BGC meeting report 30/11/20-01/12/20 (Virtual)

Actions list:

https://docs.google.com/spreadsheets/d/1hO46nTG1Bk1FL49AXzFIDH2GxzvE5qEeuYvFM UPa5uM/edit#gid=0

Attendees:

100 attendees (M. Scanderbeg will collect these after the meeting) Excused: Xiaogang Xing

DAY 1 :

Hervé Claustre / Ken Johnson. Introduction general objectives of this meeting

There are currently 377 operational BGC floats. The overall quality of the BGC-Argo dataset, including the amount of adjusted data available to users at the GDAC, has increased dramatically over the past year. The DOXY parameter represents the largest improvement with currently 80% of all profiles adjusted (a comparison of Oxygen % saturation from Argo floats and GLODAPv2 is presented highlighting the improvements to the dataset). The number of publications using BGC-Argo data is also increasing, underlining the value of the BGC-Argo dataset to the scientific community. Two virtual international workshops related to BGC-Argo are currently being organized for the near future to further the development of BGC-Argo: (1) a NSF/NOAA/NASA-led workshop to introduce makers and resource managers BGC-Argo; policy to (2) а GO-BGC/US-CLIVAR/US-OCB workshop to discuss technology, data management and science related to the growth of BGC-Argo.

First Session : National BGC Data report

Udaya Bhaskar. DAC: BGC Argo data management-India

14 new floats were deployed since the last ADMT. DOXY adjustments are being performed using the SAGE-O2 tool, modified to produce Bfile modifications directly. The DOXY audit is also being used to compare and validate derived gains. Chla correction is also being proposed and a manuscript is under review. Upon approval, the same will be applied to Chla profiles and results will be presented to ADMT. Of 67 BGC floats, 39 are still active. The procurement of 10 future floats is currently planned, although funding is tight.

Matt Donnelly. DAC: BGC Argo data management-UK

Progress was less than expected due to staff availability. A primary focus has been on the APF11 decoder as well as the adjustment of DOXY and pH using SAGE at BODC. Giorgio Dall'Olmo (PML) is also involved in the EARISE project and in the development of procedures for quality control for BBP. BODC would like to work with other DACs to share tools through agnostic infrastructure development. There are some good prospects for BGC float procurement in 2021.

Yuka Okunaka DAC: BGC Argo data management-Japan

7 BGC floats are currently in operation. RTQC for DOXY, BBP, and CDOM have been developed and they should be implemented next year by JMA. JAMSTEC has started to perform DMQC for DOXY and Nitrate. JAMSTEC will deploy 19 BGC floats planned by May, 2021. (equipped with 4 FLBBCD, 6 SEAFET, 2 SUNA, 15 ARO-FT).

Christina Schallenberg DAC: BGC Argo data management-Australia

Only 2 live BGC floats are presently operational. 5 deployments are planned in 2021 in the Southern Ocean and 3 in warmer waters (Coral Sea). Funds should be available for 3 more float deployments as well. 90% of DOXY data are DMQCed and 100% of DOXY data are provided as DOXY_ADJUSTED but not visible on Henry's plots, likely due to an issue related to metadata. CHLA and BBP RTQC and DMQC will be implemented once official Argo procedures are finalized.

Tanya Maurer / Josh Plant / Claudia Schmid DAC: BGC Argo data management-US

519 US BGC-Argo floats exist. 48 of these were deployed since the last ADMT, with the SOCCOM program being the largest contributor to the array. The management of US Argo data is a collaboration between AOML and MBARI. AOML is responsible for Core, meta and Traj file production; MBARI performs processing and QC for all BGC parameters. However, AOML is currently working on building their BGC processing capabilities in house for future NOAA deployments. MBARI-developed tools for BGC data quality control and monitoring are being used by other DACs (SAGE-O2, SAGE, and the DOXY audits). The GO-BGC array has been funded by NSF which includes the deployment of 500 additional BGC-Argo floats over the next 5 years (global extent).

Anh Tran / Chris Gordon DAC: BGC Argo data management-Canada

9 out of 48 DOXY-only BGC floats are still active. Takuvik deployed 6 floats which are no longer operational. 7 more are planned for deployment. SAGE-O2 is being used to adjust O2. The Takuvik floats are processed by Coriolis. C. Gordon was just hired at DFO and is working to move Sage-O2 from MATLAB to python. Argo Canada has a contract with NKE for supply of BGC-Argo floats that will be delivered in 2021. Katja Fennel (Dalhousie University) received some funding for BGC Argo deployments in the NW North Atlantic Ocean from the Canada Foundation for Innovation.

