new BGC-Argo BBP data have been collected. In addition, satellite estimates of BBP appear to be affected by relatively large uncertainties (Bisson et al., 2019). Finally, knowledge of previous in-situ estimates of BBP in the surface and deep open ocean has been used to define all tests, as well as some of the specific thresholds (see references to Poteau et al 2017 and Dall'Olmo et al., 2012).

ACTION: We have acknowledged better that these tests may need to be revised.

This points to the question not explicitly addressed in the manuscript on whether DMQC is only applied to profiles initially flagged as 3 or to all profiles, independently of the RTQC. If all profiles do undergo DMQC independently of RTQC then the importance of RTQC is only relevant to applications needing real-time data (e.g., operational modelers). On the contrary, if DMQC is only applied to suspicious profiles determined by the RTQC, then it is important to determine the various thresholds in a more rigorous manner.

4a) OUR ANSWER: DMQC tests for BBP have not been devised nor implemented, yet. Once defined, the DMQC will be applied to all BBP data with QC<=3.

To give the readers the flavor from one side of the importance of the expert review and on the other of the robustness of the general approach described in the manuscript, I would suggest the authors to color (or simply to provide percent numbers) the profiles shown in the various examples that effectively changed their status: for example, how many profiles were originally flagged as 2 or 1 and then turned 3 or 4 after expert judgement? And similarly how many profiles that were originally flagged as 3 or 4 actually turned 2 or 1 after expert judgement?

4b) OUR ANSWER: DMQC tests for BBP have not been devised nor implemented, yet. We are currently planning on developing these tests by not only focusing on the profiles that failed the RTQC, but also by adding additional criteria (that have not been defined yet, but that will include for example comparing a given profile to other spatially- and temporally-adjacent profiles).

ACTION: Because the BBP DMQC tests have not been defined yet (this was stated in the Introduction of the draft manuscript), it is not possible to answer the questions posed by the reviewer.

Moreover, I understand that a quasi-binary (e.g., good vs no good data) flagging system is much easier to handle than a more complex system like the one adopted by the satellite data processing in which the flags surely provide a better means to quality assess the data. In this context, I do not see any reason for keeping things easier but rather to help users be more confident in data usage.

5) OUR ANSWER: Unlike the institutions that manage satellite data that are typically centralised (e.g., ESA, EUMETSAT or NASA), the international Argo programme is a decentralised system. Eleven Data Assembly Centres (DACs) around the world are responsible for acquiring, processing and delivering Argo data in real time in a consistent manner. Importantly, unlike satellite data, Argo data come from thousands of independent sensors. Although users do not see how exactly this consistency is achieved, great efforts are spent by DACs on this. DACs are independent of each other (e.g., they use different programming languages to code their tests) and are supported by different sources of funding. As of now, most DACs are underfunded and understaffed to deal with the amount

of work that the new 6 BGC-Argo variables have added to the Argo programme. This is why it is key to "keep things as simple as possible". We do not want to further complicate operations at the DACs. We hope that this explains more clearly why we strived to "keep things simple".

One drawback of the proposed flagging system is that it does not allow users to discriminate data according to the various tests. This could also give useful feedbacks to the test developers.

6) OUR ANSWER: We agree with the reviewer that a flagging system similar to that in use in the satellite community will be very valuable to BGC Argo. It is also important to understand that data-management methods for the BGC-Argo variables are currently being developed, so the current system should not be considered in its final version. The BGC-Argo Data Management team has explored a flagging system similar to the one used by the satellite community (see page 10 in https://archimer.ifremer.fr/doc/00298/40879/42267.pdf), but this has not been implemented yet. Also, the objective of this manuscript is to describe the new BBP RTQC tests, not how data and flags are managed inside the Argo data system.

ACTION: We have started defining a system to track which BBP RTQC tests have been implemented on a given profile and which have failed, but to ensure all DACs will implement the same system, we need to first reach an agreement among most DACs and then obtain official approval from the Argo Data Management Team. This is described in a new paragraph of the results.

