

Dear Dr. Manzella

Thank you for considering our manuscript for publication in Earth System Science Data. In the following we provide a point-by-point response to the comments from the reviewers including all relevant changes made as a consequence of each, and a marked-up version of the manuscript. This does not include figures. The changes to these were minor, adding legends to Figure 8 and 10, please see uploaded manuscript for these figures.

Best wishes,  
Are Olsen

## Response to review by referee #1, Dr. Matthew Humphreys

We thank Dr. Humphreys for the helpful comments and suggestions, each one is addressed below (comment in black, response in red).

The new cruise datasets added to GLODAP in this release constitute a substantial update to this already invaluable data product. The manuscript is clearly written and virtually ready to publish as it is. The first section of my comments below raises a few minor issues that the authors should consider before publication of this paper. The second section contains broader suggestions that might benefit future releases, but which are not necessary to include in this version.

### 1 Comments for this manuscript

#### 1.1 Version naming convention

The new version number/naming convention outlined in lines 146–147 is intuitive and clear to follow. It could be more strongly emphasised here that the exact version number used should always be reported in studies, rather than making a generic reference to GLODAP.

Agreed

- Changes made: The following sentence has been added to the second final paragraph of the introduction “The exact version number and release year (if appended) of the product used should always be reported in studies, rather than making a generic reference to GLODAP.”

It might be helpful to also explicitly commit to what may and may not be changed between different levels of version release. For example, in the "minor" version increments new cruises may be added but data that was already there will not change (with the exception of bug fixes, such as described in section 3.3.1), whereas it sounds like a "major" version increment would involve a reanalysis of the entire dataset, in which the adjustments applied to existing datasets could be more fundamentally altered.

Even if it's not exactly as I've described, some sort of explicit commitment like this could be helpful — users who switch to a newer version could immediately know what they can rely on to be consistent, and what changes they need to watch out for — and now, as the new versioning system is introduced, seems like a good opportunity to do this.

This is a good suggestion.

- Changes made: The following two paragraphs have been added at the end of the introduction (part of the material appeared at the end of Section 2, which is now shorter. Being fundamental to the procedures, we believe it fits better in the introduction):  
“Within this there are two types of GLODAP updates: full and intermediate. Full updates involve a reanalysis, notably crossover and inversion, of the entire dataset (both historical and new cruises) and all adjustments are subject to change. This was carried out for GLODAPv2. For intermediate updates, recently-available data are added following quality control procedures to ensure their consistency with the cruises included in the latest GLODAP release. Except for obvious outliers and similar types of errors (Sect. 3.3.1), the data included in previous releases are not changed during intermediate updates. Additionally, the GLODAP mapped climatologies (Lauvset et al., 2016) are not updated for these intermediate products. A naming convention has been introduced to distinguish intermediate from full product updates. For the latter the version number will change, while for the former the year of release is appended. The exact version number and release year (if appended) of

the product used should always be reported in studies, rather than making a generic reference to GLODAP.

Creating and interpreting the inversions, and other checks of the full data set needed for full updates are too demanding in terms of time and resources to be preformed every year or two-years. The aim is to conduct a full analysis (i.e., including an inversion) again after the third GO-SHIP survey has been completed. This completion is currently scheduled for 2023, and we anticipate that GLODAPv3 will become available a few years thereafter. In the interim, presented here is the second intermediate update, which adds data from 106 new cruises to the last update, GLODAPv2.2019 (Olsen et al., 2019)."

## 1.2 Carbonate ion measurements

The "four variables" statement in line 360 ignores the increasing reliability of carbonate ion measurements (e.g. Sharp and Byrne, 2019). I suggest to modify this statement accordingly; it is not really necessary to specify "four" or any specific number here at all.

Agreed.

- Changes made: "four" has been deleted here, and in other places where this number was mentioned as the number of measurable sea water CO<sub>2</sub> chemistry variables.

## 1.3 pH adjustments — or not

It would be useful to recap that pH adjustments were not applied to the new data in this version where this is mentioned in the summary on lines 554–555.

Agreed

- Changes made: The following text has been added to the end of the paragraph in question: "No pH data were adjusted for this version, but we note that this is largely a consequence of problems in establishing a reasonable pH baseline level in the deep northwest Pacific (Sect. 4.2). A comprehensive analysis of all available pH data in that region should be conducted for the next update".

## 1.4 Figures

The axis labels and other text notes on a couple of the figures are a bit too small relative to the figure size, making reading difficult (e.g. Figure 3).

Indeed, this is a problem for some of the figures, Figure 3 and 6, in particular. This problem arises as a consequence of downsizing of the submitted pdf, when the ESSD header is added to convert it into a discussion paper. We will take care during the production of the final paper to ensure text and notes on all figures are legible.

Although you can work these out from context — if you are familiar with the field — several of the figures are missing axis labels and units for the variables shown (e.g. Figures 3 through 6).

Thank you for pointing this out. Figures 3-5 are produced by the various QC algorithms, where context is clear, but we readily acknowledge that labels and units should be stated in the paper, so we have included this information in the captions. For Figure 6, we have also added an explanation on what is shown for the various variables.

- Changes made: Captions for Figure 3-6 have been revised.

## 1.5 Typos

Abstract: add a comma after "discrete fCO<sub>2</sub>" on line 56. Change "bias corrected product" to "bias-corrected product" on line 60.

- Changes made: Corrected

I suggest to change "are released regularly" to "will be released regularly" on line 145. This sentence has been removed, following the changes in Sect 1 and 2 in response to your comment 2, on explicitly committing to what may and may not be changed between different levels of version release.

Summary: the sentence on lines 554–555 is missing a full stop at the end.

- Changes made: Full stop added.

## 2 Suggestions for future releases

The following points are not revisions that are necessary for this publication, but rather ideas that could be taken under consideration for future releases of GLODAP.

### 2.1 Expand dataset sourcing

The latest GEOTRACES Intermediate Data Product (Schlitzer et al., 2018) contains some datasets with the core GLODAP variables that are not included in this GLODAP release. While it's unreasonable to expect the GLODAP team to continually seek out new data from an endless list of sources, it may be worth including the GEOTRACES IDPs for future versions given the typically high quality of the carbonate system data therein, abundance of auxiliary variables to aid secondary QC, and consistent data format.

Thanks. We will scrutinize this dataset for cruises to include in the next version of GLODAP.

### 2.2 Accept carbonate ion measurements

As noted above, carbonate ion measurements are now becoming usefully reliable (e.g. Sharp and Byrne, 2019) and becoming more widespread. Accepting this type of data into GLODAP would be a natural extension to the current set of core variables, adding a new dimension to some applications of the GLODAP database such as evaluating dissociation constants based on over-determined data points (e.g. Sulpis et al., 2020).

Thanks for the suggestion. We do strive to increase the utility of GLODAP for evaluation of dissociation constants and other factors that biases the measurements. Plans are on the table for preparing a product with all of our alterations removed (adjustments, interpolations, calculations etc.); i.e. all data 'as reported', in a uniform format. The GLODAP Reference Group discussed the suggestion of including carbonate ion measurements in the product, and we came to the conclusion that it is premature as unresolved issues with these measurements remain; specifically there are too few measurements to perform secondary QC, as carbonate ion is measured by few groups and (similar to pH) there is no certified standard to evaluate accuracy. Probably the main issue is that after the seminal work by Byrne and Yao (2008), four other manuscripts (Easley et al. 2013; Patsavas et al., 2015; Sharp et al., 2017; Sharp and Byrne, 2019) were published with modifications in the reagents, equations and other method settings, consequently the method is still under development and still improving.

### 2.3 Update carbonate system calculations

The analysis here still uses CO2SYS for MATLAB v1 (van Heuven et al., 2011). Updating to at least CO2SYSv2 (Orr et al., 2018) would enable uncertainty propagation — given that some calculated marine carbonate system variables are reported, it would be useful to also propagate uncertainties from the measured variables and dissociation constants into the calculated variables.

Updating further still to the recently released CO2SYSv3 (Sharp et al., 2020) would also enable calculations with carbonate ion as an input variable, if these measurements were to be accepted in future GLODAP releases. Ammonia and sulfide speciation are also included in

the alkalinity equation as of CO2SYSv3, which could improve the accuracy of marine carbonate system calculations in areas where these species are significantly abundant  
Thanks, this is a useful reminder. We plan to use the updated CO2SYS software for future versions and inclusion of robust uncertainty estimates is a priority for GLODAP.