Thierry Carval . DAC: BGC Argo data management-France

Thierry reports that the implementation of QC=3 at coriolis was done in August 2020 for DOXY. There is some ongoing work on DOXY Adjustment in RT (automatic procedure) and in DM, based on Josh's audit, but for old floats with simple calibration, this process can be very time consuming. 10000 radiometric profiles were DModed in 2020 taking into account the temperature dependence and the sensor drift.

Xiaogang Xing. DAC : BGC Argo data management - China (presented by Catherine Schmechtig)

Due to COVID-19, many things have been postponed this year, including float deployments. Two floats were deployed in July in the Northwest Pacific and only one remains operational. 3 NKE floats will be deployed soon (in late December or early January) and they are supposed to receive 4 Navis-SL1 (with rechargeable battery) next spring. The group is looking for a summer or autumn cruise to deploy them in the Northwest Pacific.

The oxygen RT adjustment has been finished for all active floats this year, based on SAGE-O2 tools. A BGC-Argo data visualization webpage has also been developed with the technical support from Zhejiang University. Two data application studies were mentioned: a study was published in *Remote Sensing* using the global BGC-Argo radiometry data to evaluate satellite algorithms/products. Another study was published in GRL in which the authors used data from one BGC-Argo float to evaluate the exported carbon of synoptic-scale mixed-layer pump events.

Discussion

6-variable BGC floats are available from NKE and Teledyne (delivered to CSIRO but not deployed yet). MRV (Solo) are manufactured as prototypes and not much info from NAVIS.

Second session DOXY and Nitrate

Racapé/ Bittig and ALL. DOXY: Discussion on updates to documentation

Various updates to the O2 documentation are discussed and will be published soon on the Argo website. The biases in RT unadjusted DOXY data are well understood; the propagation of required adjustments to DOXY data needs to be easy for DACs to implement. A standardized adjustment equation is thus proposed. The main correction to be applied is to address the bias in sensitivity due to storage drift (applied as a slope). Additional drift and temperature correction are also supported by the proposed equation. Should the notation proposed be enforced or used only as a recommendation? The QC flag definition table is also presented and Henry outlines the rationale behind the recent decision to flag RT unadjusted DOXY data as "3" in BGC-Argo.

Maurer/Bittig DOXY: Implementation of Bittig time response correction within Argo framework

T. Maurer begins her presentation with a "sneak-peek" at the new Sea-Bird Scientific SBE83 oxygen optode for Navis floats, on behalf of SBE and MBARI. Similar to the SBE63, this optode model offers a faster response time than the Aanderaa optode, yet remains exposed to air once at the surface and is thus capable of in-air calibration. Preliminary data from a test deployment off Hawaii are very promising. Following this update, Tanya discusses the topic of optode time-response in more detail, with particular focus on remaining issues related to the implementation of the BIttig et al (2014) correction method. The effect of sample resolution on the uncertainty in the correction is discussed, as well as issues related to the use of CTD bin count information to reconstruct a time axis for use in the time-response correction. One limitation to the use of bin-counts in Apex floats is that bin count data storage saturates at 255 (data is returned only as 2-digit hex), which leads to another potential source of error in the correction. Options for implementation on select profiles are discussed, although a standardized approach across data centers will likely require a more detailed description of the adjustment uncertainties.

Gordon/Racapé DOXY:New python code for DMQC; RT Adjustment and Alerts to PI

Chris Gordon presented on `bgcArgoDMQC`, a python package being developed by Argo Canada for performing delayed-mode quality control on BGC-Argo data. The package currently works only with DOXY data, but the goal is to eventually include DMQC methods for all BGC-Argo variables. The core functionality of the package is based on SAGE-O2 matlab code by Tanya Maurer and Josh Plant. A basic example of the gain calculation was provided, and the package includes other functionality such as calculating gain with carryover (Bittig et al. 2018) and performing the response time correction (Bittig et al. 2014, Gordon et al. 2020). Validation of the code against SAGE-O2 and the DOXY audit distributed by Josh Plant is ongoing, as the package is meant to provide an open source method for performing DMQC, but to agree with previously established/currently in-use methods. Chris is seeking contributions from the community as general feedback, alpha users, or contribution of code towards other BGC variables, via the package's github page: https://github.com/ArgoCanada/bgcArgoDMQC.