Going through the manuscript, I found curious and a bit frustrating as well that at the end of "Data and methods" it was still unclear what the tests are about and what are they aimed at.

7) OUR ANSWER: The motivation and objectives of our work are clearly stated in the Introduction: "The main motivation behind this work is therefore to deliver in real time a quality-controlled BBP dataset that can be used by non-experts interested in retrieving information on suspended particles from the BGC-Argo dataset. The objective of this manuscript is to present a new suite of BBP Real-Time Quality-Control (RTQC) tests, the methodology used to devise them, and the results of implementing them on the entire BGC-Argo BBP dataset." This is why the main results of this work are the new tests themselves and that is why these tests are not described in the Methods section.

I would suggest the authors to reshape a bit the way the information is conveyed and in case to compact the relevant information about the five RTQC tests (e.g., thresholds, filtering application etc ...) into a table that could be referred to.

8) OUR ANSWER: Since the description of the new BBP RTQC tests is the main result of this work, we find it very hard to summarise it all in a single table. Instead, we prefer to maintain the current structure of the manuscript.

Information on the general Argo data handling approach could provide a context for nonexpert users or for the non-community members and help them understanding what is behind the choice of simplicity or,

9) OUR ANSWER: We understand that the Argo data system is not known to everyone, but the objective of this manuscript is not to describe again how it works. We provide here brief answers to the reviewer's questions, but we urge the interested reader to study the Argo Data Management documentation to obtain an in-depth understanding of how the Argo data system works.

,for example, how frequent are the RTQC and DMQC testing?

10) OUR ANSWER: As its name suggests, RTQC occurs in real time. In practice, DACs process, apply RTQC tests and submit newly acquired profiles to the GDACs within maximum 12-24 hours after they have been received. DMQC instead takes place on a 6-12 month basis, depending on the DAC and variable.

How many profiles the single DAC has to handle in terms of both testing (RTQC and DMQC)?

11) OUR ANSWER: This depends very much on the number of floats each DAC is responsible for. As can be seen in the figure linked, the Argo DACs handle very different percentages of the Argo dataset.

How many DACs are involved?

12) OUR ANSWER: There are 11 Argo DACs in total. ACTION: In the revised Introduction we have added a reference to the Argo Data Management Handbook that explains how the Argo data system works.

Here below more detailed comments on the various sections.

The abstract is schematic and effective.

Introduction Since the Argo variable used to represent bbp is BBP, we will use the latter in this manuscript. – Non-expert readers may surely benefit from the addition of one sentence that explains the difference between the two bbps if indeed it exists. The way it is presented this sentence may create confusion, please rephrase it.

14) OUR ANSWER: We agree. ACTION: In the revised version we have expanded on why "BBP" is used instead of "bbp" and clarified that the two variables are equivalent.

Approach section is not entirely clear and I personally find it a bit confusing. It refers to a series of details that surely provide the context in which the manuscript has developed but probably do not add any significant science to the paper. A better place where mentioning this kind of details would probably be the introduction.

15) OUR ANSWER: We disagree. The objective of the manuscript is to present the new BBP RTQC tests. The Approach section explains the general process used to come to an agreement about these tests.

I would expect Data and methods to cover aspects that help the reader discriminating whether the tests are useful, scientifically sound and operationally feasible.

16) OUR ANSWER: see answer 3.

Other things that I found confusing/not clear in this section are: the tests that are often mentioned are not yet defined nor there is a link to any table/figure or section that the reader can promptly refer to: this is also mentioned in the general comments.

17) OUR ANSWER: See our answer 15.

the authors refer to themselves as the community and this is done in a way as if the consensus reached among the coauthors of the manuscript should per se be a proof of the validity of the approach. These interactions with the community allowed us ... - this sentence does not add any particular or relevant information: that the coauthors/community of a work do interact among them is pretty obvious as it is obvious that they eventually reach an agreement.