References:

- Byrne, R. H. and Yao, W. S.: Procedures for measurement of carbonate ion concentrations in seawater by direct spectrophotometric observations of Pb(II) complexation, *Mar Chem*, 112, 128-135, 2008.
- Easley, R. A., Patsavas, M. C., Byrne, R. H., Liu, X., Feely, R. A. and Mathis, J. T.: Spectrophotometric measurement of calcium carbonate saturation states in seawater, *Environ. Sci. Technol.*, 47, 1468-1477, 2012
- Patsavas, M. C., Byrne, R. H., Yang, B., Easley, R. A., Wanninkhof, R., and Liu, X. W.: Procedures for direct spectrophotometric determination of carbonate ion concentrations: Measurements in US Gulf of Mexico and East Coast waters, *Mar Chem*, 168, 80-85, 2015.
- Sharp, J. D. and Byrne, R. H.: Carbonate ion concentrations in seawater: Spectrophotometric determination at ambient temperatures and evaluation of propagated calculation uncertainties, *Mar Chem*, 209, 70-80, 2019.
- Sharp, J. D., Byrne, R. H., Liu, X. W., Feely, R. A., Cuyler, E. E., Wanninkhof, R., and Alin, S. R.: Spectrophotometric Determination of Carbonate Ion Concentrations: Elimination of Instrument-Dependent Offsets and Calculation of In Situ Saturation States, *Environ Sci Technol*, 51, 9127-9136, 2017.

## Response to review by referee #2, Dr. Nicolas Metz

We thank Dr. Metz for the helpful comments and suggestions, each one is addressed below (comment in black, response in red).

### General comments:

Since 15 years GLODAP data-bases (from 2004 to 2019, including CARINA, PACIFICA) are widely used in the community, not only to evaluate the change of CO<sub>2</sub> in the ocean or acidification (e.g. Gruber et al 2019; Jiang et al 2019), but also to compare and validate ocean and climate models (e.g. CMIP5, Bronselaer and Zanna, 2020 for a recent publication). The GLODAP data-set is also an important synthesis for GOA-ON activities and to construct climatology (e.g. Broullón et al, 2020).

Here, authors present an updated version of the GLODAP effort. This includes 106 new cruises quality controlled (QC), inclusion of new fCO<sub>2</sub> observations (not QCed) and comparison of secondary QC with reconstructed properties using neural network methods (named CANYON-B and CONTENT).

The effort consists mainly in (i) format and check the data received from PI or available in different locations (NCEI/OCADS, PANGAEA, CCHDO), (ii) performed a secondary QC to identify data biases (if any) and separate from real temporal changes of the properties that could be low relative to the mean concentrations and (iii) construct final formatted products with adjusted data and associated flags for easy use at global or regional scales.

The paper is basically structured from the previous manuscript (Olsen et al 2019) and I therefore have only few comments regarding this new version (v2020). Most suggestions are for clarity, here thinking to readers that would discover only now the GLODAP project (e.g. new students in the field).

As fCO<sub>2</sub> data are now included, GLODAP is in a way a companion data-base to SOCAT dedicated to surface fCO<sub>2</sub> data (Bakker et al 2016) also annually updated (Bakker et al 2020). Both products were already used together for specific analysis (e.g. comparing pH fields from GLODAP and SOCAT, Jiang et al 2019). It might be useful for future to attempt incorporate fCO<sub>2</sub> data that are in GLODAP but not yet in SOCAT. In this context few words might be added at the end in the conclusions/perspectives.

This is an interesting suggestion, thanks. There are indeed many sources of fCO<sub>2</sub> data, and there are also potentially many issues related to the various measurement techniques and different levels of, and approaches to, their QC. For GLODAPv2.2020, fCO<sub>2</sub> was not quality controlled. A unified look at ocean fCO<sub>2</sub> data seems worthwhile but would be very demanding, in particular related to differences in sampling strategies.

- Changes made: The following sentence was added to the second paragraph of Sect. 6 Summary, to make it clear that the fCO<sub>2</sub> data in GLODAP have not been subjected to quality control: "The number of measured fCO<sub>2</sub> data are 33 924; note that these data were not subjected to quality control."

The following sentence has been added at the very end of Sect. 6 Summary, to make it clear that QC of fCO<sub>2</sub> data is needed, although at this stage we are not in a position to suggest any particular procedure: "As mentioned above, the included fCO<sub>2</sub> data have not been subjected to quality control, therefore no uncertainty estimate is given for this variable. This should be conducted in future efforts."

In this version, authors used CANYON-B and CONTENT methods (I think this was not systematically performed in v2019). This is a new and an elegant way to check and compare secondary control (and bias if any). This is a new step in GLODAP that might be recalled in the abstract for this version.

Thank you. We now mention this in the abstract.

- Changes made: We have added the following sentence to the abstract:  
"Comparisons to empirical algorithm estimates provided additional context for adjustment decisions, this is new to this version."

Something not very clear concerns the QC for historical cruises. With the new cruises in hand, I was not sure at the start if the QC of previous cruises in the same regions has been checked again and would lead to new corrections for cruises already in GLODAPv1, CARINA or v2019. However, as specify in the manuscript (line 145) I understand that a complete revision of QC would be performed in 2023 (after 3d GO-SHIP).

We realise that this is mentioned rather late in the manuscript, but hope that the paragraph on the different types of GLODAP updates now included in the introduction in response to the comment from Matthew Humphreys, clarifies this early on.

- Changes made: The following paragraphs have been added at the end of the introduction:  
"Within this there are two types of GLODAP updates: full and intermediate. Full updates involve a reanalysis, notably crossover and inversion, of the entire dataset (both historical and new cruises) and all adjustments are subject to change. This was carried out for GLODAPv2. For intermediate updates, recently-available data are added following quality control procedures to ensure their consistency with the cruises included in the latest GLODAP release. Except for obvious outliers and similar types of errors (Sect. 3.3.1), the data included in previous releases are not changed during intermediate updates. Additionally, the GLODAP mapped climatologies (Lauvset et al., 2016) are not updated for these intermediate products. A naming convention has been introduced to distinguish intermediate from full product updates. For the latter the version number will change, while for the former the year of release is appended. The exact version number and release year (if appended) of the product used should always be reported in studies, rather than making a generic reference to GLODAP.  
Creating and interpreting inversions, and other checks of the full data set needed for full updates are too demanding in terms of time and resources to be performed every year or two-years. The aim is to conduct a full analysis (i.e., including an inversion) again after the third GO-SHIP survey has been completed. This completion is currently scheduled for 2023, and we anticipate that GLODAPv3 will become available a few years thereafter. In the interim, presented here is the second intermediate update, which adds data from 106 new cruises to the last update, GLODAPv2.2019 (Olsen et al., 2019)."

Also, many colleagues used the GLODAP gridded products that were constructed from GLODAP-v2 (Lauvset et al 2016). Will you also revisiting this gridded product now or wait for the 2023 version ? This might be specified in the manuscript.

The gridded product will not be updated now. The changes would likely be rather small, as the main source of uncertainty in the gridded product is lack of observations in certain regions. The data added in GLODAPv2.2019 and GLODAPv2.2020 are mostly repeat observations, extending the coverage in time and not in space. We cannot commit, now, to making new climatologies for v3. This depends on funding. Therefore, we simply add a statement that the intermediate products are not accompanied by a gridded product

update.

- Changes made: The sentence “Additionally, the GLODAP mapped climatologies (Lauvset et al., 2016) are not updated for these intermediate products.” has been included in the second final paragraph of the introduction.

Another remark concerns the new cruises to be added in GLODAP. I understand that new cruises (106) were recently obtained from NCEI or PANGAEA or from PIs. However, I suspect there are many other cruises in the community (published) and it would be useful to find the best way to get more cruises in the future and invite new PIs to contribute.

Yes, there is certainly room for improvement. Right now, apart from close interaction with GO-SHIP and CCHDO, the level of formalization for addition of data is very low. While no changes were made to this end in the manuscript, we will explore ways to obtain more publicly available datasets.

Overall, I recommend publication after few minor revisions.

Below I list specific and minor comments (mostly details for clarity for a reader who discover Glodap for the first time). At the end of the review few technical questions regarding the files on-line.

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Specific comments:

C-01: Title: The title includes only acronyms of the project (GLODAP). Would it be useful to recall that this concerns Ocean biogeochemical observations in the water column? A Suggestion for a title: “An updated version of global interior ocean biogeochemical observations, GLODAPv2-2020”.

That is a good suggestion

- Changes made: Title has been changed to “An updated version of the global interior ocean biogeochemical data product, GLODAPv2.2020”

C-02: Page 2, line 44: “the inclusion of available discrete fugacity of CO<sub>2</sub> (fCO<sub>2</sub>) values in the merged product files”. Does this new inclusion concerns only the new cruises added in v2020 or did you also add this parameter for historical cruises ? (this is specify later, Line 369).

- Changes made, added “(also for historical cruises)” to sentence in question.

C-03: Page 4, Line 121: “The data collected across the Davis Strait”. Maybe specify where is the Davis Strait for those not familiar with the Indian Ocean....(.....Atlantic of course)

☺

- Changes made, added “between Canada and Greenland” after “Davis Strait”

C-04: Page 5, Line 175: For new users: Not sure to clearly understand all Flag definitions listed in Table 2.