Virginie R. presents the real time adjustment procedure and alerts to PI set up by the DAC Coriolis to improve DOXY quality. This procedure follows most of the recommendations of the Argo QC manual for dissolved oxygen and provides DOXY_ADJUSTED with mode 'A' within two months of float deployment if no previous delayed-mode adjustment is available. The adjustment is then checked by a set of Go/No Go criteria and, depending on results, propagated on subsequent cycles until it raises a new alert. Based once again on the estimate of gain for each cycle, this new alert informs PI that his float needs a delayed mode adjustment.

Plant NITRATE: Presentation of updated algorithm

Josh Plant presented an updated version of the temperature correction for calculating the NITRATE concentration. At the time of the ADMT21 meeting there were 336 profiling floats

equipped with nitrate sensors encompassing 6 different DACs (aoml: 245; coriolis: 74; csiro: 7; csio: 5; jma: 4; incois: 1). These floats have resulted in over 36,000 nitrate profiles throughout the world oceans. Some of these floats profile in warmer surface water with zero or near zero nitrate concentrations at the surface. These deployments illuminated a small bias in the surface nitrate estimates resulting from the temperature correction component of the nitrate calculation. An update to this temperature correction is proposed and the BGC Argo community was notified of this proposal via email on November 25, 2020.

In open ocean waters the dominant absorbers of UV light in the 217-240 nm range are the bromide and nitrate ions. Absorption can be related to concentration via the Beer-Lambert law if the molar extinction coefficients are known. If salinity is known so is the bromide ion concentration, but in practice the extinction coefficient of nitrate free seawater (ESW) is used when calculating nitrate rather than the extinction coefficient of bromide itself. For a given sensor, ESW and the nitrate extinction coefficient are determined in the lab, usually at 20C before deployment. The general procedure to calculate nitrate is to use the known salinity of the sample to first subtract off the seawater absorption component of the sample spectrum and then model the remaining spectrum as a combination of nitrate absorption plus absorption due to a linear baseline component. Nitrate concentration and the baseline slope and intercept are determined by solving the system of linear equations in a least squares sense.

Before this can be done though, the effects of temperature must be considered. The bromide ions ability to absorb UV light is very temperature dependent, increasing with increasing temperature & decreasing with decreasing temperature. Since the calibration is determined in the lab at 20C, an adjustment needs to be applied to these calibration ESW values to bring them in line with the in situ sample temperature. The current correction to ESW, which follows Sakamoto et al. (2009), works well except for very warm surface water where it tend to bias the nitrate values about 1 µmol/kg high when compared to reference estimates such as CANYONB and LINR. An improved empirical temperature correction approach was developed using an augmented temperature experiment data set that also maintained better control over the sample temperature during these experiments. The newly proposed correction is based on the realization that for a given wavelength, dLN[ESW)/dT is constant. The new approach removes most of the surface bias observed with the existing method, better models the laboratory experimental data, and reduces the fit error when calculating nitrate in warm waters, especially at the surface. It was proposed that this new approach should be implemented as a direct replacement to the current temperature correction. It was also noted that DM operators should remember that when measuring low nitrate concentrations, one is measuring a very small signal on a large background (sea water absorbance spectrum), and small changes in instrument performance or small errors in calibration values can potentially add variability to the measurement.

Schmechtig NITRATE: DM challenges for selected floats

34 floats equipped with SUNA sensors were D-moded during summer 2020 at the Coriolis DAC. 8 of them presented a "depth surface" issue, which means that adjusted at depth using CANYON-B, they exhibit a NITRATE concentration around -2 umol/kg. Catherine got around this issue by applying a gain-correction to the raw nitrate concentrations. Using the new version of the temperature correction (presented by Josh Plant) can solve the issue for 4 of

the floats. For the 4 remaining floats, Josh Plant offered his collaboration to investigate the topic.

Maurer/Plant. PH: pH "pump offset" issue and potential RT solution

pH profiles exhibit a step change for some MBARI APEX floats when CTD shifts to constant profiling mode (CTD pump continuously on) at 985m. The magnitude of this offset can vary from float to float, as well as through time from profile to profile. It has been rarely seen in NAVIS floats. This issue seems partially related to flow over reference electrode or FET and is mostly isolated to the MBARI 2018-2019 deployment season. The new GDF pH sensor design at MBARI may eliminate the problem completely.