18) OUR ANSWER: We wrote this section to describe the process through which we, as a community, have reached a consensus about the proposed BBP RTQC tests. As already mentioned in this response and already acknowledged in the manuscript, we are fully aware that the proposed tests are likely imperfect and will require fine tuning.

ACTION: We have added a sentence that clarifies this in section 4.4.

It is not clear why the overlap among tests should be minimized. Having more than one test telling that the profile is not the best you might have measured is probably better, especially if the goal is to worn non-expert users on their usage. I suggest here to add a sentence to better explain why it is advisable that the tests do not overlap, if that is the case.

19) OUR ANSWER: We agree, it was not clear why we needed to check how much overlap there was among tests. Although tests that confirm results from other tests can increase confidence in the results, they also mean that a greater number of tests is needed. Even if the same tests flag the same data. Again, to minimise the burden on DACs, we have decided to minimise the number of tests by also screening for overlapping results.

ACTION: we have clarified, in the Approach section, why we screened for overlapping tests.

The link between the different sampling rate and the vertical resolution of the various sensors and missions with the need of smoothing the data with a median filter is not entirely straightforward. I can understand that for the sake of QC tests the application of a median filter to smooth the profile could be useful, advisable and foreseeable, but this should be properly justified.

20) OUR ANSWER: Since the manuscript was submitted, one of the DACs has started implementing these tests and has verified that using a median filter with a single window of

11 points to smooth the data generates the same results as with the adaptive median filter.

ACTION: We have now repeated all tests with the single-window median filter and the revised manuscript has been updated accordingly.

Probably a better title for this section could be "background".

21) OUR ANSWER: We disagree.

Results Very often, to explain the various tests, English is substituted by a sort of programming language notation: although most of the times the meaning is intuitive it still distracts and one often has to go back and forth reading the same sentence to make sure the meaning is appropriately taken. I recommend the authors to use English and where necessary or helpful to add the "programming language" notation. I found this particularly true in correspondence of the implementation of the parking-hook test.

22) OUR ANSWER: We have added specific parameter names for each test in a different font to ensure readers can more easily link the manuscript to the code related to this manuscript. We have now realised that this was not explained. We believe this link is fundamental.

ACTION: We have kept specific parameter names in a different font, but have now clarified why this is done at the beginning of the Results section. We have also improved the description of each test by minimising the use of the "programming language notation" and by adding flow charts.

Missing-Data test Since the 10 bins are quite large (50 to 100 m), I would expect data abundance per bin to be higher, so perhaps MIN_N_PERBIN should be set larger than 1 according with the rate of acquisition and the float vertical velocity.

23) OUR ANSWER: The bins widths are not necessarily "quite large". Some groups collect measurements at 50-100-200 dbar resolution in the deep ocean. That is why MIN_N_BIN was set equal to 1.

High-deep-value test My understanding is that the rationale for the high-deep-value test is to spot profiles affected by any kind of sensor issues. In this view, it would probably make sense, once a profile is flagged, to also look at the temporal variability of the closest profiles acquired with the same float.

24) OUR ANSWER: We agree, but, for the sake of simplicity, we have decided to leave this type of quality control to the DMQC step.

Similarly, the overall shape of the profile should somehow suggest whether the profile should be flagged as 2 or 4, thus removing the need of the expensive expert judgement. Right out of my curiosity (other readers could find it interesting as well), how would the profile of Figure 3 be flagged by an expert? At a very first sight the profile looks absolutely reasonable but probably affected by a bias depending whether or not it was acquired in a

high productive area.

25) OUR ANSWER: The profile in figure 3 has a potentially reasonable shape, but it shows unreasonably elevated values at depth. As explained in the "Objective" subsection of this test, these values are not plausible for BBP values in the deep open-ocean. These types of "biases" can arise from biofouling, that is why the entire profile is flagged as probably bad.

Noisy-Profile test Why is this test based on the absolute residuals and not over a percent or relative units threshold? The percent threshold is probably easier to implement especially if the test is meant to be applied to all sensors deployed globally.