Indeed, this Table is a bit brief, and may lead to misunderstandings, as also pointed out by Jens Muller in his short comment.

- Changes made:
  - We have added a citation to Swift (2010) in the Table header, which provides full details on the flags used in the exchange format original data files
  - We have expanded the table caption to make it clear that the flagging scheme in the merged product files is simplified (added text is underlined):



“Table 2. WOCE flags in GLODAPv2.2020 exchange format original data files (briefly; for full details see Swift, 2010) and the simplified scheme used in the merged product files”

- We have added the underlined text in the paragraph of section 3.1 where Table 2 is first mentioned: “Each data column (except temperature and pressure, which are assumed “good” if they exist) has an associated column of data flags. For the original data exchange files, these flags conform to the WOCE definitions for water samples and are listed in Table 2. For the merged and adjusted product files these flags are simplified: questionable (WOCE flag 3) and bad (WOCE flag 4) data are removed and their flag set to 9. The same procedure is applied to data flagged 8 (very few such data exist). WOCE flags 1 (Data not received) and 5 (Data not reported) are also set to 9, while 6 (Mean of replicate measurement) and 7 (Manual chromatographic peak measurement) are set to 2, if the data appear good. Also, in the merged product file a flag of 0 is used to indicate a value that could be measured but is somehow approximated: for salinity, oxygen, phosphate, nitrate, and silicate, the approximation is conducted using vertical interpolation; for seawater CO<sub>2</sub> chemistry variables (TCO<sub>2</sub>, TALK, pH, and fCO<sub>2</sub>), the approximation is conducted using calculation from two measured CO<sub>2</sub> chemistry variables (Sect 3.2.2). Importantly, interpolation of CO<sub>2</sub> chemistry variables is never preformed and thus a flag value of 0 has unique interpretation.”
- For the ‘Merged product files’ column in Table 2 we have changed “Not used” to “Flag not used”

C-05: Table 2: for clarity, it might be useful to assign different flag for interpolated and calculated values (both flag 0). Maybe for the next version.

- Changes made. To be clear about the unique interpretation of the 0 flag for different variables, we have added the following sentences in Sect. 3.1: “Also, in the merged product file a flag of 0 is used to indicate a value that could be measured but is somehow approximated: for salinity, oxygen, phosphate, nitrate, and silicate, the approximation is conducted using vertical interpolation; for seawater CO<sub>2</sub> chemistry variables (TCO<sub>2</sub>, TALK, pH, and fCO<sub>2</sub>), the approximation is conducted using calculation from two measured CO<sub>2</sub> chemistry variables (Sect 3.2.2). Importantly, interpolation of CO<sub>2</sub> chemistry variables is never preformed and thus a flag value of 0 has unique interpretation.”

C-06: In table 2, you list “b” “Data are not included in the GLODAPv2.2020 product files and their flags set to 9. “ Does that mean that original flag 3 (Questionable but sometimes maybe real signal) are not included in the files ? However this is explained later, line 395 Yes, these are removed from the product file. We now explain this in the paragraph that introduces the table (see response to C-04).

C-07: In table 2, you list “c” for replicate: “Data are included, but flag set to 2 “. This suggests that all replicate are acceptable (or some were also identify as outliers and thus moved to flag 9 or deleted ?).

We now clearly state in the paragraph that introduces this table, that replicates are only kept if the value appears valid, please see response to C-04.

C-08: Page 6, Line 197: “comparison of deep-water averages”. Specify the layers here ? How this is selected in the high latitude (e.g. bottom water formations, where anthropogenic CO<sub>2</sub>

is found to be relatively high in water column ?).

This is the introductory paragraph for Section 3, stating what is to be presented in the subsections to come, among them Sect. 3.2.2, where the full details of the comparisons and what depth layers are used are provided. To avoid repetition, we do not go into these details here.

C-09: Page 6, Line 200: Add reference to CANYON-B and CONTENT (first time listed here) ?

- Changes made: Reference to Bittig et al., 2018, added.

C-10: Page 6, Line 226: “In areas where a strong trend in salinity was present”. Any example for this version ?

This is a leftover from the earlier versions of this paper; no strong salinity trends were present in the crossovers evaluated.

- Changes made: sentence deleted.

C-11: Page 7, Line 235: “convection occurs (such as the Nordic, Labrador, and Irminger seas)”. How do you select the layer in region of bottom water formation (e.g. SR03 for this version) ? Might be interesting for new readers to show another QC example (as presented in Figure 3 for the North Pacific).

Whether to use 1500 or 2000 dbar is determined on a case by case basis, by looking at the crossover comparisons for the two options, with respect to the accuracy of the information provided on the comparability between the data and whether changes in some layers seems related to actual change. In regions of bottom water formation change is expected, and results are scrutinized in light of this. We have revised the text to make it clear that subjective choices are involved, and that we always evaluate the results for presence of actual change, in order to not adjust this away.

- Changes made: The text on depth limits for crossover analysis has been extended and revised:  
“Either the 1500 or 2000 dbar depth surface was used as upper bound, depending on the number of available data, their variation at different depths, and the region in question. This was evaluated on a case-by-case basis by comparing crossovers with both depth limits and using the one that provided the most clear and robust information. In regions where deep mixing or convection occurs, such as the Nordic, Irminger and Labrador seas, the upper bound was always placed at 2000 dbar; while winter mixing in the first two regions is normally not deeper than this (Brakstad et al., 2019; Fröb et al., 2016), convection beyond this limit has occasionally been observed in the Labrador Sea (Yashayaev and Loder, 2016). However, using an upper depth limit deeper than 2000 dbar will quickly give too few data for robust analysis. In addition, even below the deepest winter mixed layers properties do change over the time periods considered (e.g., Falck and Olsen, 2010), so this limit does not guarantee steady conditions. In the Southern Ocean deep convection beyond 2000 dbar seldom occurs, an exception being the processes accompanying the formation of the Weddell Polynya in the 1970s (Gordon, 1978). Deep and bottom water formation usually occurs along the Antarctic coasts, where relatively thin nascent dense water plumes flow down the continental slope. We cautiously avoid such cases, which are easily recognizable. In order to avoid removing persistent temporal trends, all crossover results are also evaluated as a function of time (see below).”

C-12: Page 7, Line 238: Maybe recall that 49UP20160109 is new while 49UP20160703 was QCed in v2019.

- Changes made: The underlined text has been added to this sentence: “As an

example of crossover analysis, the crossover for TCO<sub>2</sub> measured on the two cruises 49UP20160109, which is new to this version, and 49UP20160703, which was included in GLODAPv2.2019, is shown in Fig. 3.”

C-13: The example in Figure 3 shows in 3a blue dots on the map, but I suspect these stations (far east) were not used to evaluate the QC.

This is correct indeed. Thank you for pointing this out, it is certainly worthwhile to mention that only stations shown in panel b are used for the crossover analysis.

- Changes made. The following clarification has been made in the caption of Figure 3: “Panel (a) show all station positions for the two cruises and (b) show the specific stations used for the crossover analysis.”

C-14: Page 7, Lines 245-250: For 49UP20160109, maybe specify that no temporal changes was observed for salinity (i.e. you used TCO<sub>2</sub> here, not normalized TCO<sub>2</sub> as suggested in Line 227 for some cruises).

As mentioned under C-10, salinity normalization was not needed for any crossover, and therefore not mentioned in this manuscript anymore. Thus, we did not mention here that the data were not salinity normalized.

C-15: Page 7, Line 245: Figure 4 shows the TCO<sub>2</sub> cross-over for 49UP20160109 versus GLODAPv2-v2019. The cruise 49UP20160703 is also plotted and thus was in GLODAPv2-v2019, although conducted after 49UP20160109 (just to clarify for a new user).

In response to comment C-12, we now mention that 49UP20160703 was included in GLODAPv2.2019.

C-16: Page 7, Line 256: “they are included in the product but with a secondary QC flag of 0 (Sect.6)”. Sect 6 (?)

The statement on the lack of full QC on the Davis Strait cruises and the consequential assignment, and interpretation of, secondary QC flag 0 has been moved to Section 4.2 Adjustment Summary.