To correct the profiles already at the GDAC, the following solution is presented :

- 1. Assume pH is a smooth function of pressure over a narrow data window centered at 985m
- 2. Break data window above & below 985m
- 3. Add offset to shallower part of data window
- 4. Iterate offset value to optimize polynomial fit over data window (minimize SSR)
- 5. Calculate a signal to noise ratio = offset / std(fit residuals)
- 6. Set offset & signal to noise thresholds (exact thresholds TBD)
- 7. Add offsets which exceed thresholds to all data shallower than 985m

This correction protocol is a working research topic. No official recommendation was proposed for direct implementation into the BGC-Argo data system across data centers at this time.

Johnson. PH: Next-gen pH sensor design (MBARI) update

The number of pH sensors in the BGC Argo array is improving which allows for global analyses that were not possible a few years ago. pH sensors have a few remaining issues, including difficulties in manufacturing and a relatively high failure-rate. New designs are being tested at both MBARI and Sea-Bird. MBARI's new GDF design has been deployed and recovered, and looks promising although further testing will be forthcoming. Ken stresses the importance of diagnostic variables and that SBE sensors on NAVIS floats are now returning such diagnostics. Ken proposes the addition of VK_PH as an Argo intermediate parameter. These should ideally be returned at every measurement level (spot sampling and CP mode).

Organelli E. / Jutard Q. RADIOMETRY: Discussion of DMQC

Quentin presents a Delayed Mode Quality Control (DMQC) method to correct radiometry profiles for sensor temperature and drift effects. The main recommendation to obtain radiometry data with the highest accuracy is to plan acquisitions also of night profiles and during drift at the parking depth. The established DMQC procedure has been already implemented on several floats and is envisaged for all future missions. In addition, alternative protocols for correction of sensor temperature and drift effects have been implemented with the only aim to QC oldest float missions, for which neither night profiles nor drift measurements have been acquired.

DAY 2 : 97 participants

BBP session

Giorgio Dall'Olmo and ALL . Status of on RTQC BBP methods.

Based on the assumption that RTQC tests should aim at generating a globally-consistent data set for non-expert users, Giorgio proposed a set of RT tests that would flag at 2 or 3 or 4 that can be put back as good in delayed mode by BBP experts. Such tests can also flag bad calibration or biofouling. These new tests were applied to all the BBP data resulting in ~91% of the data passing the tests (thus, ~9% of the data was flagged as a result of the tests).. The quality of the resulting dataset has thus improved, but there are still some issues that need to be addressed through additional tests (for example, the surface and deep "hooks", animal spikes, and hooks resulting from sensor initialization)

Sauzède. BBP: presentation of BBP "audit" methodology

Raphaëlle proposes a method to detect anomalous BBP profiles as already done for T&S or DOXY by comparison with reference data. The reference database used for the BBP audit is the SOCA2020 method-derived product (i.e. bbp weekly climatologies computed using a neural network based method called SOCA that merges ocean color and Argo data to retrieve the vertical distribution of bbp). First, to validate the audit methodology, the anomalous bbp detected profiles have been visualized and more than 95% of the detected data are bad or suspicious data. Results of the BBP audit per DAC have been presented by removing all already bad flagged data in the BGC-Argo database. The BBP audit allows for the detection of noisy profiles in a time series due to sensor shifts, drift, etc. A BBP audit will be available for access together with the DOXY audit at the same web location and a report of profile anomalies will be sent to the Argo mailing lists every 4/6 months. The development of a similar audit for CHLA is planned for next year.

Giorgio Dall'Olmo. BBP Error estimation, and sensor failure rates

A proposal on how to estimate uncertainties for BBP was presented. The method relies on the standard law for the propagation of uncertainties (<u>BMIP 2008</u>). The most critical part of the method is identifying the main sources of uncertainty and assigning realistic uncertainties to them. The need to make decisions based on published information was stressed. Discussion centered on comparing these modelled uncertainties with experimental estimates of the uncertainty which could be derived by analysing the statistical distribution of BBP values at depth, even though these empirical estimates may not allow one to estimate the full BBP uncertainty.

An analysis of failure rates of BBP meters installed as part of REM-A sensors vs. independently-installed BBP was presented. The analysis assumes that BBP meters on REM-A sensors can be identified by selecting PROVOR floats that have BBP, CHLA and IRRADIANCE. Results show that BBP meters on REM-A sensors are ~3.5 times more likely to fail than BBP meters that are not part of a REM-A sensor.