26) OUR ANSWER: Relative residuals are inappropriate, because they are "relative". In other words, there could be relatively high relative residuals in a profile that are simply due to the intrinsic variability of the sensor around a very low signal (typical of mesopelagic waters). On the other hand, absolute residuals allow us to identify spikes in the data that are significant with respect to the values expected for the BBP signals in the open ocean. ACTION: We have added a sentence to explain this.

Parking-Hook test The implementation part should be rewritten. Many times the authors refer to variables that have not previously defined making the reading heavier than necessary. Similarly, as already mentioned, the authors should write in proper English avoiding coding language where possible. The addition of equations could go in the right direction.

27) OUR ANSWER: See answer 22.

ACTION: We have improved the description of the implementation of this test.

Test overlap Before reading about the example provided by the authors to interpret figure 11, I understood that the test overlap was computed over single measurements (points).

28) OUR ANSWER: We are confused by this statement ("single measurements" seems an oxymoron). Also, if only single pairs of points are used, how can a percentage be computed?

ACTION: We have clarified in section 3.2 that the flagging is based from "points from the entire GDAC dataset"

Then I wonder, how can a data point fail both the missing data test and the parking hook test, especially because the missing data test is applied over a depth range totally different than the parking-hook test?

29) OUR ANSWER: If a profile has missing data, for example, at the surface and a parking hook at depth, then the data in this profile will be flagged by both tests.

I am confused perhaps because I still don't understand the point of considering the test overlap. One consideration is that perhaps there should be two different flagging systems: one for the profile and the other for the single measurement. 30) OUR ANSWER: We have explained the reasoning beyond the test overlap in our response above. Also, the new tests need to be adapted to the existing Argo Data Management system. We cannot change the system altogether. We also note that Argo also does have a system for flagging profiles, depending on the fraction of flagged points in a given profile (see Argo Data Management Handbook). However, once the points in a profile are flagged, this additional "profile flagging" occurs automatically and therefore this additional flagging is out of the scope of this paper.

Moreover, the authors may want to consider the additive flagging system method used, for example, in the Level-1 to Level-2 satellite data processing. The advantage of this method is that each test has its own value which can then be added to the others and independently of the others; the result is that pixel (data point in this case) can be flagged with and thus sorted according to any of the applied tests.

31) OUR ANSWER: See our response above.

Comments on selected proposed tests One important remark is about the authors' choice (driven by the Argo community feedback) of keeping the various tests as simple as possible even if more complex and likely more robust tests can be envisaged also in real-time. These tests should be as robust and reliable as possible with the general aim of minimizing as much as possible the expensive human intervention. Given the general simplicity of the shown tests, it is hard to see how a "more complex" test could overburden DACs.

OUR ANSWER: We have already explained why it is important to keep these tests simple. Adding a real time check on bathymetry would require additional programming and coordination between the DACs. Because such a test would not add significant benefits to the resulting dataset, we have decided to leave this type of testing to the DMQC step.

The point here is to operationally run the RTQC procedure (i.e., a python script?) to assign a specific value to the profile or to each of its data points. This has little or nothing to do with the complexity of the test which could also take account of the local bathymetry or climatology, which could and actually should be generated at GDAC level and disseminated to local DACs. Lack of ancillary data at the time of RTQC appears a much solid reason for not running the test, not simplicity.

OUR ANSWER: We have already explained why it is important to keep these tests simple. The problem is not a simple "lack of ancillary data".

Missing-Data test. An additional reason for ... - this is connected to one of my previous comments on the need of either splitting the QC flagging system into two (profile and single data record) or to adopt an approach similar to satellite data processing.

OUR ANSWER: See our response above.

High-Deep-Value test I do not see any inconvenience nor complexity in using the bathymetry also in real-time quality testing.

OUR ANSWER: We have already explained why it is important to keep tests simple. Adding a real time check on bathymetry would require additional programming and coordination between the DACs. Because such a test would not add significant benefits to the resulting dataset, we have decided to leave this type of testing to the DMQC step.

Competing Interests: No competing interests were disclosed.