- Changes made: The following paragraph has been added at start of Section 4.2: “The secondary QC has 5 different outcomes, provided there are data. These are summarized in Table 5, along with the corresponding codes that appear in the online Adjustment Table and that are also occasionally used as shorthand for decisions in the coming text. The level of secondary QC varies among the cruises. Specifically, in some cases data were too shallow or geographically too isolated for full and conclusive consistency analyses. A secondary QC flag has been included in the merged product files to enable their identification, with “0” used for variables and cruises not subjected to full secondary QC (corresponding to code -888 in Table 5) and “1” for variables and cruises that were subjected to full secondary QC. The secondary QC flags are assigned per cruise and variable, not for individual data points and are independent of—and included in addition to—the primary (WOCE) QC flag. For example, interpolated (salinity, oxygen, nutrients) or calculated (TCO<sub>2</sub>, TALK, pH) values, which have a primary QC flag 0, may have a secondary QC flag of 1 if the measured data these values are based on have been subjected to full secondary QC. Conversely, individual data points may have a secondary QC flag of 0, even if their primary QC flag is 2 (good data). A 0 flag means that data were too shallow or geographically too isolated for consistency analyses or that these analyses were inconclusive, but that we have no reasons to believe that the data in question are of poor quality. Prominent examples of this for this version are the 10 new Davis Strait cruises: no data were available in this region in GLODAPv2.2019,

which, combined with complex hydrography and differences in sampling locations, rendered conclusive secondary QC impossible. As a consequence, most, but not all, of these data (some being excluded because of poor precision after consultation with the PI) are included with a secondary QC flag of 0.”

C-17: Page 7, Line 259: “A few new cruises had no or very few valid crossovers with GLODAPv2 data.” Which cruises ? Would it be relevant to add a column in Table- Annexe 1 with a remark specifying what kind of secondary QC has been performed for each cruise (e.g. Standard QC, MLR, no QC) ?

For the 106 new cruises, MLR and deep water averages were used in a complimentary fashion, i.e., none of secondary QC were only based on these types of analyses. We have revised Sect. 3.2.3 to convey this.

The type of secondary QC varies not only per cruise, but also per variable. Different types of QC (e.g. Standard QC, MLR, no QC) can be applied for different variables on certain cruises. The various QC types can also be applied in combination. It is not practically possible to include this information in Table – Annexe 1. The most important information regardless appears in the online adjustment table.

- Changes made: The first sentences of Section 3.2.3 have been revised to: “MLR analyses and deep water averages, broadly following Jutterström et al. (2010), were also used for the secondary QC of salinity, oxygen, nutrients, TCO<sub>2</sub>, and TAlk data. These approaches are particularly valuable when a cruise has either very few or no valid crossovers with GLODAPv2, but are used more generally to provide more insight on the consistency of the data. The latter was the case for the 106 new cruises; i.e., no adjustments were reached on the basis of MLR and deep water average analyses alone. “

C-18: Page 8, Section 3.2.3: I understand the description but what are the results and which cruise ? Would be interesting to show an example for a cruise that is QCed using MLR. As no cruise was fully QC'd using MLR, we have not included such an example, but will consider this for the next version of GLODAP.

C-19: Page 8, Line 277: “Altogether 82 of the 106 new cruises included pH data.” Here specify this is measured pH, not calculated (so there is no confusion with pH calculated for other cruises).

- Changes made: Sentence revised to (new word underlined) “Altogether 82 of the 106 new cruises included measured pH data.”

C-20: Page 8, Line 291: “The pH data of 840 of the 936 cruises in GLODAPv2.2020”. Again, specify if pH data here were measured or calculated or both.

We agree that this is not clear, and not all of the 840 cruises included measured pH. This paragraph has been extensively expanded following comments from Dr. Williams, and the specific sentence has been altered to: “In contrast to past GLODAP pH QC, evaluation of the internal consistency of CO<sub>2</sub> system variables was not used for the secondary quality control of the pH data of the 106 new cruises.”

C-21: Page 8, Line 305: Maybe recall the mean uncertainty associated to CANYON-B and CONTENT (see table 1 in Bittig et al 2018, i.e. about twice the adjustment limits fixed for GLODAP listed in Table 3).

We are reluctant to mention specific uncertainties for CANYON-B and CONTENT. These vary with depth and with location, and specifically for nutrients, are stated in absolute terms (concentration) in Bittig et al. (2018), rather than relative as used for the adjustment limits,

so the comparability and transferability of directly stating these values is small. We do recognize the need for more clearly relaying that we did in fact explicitly consider these uncertainties in our assessment, however. Therefore we have revised and expanded the sentence in question.

- Changes made: The sentences:  
“Of course, we kept in mind that this relies on the accuracies of the T, S, and O<sub>2</sub> data and of CANYON-B and CONTENT in themselves. Used in the correct way and with caution this tool is a powerful supplement to the traditional crossover analyses. “

has been replaced with the following:

“Used in the correct way and with caution this tool is a powerful supplement to the traditional crossover analyses. Specifically, we gave no weight to comparisons were the crossover analyses had suggested that the S and/or O<sub>2</sub> data were biased as this would lead to error in the predicted values. We also considered the uncertainties of the CANYON-B and CONTENT estimates. These uncertainties are determined for each predicted value, and for each comparison the ratio of the difference (between measured and predicted values) to the local uncertainty was used to gauge the comparability.”

C-22: Page 8, Line 305: As it is new results presented here (and probably also used in the next version), I think some more information is needed. For CANYON-B and CONTENT are you using results based on GLODAP-v2 data (Bittig et al 2018) or an updated version using GLODAPv2-2019. Is the comparison presented here (Figure 5) validate the QC for the new cruises or validate CANYON-B and CONTENT reconstructed fields? It is reassuring to get about the same results as CANYON-B and CONTENT were trained with GLODAP. We already state that “These approaches were developed using the data included in the GLODAPv2 product” (line 299-300 in discussion paper). Moreover, from the text and context it is apparent that we validate the new cruises. Finally, we agree that the agreement is reassuring.

C-23: Page 8, Line 308: Figure 5: not easy to see the black dots (measured values). This is true, and in large part a consequence of the overlap between the predicted and measured values. We prefer not editing the figure. One can see the black dots zooming in. We will add a sentence in the caption to explain that the black dots are in large part hidden by the red/blue dots.

- Changes made: The sentence in the caption explaining the color scheme, has been revised, new text underlined: “Black dots (which to a large extent hidden are by the predicted estimates) are the measured data, blue dots are CANYON-B estimates and red dots are the CONTENT estimates.”

C-24: Figure 5: there is no units (to be added in captions ?).

- Changes made: Units have been stated in the caption.

C-25: Figure 5: Like for Figure 3 and 4, it would be nice to show another example, e.g. SR3 or Davis Strait ? Or an example where the comparison between QC from GLODAP and CANYON-B/CONTENT does not work (if any). This is a suggestion not absolutely needed. Based on the current large numbers of figures in this manuscript, we chosen to not follow this suggestion.

C-26: Page 9, line 320: “Another advantage of CANYON-B and CONTENT is that by

considering the each data point in it self, primary QC issues has been revealed and corrected for some of the cruises.” Which cruises ? Give some examples ?

We have revised the sentence and added an example.

- Changes made: The sentence in question has been revised to: “Another advantage of CANYON-B and CONTENT is that these procedures provide estimates at the level of individual data points, e.g., pH values are determined for every sampling location and depth where T, S, and O<sub>2</sub> data are available. Cases of strong differences between measured and estimated values are always examined. This has helped to identify primary QC issues for some variables and cruises, for example a case of an inverted pH profile at cruise 32PO20130829, which has been amended.”

C-27: Page 9-10: Section 3.3.1. Lines 332-358: This is a list of revisions and would be better to move this section in an Annex but keep in Section 3.3.1 the fCO<sub>2</sub> information (lines 359-375) as it is new data added in v2020.

While we agree that the list is tedious, we prefer to keep it the main text as this is very much what the intention of the manuscript is, documenting significant additions and *changes* to the dataset.

C-28: Page 10: Concerning fCO<sub>2</sub>, in the GLODAP files there are now both fCO<sub>2</sub> measured and calculated in the same column. Authors indicate that all values were converted to 20\_C. However, in the data-files, there are fCO<sub>2</sub> values with fCO<sub>2</sub>temp fixed at -9999. I missed something here and not sure if all fCO<sub>2</sub> values in the files are at the same temperature, pressure or at local temperature etc. : : Also, there are fCO<sub>2</sub> values with flag 0 or 2. What was the criteria for fCO<sub>2</sub> with flag 2 ? How users can easily separate the fCO<sub>2</sub> measured and calculated in the files ? This is important to clarify if one uses both GLODAP (in surface) and SOCAT to merge both products.

We thank you for checking the product files carefully. Indeed, fCO<sub>2</sub> data without accompanying temperatures occurred. This is an error. The product files have been corrected now. fCO<sub>2</sub> data flagged 2 are measured, while fCO<sub>2</sub> values with flag 0 are calculated, as is the case for all seawater CO<sub>2</sub> data.

C-29: Page 10, line 364: “These calculated TALK values were, however, not included in v2.2019.” Does that mean that all TALK values with flag 0 in the files are only interpolated values (i.e. not calculated as an option suggested in table 2).