Session Chlorophyll

Schallenberg: CHLA: Discuss document updates, final recommendations & remaining questions

A lively discussion ensued after the presentation. No conclusions were reached, but a number of things became clear, and a way forward was also devised:

- The question of the end users is an important one and has a strong influence on how we think about our data and the tests we need to conduct. We might even have different end users for the CHLA_ADJUSTED variable in A (data assimilation) and D mode (scientific applications).
- The main sticky points in how to adjust the CHLA variable relate to issues that are not sensor failures but physiology (NPQ, Roesler factor); while the CHLA variable isn't the only one where a derived parameter is reported (see subtraction of seawater backscatter for BBP, and absorption translated to NITRATE), it's probably the only one where QC is heavily affected by issues that aren't ultimate sensor issues. Regardless: good points can be made in defence of either option, i.e. to only QC instrument failures, or to report a variable that users expect and frequently use, such as CHLA as we currently treat it. One point that was made: if we stop reporting CHLA the way we do, will that affect data uptake?
- One possible way out of the conundrum: have two separate variables, CHLA and FLUORESCENCE_CHLA, which both get QC'ed in their respective ways, with CHLA continuing along the trajectory we've been on (i.e., NPQ correction and Roesler factor), and FLUORESCENCE_CHLA only receiving the dark correction and QC that relates to instrument failure. Importantly, FLUORESCENCE_CHLA should become an essential B variable that is also carried into the Sfile.

- With respect to NPQ correction: the main question is whether it should only be done at night.
- The treatment of spikes relative to the NPQ correction is also not clear. The NPQ-corrected part of the profile should probably not get spikes added back in, as they will be affected by NPQ in some way. So maybe just deal with the fact that spikes are lost from NPQ-corrected parts of profiles and leave them in for the rest? And document this very clearly?
- The way forward: Christina (in consultation with a small group of experts) is to come up with questions that will be presented in a survey to the larger group with the objective of reaching some decision on some of the issues presented above. Decisions will be made based on inputs from the survey and then implemented in an updated RTQC document. The aim is to have this all sorted by Feb 2021.

Maurer. Suggested updates to select BGC <PARAMETER>_ACCURACY and <PARAMETER>_ADJUSTED_ERROR fields.

T. Maurer presents recommended updates to BGC <PARAMETER>_ACCURACY AND <PARAMETER>_ADJUSTED_ERROR fields based on an assessment of required adjustments upon deployment for nitrate and pH data within the SOCCOM array. It is suggested that statistics on the magnitude of adjustments required across an array can serve as a guide to DMQC operators, assisting in the evaluation of sensor health/performance. A slide is also presented showing histograms of the offsets applied to nitrate data within the Argo array, separated by sensor type (SBE/SUNA, MBARI/ISUS). The magnitude of the difference in mean offset among the two groups warrants further investigation.

ALL (Racapé/Schmechtig) Group discussion of potential for a BGC Argo reference database.

Catherine S. opens the reference database discussion by reminding all of the need for BGC-Argo to formalize a reference database for standardized handling and storage of shipboard data, but also to extend to other datasets to use for float calibration and/or validation. GLODAP is presented as a logical partner but issues related to cost, sustainability (as illustrated by Siv L.), data in marginal seas, cruises that do not have a direct pathway to GLODAP, and the handling of biooptical data (HPLC, POCS, Radiometry) are apparent. Use of additional reference data sets requires standardized format, units, vocabulary, embargo, and citation. Catherine finishes her introduction by highlighting the need for easy and formatted access to each data type for float calibration and/or validation. ERDDAP software seems to be a "good candidate". Through the chat, two essential notions have been evoked: (by Toste T.) What do you mean with "reference data set" as opposed to a data set ?, (and by Siv L.) The profiles taken on deployment are not necessarily the reference data. In addition, S. Diggs informs that "CCHDO is very interested in incorporating the casts at float deployment locations and assembling them into an additional, supported reference data set

for cal/val for BGC-Argo as well as for Deep Argo". At the end of the discussions, a working group was formed to move forward on the subject for the next ADMT.

ALL (Sauzède / Plant) Group discussion of coordinating anomaly reports; closing discussion.

Anomaly reports and BGC audits are a good tool to improve the quality of the BGC-Argo database, it is useful and efforts have to continue in this way. All BGC audits should be at the same location on the web and with easy access (BGC-Argo website, as well as the ADMT website).

ALL (Maurer/Schmechtig) closing discussion.