With the more extensive explanations of the flags added in Section 3.1 (see response to C-05) we hope that it has become clear that seawater CO<sub>2</sub> chemistry variables, such as TALK, flagged 0, are not interpolated, only calculated.

Moreover, the sentence in question relates to the previous version of this product, v2.2019. We realize now, that this sentence might cause confusion and is unnecessary.

- Changes made: The sentence has been removed.

C-30; Page 11, Lines 397-398: For flags 6 and 7 now set to flag 2, recall that this only applied for valid data (i.e. obvious outliers deleted also for these replicates ?).

- Changes made: The underlined text has been added to the sentence: “All flags 6 (replicate measurement) and 7 (manual chromatographic peak measurement) were set to 2, provided the data appeared good.”

C-31: Page 11, Line 399: “Missing sampling pressures or depths were calculated following UNESCO (1981).” This is obvious but maybe rewrite following: “Missing sampling pressures (resp. depths) were calculated from depths (reps. pressures) following UNESCO (1981).”

- Changes made: Revised according to suggestion.

C-32: Page 11-12, Lines 405 and 432: Flag 0 is used for both interpolated and calculated values. Why not using different flag ? (for next version)

As explained in response to comment C-05, interpretation of WOCE flag 0 is unique, and this is now clearly stated in Section 3.1. Nevertheless, we now also reiterate these principles in this section.

- Changes made: The underlines text has been added to the sentences in question:

(Line 405) “Missing salinity, oxygen, nitrate, silicate, and phosphate values were vertically interpolated whenever practical, using a quasi-Hermetian piecewise polynomial. “Whenever practical” means that interpolation was limited to the vertical data separation distances given in Table 4 in Key et al. (2010). Interpolated salinity, oxygen, and nutrient values have been assigned a WOCE quality flag 0.”

(Line 432)“Calculated seawater CO<sub>2</sub> chemistry values have been assigned WOCE flag 0. Seawater CO<sub>2</sub> chemistry values have not been interpolated, so the interpretation of the 0 flag is unique.”

C-33: Page 11, Line 416. Concerning the “Missing seawater CO<sub>2</sub> chemistry variables”. Are the calculated properties used only measured data (i.e. TALK and TCO<sub>2</sub>) or also interpolated values ? In other words, are the fCO<sub>2</sub> and pH interpolated values based on calculated fCO<sub>2</sub> and pH or recalculated with interpolated TALK/TCO<sub>2</sub> ?

We hope that it is clear now, and also in the manuscript, that no seawater CO<sub>2</sub> chemistry variables were interpolated.

C-34: Page 13, Line 486: “For example, Arctic Ocean phosphate, Indian Ocean silicate and TCO<sub>2</sub>, and Pacific Ocean pH data all show considerable improvements.” For Indian, in Table 6 improvement is for TALK, not TCO<sub>2</sub> ?

Indeed, this is correct and has been amended.

- Changes made: TCO<sub>2</sub> has been replaced with TALK in the sentence in question.

C-35: Page 15, Line 544: Weatherall et al., (2015): not in references.

Thank you for pointing this out.

- Changes made: Weatherall et al., (2015) has been added to the reference list.

C-36: Now concerning the files, for curiosity I had a look at the Indian.cvs file and have few questions that could be also valid for other basin. The questions below are obvious for someone familiar with Glodap, but mainly addressed here to help new users.

C-36a: Why the QC flags for S or O<sub>2</sub> are 0 for several cruises although flag WOCE are 2 ? Is it because the secondary QC is not available for these cruises ?

This is correct. We have added text in Sect. 4.2 to explain this (see response to C-16).

C-36c: There are data with WOCE flag=0 for O<sub>2</sub>, Nitrate, Silicates, Phosphates, TCO<sub>2</sub>, TALK, pH, and associated to QC flag = 1. Is it because these are interpolated values for a cruise/station for which a secondary QC was performed ? If QC has been performed (QCF=1) one would expect a WOCE flag different from 0 ? I thought the QC is based on original data (not interpolated or calculated). Could that be clarified ?

This is correct. We have added text in Sect. 4.2 to explain this (see response to C-16).

C-36d: There are data with flag 9 associated to QC flag=1. Again, is it because QC flag (0,1)

are assigned for a cruise/station not for each data?

This is correct. We have added text in Sect. 4.2 to explain this (see response to C-16).

C-37: In the data files on-line (e.g. GLODAPv2.2020\_Indian\_Ocean.cvs) I would suggest to add units for each column.

Yes, and this has been discussed in the GLODAP group as well, and will likely be done for the next update.

C-38: And for next versions, I think for clarity a different flag should be assign for calculated (e.g.  $f\text{CO}_2$ , pH) and interpolated values. This might help some users to select only measured+interpolated values. In references:

As stated earlier, the interpretation of WOCE flag 0 is unique for the different variables. As such there is no need to having a different flag for interpolated (salinity, oxygen, nutrients) vs calculated values ( $\text{TCO}_2$ , TALK, pH,  $f\text{CO}_2$ ). We hope this, now, is clear in the manuscript as well.

I think each reference should now have a DOI

Line 663: "Hood, E. M., Sabine, C. L., and Sloyan, B. M.: The GO-SHIP hydrography manual: A collection of expert reports and guidelines, 2010." Specify the publisher ?

DOI ?

- Changes made: publication information has been completed to:  
Hood, E. M., Sabine, C. L., and Sloyan, B. M. (Eds.): The GO-SHIP hydrography manual: A collection of expert reports and guidelines, IOCCP Report Number 14, ICPO Publication Series Number 134, available at <http://www.go-ship.org/HydroMan.html> (last access: 16 October 2020), 2010.



Response to review by referee #3.

We thank the referee for the helpful comments and suggestions, each one is addressed below (comment in black, response in red).

This is a “living data” update document that discussed the addition of 106 cruises to the GLODAPv2.2019 data set. These data have been extremely valuable to the community and represent an important asset to maintain and update. The manuscript is well written and informative. I only have a few minor comments below.

Line 92-93: The authors don’t distinguish between discrete and in situ sensor measurements here. I assume they are referring to CTD calibration problems with respect to the sensor measurements of salinity and oxygen, not the measurements of collected samples. Please clarify, particularly in light of the merging discussed in section 3.2.1.

Yes, indeed, we are referring to lacking calibration of the data from CTD mounted sensors.

- Changes made: Sentence revised to “For salinity and oxygen, lack of calibration of the data from the conductivity-temperature-depth (CTD) profiler mounted sensors is an additional and widespread problem, particularly for oxygen (Olsen et al., 2016).”

Lines 95-99: The manuscript uses some rather subjective terms without defining their meaning in this context. For example, “poor precision can render a set of data unusable” or “to minimize severe cases of bias”. What is the definition of poor precision or severe bias?

We now provide more concrete information on what is meant with these terms, without going overboard with numbers and definitions as this is a general introduction, and as such we are reluctant to discuss details about each and every variable considered. Besides, the data are evaluated on a case-by-case basis, depending on region and availability of already existing data, for instance; we do not have a strictly enforced global set of limits.

- Changes made:  
The sentence “In rare cases poor precision can render a set of data unusable” has been revised to:  
“In rare cases poor precision - many multiples worse than that expected with current measurement techniques - can render a set of data of limited use.”

The sentence: Adjustments are applied on the data to minimize severe cases of bias”

has been revised to:

“Adjustments are applied to the data to minimize cases of bias that could be confidently established relative to the measurement precision for the variables and cruises considered. “

Lines 98, 108: There are a notable number of grammatical errors in the text that should be fixed. A couple of examples are, “Adjustments are applied on the data”(should be ‘to the data’) or “A particular important source” (should be ‘A particularly important source’). Please review the entire document for these grammatical errors.

Thank you for pointing out these errors, which have been corrected. The text has been carefully read and corrected by all authors, many of whom are native English speakers. We hope the number of grammatical errors has been minimized.

Line 123-124: The authors decided to include cruises on the Merian, Meteor, and the Garcia del Cid that did not have any nutrient or carbon data. I thought nutrients and carbon were

the primary parameters for this data set. Why did the authors decide to include these data and not the thousands of other cruises that also do not have carbon data. This seem inconsistent with the goal of this project.

The emphasis for GLODAP is seawater inorganic carbon chemistry, as well as other carbon-relevant and related variables. This includes the transient tracers CFC-11, CFC-12, CFC-113 and SF<sub>6</sub>, as these are frequently used to determine ocean inventories of anthropogenic carbon (e.g., Waugh et al., 2006). Rarely measured stable carbon isotopes are also relevant, as these are often used for the same purpose (e.g., Quay et al., 2017), and while we do not quality control such data, they are included to ensure their wider availability. There are not thousands of other cruises with such data. We have now included some text on these deliberations:

- Changes made: The following sentences have been included at the start of Section 2: “Not all cruises have data for all of the above-mentioned 12 core variables; for example, cruises with only seawater CO<sub>2</sub> chemistry or transient tracer data are still included even without accompanying nutrient data due to their value towards computation of, for example, carbon inventories. In some other cases, cruises without any of these properties measured were included – this was because they did contain data for other carbon related tracers such as carbon isotopes, with the main intention of ensuring their wider availability.”

Line 150: define data center acronyms the first time they are used, or at least provide links to the data centers.

- Changes made, links to the data centers are now provided

Line 193-195: Were the original data generators consulted before adjustments were made to the data? I believe in the past there was a step that involved checking with the people that originally made the measurement to get their perspective on possible offsets.

Indeed, during preparation of the first version of GLODAP (Key et al., 2004), data originators were contacted for consultation on possible offsets. This practice was abandoned for GLODAPv2, with more than 700 cruises and over 1200 adjustments made, this became impractical. GLODAP is presently a volunteer effort and there is no capacity for routinely approaching principal investigators for every adjustment considered. However, members of the GLODAP Reference Group (i.e., the authors of this contribution) frequently possess first hand experience with the data, or are even the cruise PIs. In exceptional cases, for example where no primary QC seems to have been applied, we do reach out to the PIs.

Line 256: This is the first time that a -888 label is discussed in the text. What does this mean? The same comes in later with -777 and -666 labels.

Thank you for pointing this out. These labels hadn't really been properly explained in this manuscript, only in the GLODAPv2 article (Olsen et al., 2016). In addition, the text in the passage in question (i.e., line 256) better belong in Section 4.2, Adjustment summary as it mostly pertain results.

Changes made: The labels are now explained at the very start of Section 4.2, and presented in a new Table (Table 5). The text on the Davis Strait cruises, pointed out by the reviewer, has been moved from Sect 3.2.3, and used as an example of cruises not fully QCd. The first paragraph in Sect. 4.2 is now: “The secondary QC has 5 different outcomes, provided there are data. These are summarized in Table 5, along with the corresponding codes that appear in the online Adjustment Table and that are also occasionally used as shorthand for decisions in the coming text. The level of secondary QC varies among the cruises.

Specifically, in some cases data were too shallow or geographically too isolated for full and conclusive consistency analyses. A secondary QC flag has been included in the merged

product files to enable their identification, with “0” used for variables and cruises not subjected to full secondary QC (corresponding to code -888 in Table 5) and “1” for variables and cruises that were subjected to full secondary QC. The secondary QC flags are assigned per cruise and variable, not for individual data points and are independent of—and included in addition to—the primary (WOCE) QC flag. For example, interpolated (salinity, oxygen, nutrients) or calculated (TCO<sub>2</sub>, TAlk, pH) values, which have a primary QC flag 0, may have a secondary QC flag of 1 if the measured data these values are based on have been subjected to full secondary QC. Conversely, individual data points may have a secondary QC flag of 0, even if their primary QC flag is 2 (good data). A 0 flag means that data were too shallow or geographically too isolated for consistency analyses or that these analyses were inconclusive, but that we have no reasons to believe that the data in question are of poor quality. Prominent examples of this for this version are the 10 new Davis Strait cruises: no data were available in this region in GLODAPv2.2019, which, combined with complex hydrography and differences in sampling locations, rendered conclusive secondary QC impossible. As a consequence, most, but not all, of these data (some being excluded because of poor precision after consultation with the PI) are included with a secondary QC flag of 0. “

Lines 280-282: Why did the authors use the full GLODAPv2 data to estimate TAlk from Salinity. Wouldn't it make more sense to calculate an average ratio for the data from that cruise rather than use a global ratio that includes data from other oceans? Also, doesn't the ratio change with depth

TAlk is estimated here, with the purpose of converting pH measurement scale and/or reporting temperature/ pressure. The uncertainties introduced by a using global ratio instead of actually measured TAlk are very small. For the scale conversions the uncertainties are on the order of 10<sup>-7</sup> pH units, which is fully negligible. For the temperature and pressure conversions the uncertainties are 0.001 pH units (evaluated using 2 standard deviations around the 67 ratio, i.e. TAlk/S = 67 ± 4.1 μmol/kg/permil). This is an order of magnitude smaller than the stated uncertainty for the pH in the merged product, 0.01-0.02 units.

Calculating the TAlk vs. Salinity ratio for the cruise in question is usually not possible since TAlk often has not been measured at all at these cruises (or very few measurements exist).

We do agree, though, that more sophisticated approaches exist for estimating alkalinity (Bittig et al., 2018; Broullon et al., 2019), and since Bittig et al. (2018) is already used to estimate missing PO<sub>4</sub> and Si, it will be considered for missing TAlk data in future GLODAP updates.

- Changes made: We provide more quantitative information on the uncertainties introduced by the approximation, in section 3.2.4.

#### References:

- Bittig, H. C., Steinhoff, T., Claustre, H., Fiedler, B., Williams, N. L., Sauzède, R., Körtzinger, A., and Gattuso, J.-P.: An alternative to static climatologies: Robust estimation of open ocean CO<sub>2</sub> variables and nutrient concentrations from T, S, and O<sub>2</sub> data using Bayesian Neural Networks, *Frontiers in Marine Science*, 5, 2018.
- Broullon, D., Perez, F. F., Velo, A., Hoppema, M., Olsen, A., Takahashi, T., Key, R. M., Tanhua, T., Gonzalez-Davila, M., Jeansson, E., Kozyr, A., and van Heuven, S.: A global monthly climatology of total alkalinity: a neural network approach, *Earth Syst Sci Data*, 11, 1109-1127, 2019.
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- Quay, P., Sonnerup, R., Munro, D., and Sweeney, C.: Anthropogenic CO<sub>2</sub> accumulation and uptake rates in the Pacific Ocean based on changes in the C-13/C-12 of dissolved inorganic carbon, *Global Biogeochem Cy*, 31, 59-80, 2017.
- Waugh, D. W., Hall, T. M., McNeil, B. I., Key, R., and Matear, R. J.: Anthropogenic CO<sub>2</sub> in the oceans estimated using transit time distributions, *Tellus B*, 58, 376-389, 2006.

## Response to review by referee #4, Dr. Nancy Williams

We thank Dr. Williams for the helpful comments and suggestions, each one is addressed below (comment in black, response in red).

### General Comments:

This is an update to the GLODAPv2.2019 by adding 106 new cruises from 2004-2019, expanding the coverage of GLODAP to 946 cruises over 47 years, 1972–2019. Most of the new cruises are from the western North Pacific and the Davis Strait, with a few from the Atlantic, South Indian, and U.S. West coast. The methods for primary and secondary quality control (QC) are essentially the same as in the earlier version. However, there has been no full consistency analysis of the entire data product as was done with the original GLODAPv2 product. A full consistency analysis will be performed in the future for the next GLODAP update (will be termed “GLODAPv3”) which is set to occur after the completion of the third GO-SHIP survey around year 2023. The researchers have also fixed some minor errors in the GLODAPv2.2019 dataset.

Throughout the manuscripts the researchers discuss alternate ways of adjusting the dataset, and tend to take a conservative approach, saving any major changes for the next full GLODAP update, i.e., GLODAPv3. As such, this update could be considered by some to be incremental, but it should be noted that incremental and timely updates to GLODAP are critical to advancing ocean observing. GLODAP, and other such data products that have come before it, forms the backbone for studying largescale changes in water column properties and has also become increasingly important as autonomous platforms and sensors rapidly begin to fill the world’s oceans. Many autonomous biogeochemical sensors are prone to drift and rely on GLODAP data and methods such as linearly interpolated regressions (LIRs; Carter et al. (2016, 2018) or machine-learning methods such as CANYON/CONTENT (Bittig et al., 2018, Sauzède et al. 2017) for ongoing quality control after deployment. GLODAP also serves as a benchmark for background concentrations in ocean and earth system models.

Where available, the researchers have also added isotopic data for  $\delta_{13}\text{C}$ ,  $\delta_{18}\text{O}$ , and  $\text{D}_{14}\text{C}$  which are not quality controlled/adjusted in the same way as the core GLODAP variables but can provide context for the other data.

They have also added discrete  $f\text{CO}_2$  values which will be useful in addressing inconsistencies in the carbonate system variables. Importantly,  $f\text{CO}_2$  has not been subjected to any secondary QC. There has also been more extensive use of CANYON-B and CONTENT predictions to evaluate offsets in nutrients and  $\text{CO}_2$  data.

One important change that has been made to this version is that there is no internal consistency evaluation of seawater  $\text{CO}_2$  chemistry variables to evaluate pH. This leads to an inconsistency between the pH data for cruises added in this version, and pH data in previous versions of GLODAP. My understanding is that this will likely manifest as a bias, and not a random uncertainty. This potential bias is indeed encompassed by the stated consistency of “0.01 to 0.02 pH units,” but will be critically important for those using this dataset and should be explained more clearly earlier in the manuscript, and perhaps even in the abstract. I also do not think that the consistency for pH should be stated as a range. Yes, it varies by region but unless each region/cruise/data point has its own uncertainty estimate, the overall consistency should be stated as  $\pm 0.02$  pH units. If it is the case that there is only

one region where the consistency is  $\pm 0.02$  pH units, and the rest of the ocean is closer to  $\pm 0.01$ , then that region should be explicitly defined.

Indeed, no internal consistency evaluation was conducted for pH for the data added in this version. No pH data were adjusted either. If adjustments had been made, they would adjust the data from the new cruises, to the pH values of cruises already part of GLODAP (which are used as reference) and evaluated in the earlier efforts. As such, this would not have led to inconsistencies between the pH data for cruises added in this version, and pH data in previous versions of GLODAP.

Regarding stating the consistency for pH as a range. We agree that this was somewhat murky in the submitted manuscript, and we now provide clearer reasoning and identify regions of high vs low uncertainty.

Changes made: The final paragraph of section 3.2.4, where these issues were discussed, have been substantially expanded, to: "In contrast to past GLODAP pH QC, evaluation of the internal consistency of CO<sub>2</sub> system variables was not used for the secondary quality control of the pH data of the 106 new cruises; only crossover analysis was used as supplemented by CONTENT and CANYON-B (Sect. 3.2.5). Recent literature has demonstrated that internal consistency evaluation procedures are subject to errors owing to incomplete understanding of the thermodynamic constants, major ion concentrations, measurement biases, and potential contribution of organic compounds or other unknown protolytes to alkalinity (Takeshita et al., 2020), which lead to pH dependent offsets in calculated pH (Álvarez et al., 2020; Carter et al., 2018): these may be interpreted as biases and generate false corrections. The offsets are particularly strong at pH levels below 7.7, when calculated and measured pH are different by on average between 0.01 and 0.02 units. For the North Pacific this is a problem as pH values below 7.7 can occur at the depths interrogated during the QC (>1500 dbar for this region, Olsen et al., 2016). Since any corrections, which may thus be an artifact, are applied to the full profiles, we assign an uncertainty of 0.02 to the North Pacific pH data in the merged product files. Elsewhere, the uncertainties that have arisen are smaller, since deep pH is typically larger than 7.7 (Lauvset et al., 2020), and at such levels the difference between calculated and measured pH is less than 0.01 on average (Álvarez et al., 2020; Carter et al., 2018). Outside the North Pacific, we believe, therefore that the pH data are consistent to 0.01. Avoiding interconsistency considerations for these intermediate products helps to reduce the problem, but since the reference data set (also as used for the generation of the CONTENT and CANYON-B algorithms) has these issues, a full re-evaluation, envisioned for GLODAPv3, is needed to address the problem satisfactorily."

The original and adjusted data, a detailed adjustment table, and a "known issues" document are available online at the links provided in several formats, and as both global and regional subsets. The "known issues document" is updated regularly and users are encouraged to consult that document when using the data products and identify new issues when they find them.

I was also expecting to hear if/when the next GLODAP gridded product will be produced. Will it always only come with "major" GLODAP updates or are there any plans to do incremental updates?

There are no plans for making incremental updates to the GLODAP gridded product. The changes would likely be rather small anyhow, as the main source of uncertainty in the gridded product is lack of observations in certain regions. The data added in GLODAPv2.2019 and GLODAPv2.2020 are mostly repeat observations, extending the coverage in time and not in space. We cannot commit, now, to making new climatologies for the next full update. While we hope it will be possible, it will depend on the funding situation. Therefore, we

simply add a statement that the intermediate products are not accompanied by a gridded product update.

- Changes made: The sentence “Additionally, the GLODAP mapped climatologies (Lauvset et al., 2016) are not updated for these intermediate products.” has been included in the second final paragraph of the introduction.

Specific comments:

Line 249: An adjustment of  $-3 \mu\text{mol}/\text{kg}$  is made for a cruise which has a mean offset of  $3.68 \mu\text{mol}/\text{kg}$ . Are adjustments always whole numbers? If so, do you always round down?

Adjustments are typically round numbers relative to the precision of the variable considered. There are no particular rules about rounding down or up; we look for example, on whether there is a difference in the offset in recent vs older crossovers. We also consider additional evidence from the other methods. Here, we settled for  $-3 \mu\text{mol}/\text{kg}$ , as the CANYON-B and CONTENT analyses suggested a bias of  $3.4$  and  $2.7 \mu\text{mol kg}^{-1}$ , respectively. This also helps to make the adjustment as small as meaningfully possible, in case there actually is an increasing trend in  $\text{TCO}_2$  from uptake of anthropogenic carbon.

Changes made: The sentence in question has been revised to : “In this case  $-3 \mu\text{mol kg}^{-1}$  was applied: this is somewhat less than indicated by the crossover analysis, but a smaller adjustment is supported by the CANYON-B and CONTENT results (Sect. 3.2.3). Adjustments are typically round numbers relative to the precision of the variable being considered (e.g.,  $-3$  not  $-3.4$  for  $\text{TCO}_2$  and  $0.005$  not  $0.0047$  for pH) to avoid the communicating that the ideal adjustments are known to high precision.”

Line 251: Because they are an exception, provide more detail about how these eight Japanese Sea cruises were adjusted.

Changes made: The following paragraph has been added in section 4.2: “For the Sea of Japan cruises, (where two existed in GLODAPv2.2019 and six were added in this version - Sect. 3.2.2), the crossover results showed biased  $\text{TCO}_2$  data for one of the older cruises (49HS20081021, which is now adjusted up by  $6 \mu\text{mol kg}^{-1}$ ), and biased TALK data for two of the presently added cruises (49UF20111004 and 49UF20121024, adjusted up by  $5$  and  $6 \mu\text{mol kg}^{-1}$ , respectively).”

Line 319-320: Needs editing for clarity.

This has now been edited for clarity, and we have included an example as well, following a suggestion by reviewer 2.

- Changes made: The text has been revised to: “Another advantage of CANYON-B and CONTENT is that these procedures provide estimates at the level of individual data points, e.g., individual pH values are determined for every sampling location and depth were T, S, and  $\text{O}_2$  data are available. Cases of strong differences between measured and estimated values are always examined. This has helped to identify primary QC issues (outliers) for some variables and cruises, for example a case of an inverted pH profile at cruise 32PO20130829, which has been amended.”

Lines 280-282: While it is stated that TALK estimated from 67 times salinity is sufficient for such pH conversions, it would be useful to explicitly state the amount of uncertainty introduced to pH by such a TALK approximation.

Yes, we agree.

- Changes made: The following text has been added in Sect. 3.2.4: “The uncertainties introduced with this approximation are negligible (order  $10^{-7}$  pH units) for the scale conversions and order  $10^{-3}$  pH units for the temperature and pressure conversion (evaluated by repeating conversions with 2 times the standard deviation of the ratio,

i.e.,  $67 \pm 4.1$ ). This is sufficiently accurate relative to other sources of uncertainty, which are discussed below.”

Lines 427-429: Why was this decision made to replace measured values with calculated values?

This decision was made when GLODAPv2 was prepared. Often, for such cruises where the number of measured data points for a CO<sub>2</sub> chemistry variable is much less than the number that can be calculated, the accuracy of the measured data cannot be confidently established – there are too few data for good crossover analyses – and it makes most sense replacing these with values calculated from the two other better QC'd variables. Evaluating the appropriate action on a per cruise basis is time consuming, so we made the decision to draw the line at less than 1/3 (of the combined number of calculated and measured values)

- Changes made: We have simplified the sentences a bit, and added the reason for replacing measured values “For calculations involving TCO<sub>2</sub>, TAlk, and pH, if less than a third of the total number of values, measured and calculated combined, for a specific cruise were measured, then all these were replaced by calculated values. The reason for this, is that secondary QC of the few measured values was often not possible in such cases, for example due to a limited number of deep data available”

Lines 537-541 and 558-559: It is acknowledged twice in the summary that the surface data are both seasonally biased and not examined for consistency in GLODAP. This is an important caveat and should be stated in the introduction.

- Changes made: We have added the following sentence to the introduction (in former line # 98: “The secondary quality controlled focused on deep data, where natural variability is minimal”

Figures 3, 5, 8, 10: Include a legend for the colors

Figure 3 and 5 are produced by the crossover and CANYON-B/CONTENT software. It is not possible to add legends at this stage. The meaning of the colors are now explained in the caption.

- Changes made: Legends have been added to Fig. 8 and Fig 10.



## Response to short comment #1, by Dr. Jens Müller

We thank Dr. Müller for the helpful comments and suggestions, each one is addressed below (comment in black, response in red).

### ### Short summary

The authors present an update of the GLODAPv2.2019 data product, by adding new data from 106 cruises. Before addition, observations of 12 core variables have undergone a primary (f flag) and secondary (qc flag) quality control. The secondary quality control is based on the comparison of new data with those contained within GLODAPv2.2019. Adjustments were - if necessary - applied to the new data, in order to correct for biases between measurements from different cruises, but preserve temporal trends in the variables. The merged data product includes observations from 946 cruises and extends until 2019.

### ### General comments

The overall quality of this data product and its description in the companion manuscript appear very high. I have no general comments which would require a revision of fundamental aspects of the data set as a whole. The updated product GLODAPv2.2020 is an invaluable contribution for the scientific community and an essential prerequisite to reach the stated goal of documenting “the state and the evolving changes in physical and chemical ocean properties, e.g., the inventory of the excess CO<sub>2</sub> in the ocean”. This review is written from the perspective of a new user of the product.

### ### Specific comments

Following specific issues were identified and might (if taken into account) require a revision of some aspects of the data product:

-I.412: “Neutral density was calculated using Sérazin (2011).” It should be noted that the reference given here refers to a master thesis and that the proposed polynomial approximation of neutral density in this thesis has not undergone peer review. Furthermore, polynomials were fitted to a preliminary neutral density data set with known issues (pers. comm. P. Barker and G. Sérazin). To take those limitations into account, the computed density variable gamma could either be revised, removed or labelled as preliminary in the main text.

Thank you for alerting us on this issue.

- Changes made: We have replaced the neutral density values in the merged product files with values calculated according to Jackett and McDougall (1997). This is described in Sects. 3.3.1 and 3.3.2.

-It might be helpful for some users if the f flag value would distinguish between interpolated and calculated values.

A WOCE flag value of 0 does indeed indicate values that either have been interpolated or calculated. Interpolation is only carried out for salinity, oxygen and nutrients while calculations are only carried out for seawater CO<sub>2</sub> chemistry variables. As such, interpretation of the 0 flag is unique. This is now clearly stated in the manuscript, in section 3.1, 3.3.2 and 6. Whether to change this and introduce a new flag, is a topic that will be considered for future updates.

-I.190: It is stated that “not all offsets larger than the initial minimum limits have been

adjusted for.... Conversely, in some cases where data and offsets were very precise and the cruise had been conducted in a region where variability is expected to be small, adjustments lower than the minimum limits were applied.” I was wondering whether at all an initial minimum adjustment limit needs to be defined and what the added value of this definition is. Would it be possible to define an offset-to-precision ratio that could rigorously be applied to all decisions?

This is true, a limit based on the criteria mentioned (offset-to-precision ratio) seems more meaningful, and we will explore ways to implement this for future versions of this data product.

-1.249: An adjustment of  $-3 \mu\text{mol kg}^{-1}$  was applied, although an offset of  $3.68 \pm 0.83 \mu\text{mol kg}^{-1}$  was found. Is this difference intentional? What is the general rule on how the adjustment values are set?

Adjustments are typically round numbers relative to the precision of the variable considered. There are no particular rules about rounding down or up; we look for example, on whether there is a difference in the offset in recent vs older crossovers. We also consider additional evidence from the other methods. Here, we settled for  $-3 \mu\text{mol/kg}$ , as the CANYON-B and CONTENT analyses suggested a bias of  $3.4$  and  $2.7 \mu\text{mol kg}^{-1}$ , respectively. This also helps to make the adjustment as small as meaningfully possible, in case there actually is an increasing trend in  $\text{TCO}_2$  from uptake of anthropogenic carbon.

- Changes made: The sentence in question has been revised to : “In this case  $-3 \mu\text{mol kg}^{-1}$  was applied. This is somewhat less than indicated by the crossover analysis, but such a small adjustment is supported by the CANYON-B and CONTENT results (Sect. 3.2.3).”

### ### Technical corrections

Following comments address the presentation of the data product, and cover also aspects that are not purely technically:

-The presentation of the flagging scheme could be improved, aiming at clarity from a user perspective. Taking table 2 as an example, it confused me that labels 0-9 are presented, whereas the data product only uses flag values 0, 2, and 9. Readers currently need to refer to footnotes in column “Merged product files” to find out that WOCE flags 6 and 7 were set to 2, whereas 3, 4, 5, and 8 were set to 9. Furthermore, the term “Not used” might add to the confusion, as it can easily be misinterpreted as “observations were not used” rather than the intended “the flag value was not used”. Starting table 2 with the first column indicating flag values that are actually used in the data product would greatly improve clarity and avoid potential misinterpretation of the flagging scheme.

We agree that this should be better described and have made changes in the text and in table 2, which hopefully convey differences in flagging schemes between the original exchange formatted data files and the merged product files.

- Changes made: The underlined text has been added to the paragraph where the WOCE flags are first mentioned in Sect. 3.1: “Each data column (except temperature and pressure, which are assumed “good” if they exist) has an associated column of data flags. For the original data exchange files, these flags conform to the WOCE definitions for water samples and are listed in Table 2. For the merged and adjusted product files these flags are simplified: questionable (WOCE flag 3) and bad (WOCE flag 4) data are removed and their flags are set to 9. The same procedure is applied to data flagged 8 (very few such data exist). WOCE flags 1 (Data not received) and 5 (Data not reported) are also set to 9, while 6 (Mean of replicate measurement) and 7 (Manual chromatographic peak measurement) are set to 2, if the data appear

good. Also, in the merged product file a flag of 0 is used to indicate a value that could be measured but is somehow approximated: for salinity, oxygen, phosphate, nitrate, and silicate, the approximation is conducted using vertical interpolation; for seawater CO<sub>2</sub> chemistry variables (TCO<sub>2</sub>, TAlk, pH, and fCO<sub>2</sub>), the approximation is conducted using calculation from two measured CO<sub>2</sub> chemistry variables (Sect 3.2.2). Importantly, interpolation of CO<sub>2</sub> chemistry variables is never performed, and thus a flag value of 0 has unique interpretation.”

- Changes have also been made in Table 2, specifically, we have replaced ‘Not used’, in the third column, with ‘Flag not used’, to make it more clear that it is the flags that are not used. We prefer to leave the column order unchanged, as having the scheme for original files first and product files last, aligns with the extent to which files are modified with our procedures.

Likewise, in table 5 rownames (first column) are not intuitive. I was wondering what -888 does stand for. Does this label occur in the data set?

Reviewer 3 also pointed out lacking explanation of the -888, and similar, codes, which are used in the online Adjustment Table, and as shorthand for various actions in the manuscript. We agree these needs explanation.

- Changes made: the meaning of -888 and the other codes are now explained in a new paragraph added to the start of Section 4.2: “The secondary QC has 5 different outcomes, provided there are data. These are summarized in Table 5, along with the corresponding codes that appear in the online Adjustment Table and that are also occasionally used as shorthand for decisions in the coming text. The level of secondary QC varies among the cruises. Specifically, in some cases data were too shallow or geographically too isolated for full and conclusive consistency analyses. A secondary QC flag has been included in the merged product files to enable their identification, with “0” used for variables and cruises not subjected to full secondary QC (corresponding to code -888 in Table 5) and “1” for variables and cruises that were subjected to full secondary QC. The secondary QC flags are assigned per cruise and variable, not for individual data points and are independent of—and included in addition to—the primary (WOCE) QC flag. For example, interpolated (salinity, oxygen, nutrients) or calculated (TCO<sub>2</sub>, TAlk, pH) values, which have a primary QC flag 0, may have a secondary QC flag of 1 if the measured data these values are based on have been subjected to full secondary QC. Conversely, individual data points may have a secondary QC flag of 0, even if their primary QC flag is 2 (good data). A 0 flag means that data were too shallow or geographically too isolated for consistency analyses or that these analyses were inconclusive, but that we have no reasons to believe that the data in question are of poor quality. Prominent examples of this for this version are the 10 new Davis Strait cruises: no data were available in this region in GLODAPv2.2019, which, combined with complex hydrography and differences in sampling locations, rendered conclusive secondary QC impossible. As a consequence, most, but not all, of these data (some being excluded because of poor precision after consultation with the PI) are included with a secondary QC flag of 0. “
- A new table 5 has been added:

**Table 5: Possible outcomes of the secondary QC and their codes in the online Adjustment Table**

Secondary QC result	Code
The data are of good quality, consistent with the rest of the dataset and should not be adjusted.	0/1 <sup>a</sup>
The data are of good quality but are biased: adjust by adding (for salinity, TCO <sub>2</sub> , TAlk, pH) or by multiplying (for oxygen, nutrients, CFCs) the adjustment value	Adjustment value
The data have not been QC'd, are of uncertain quality, and suspended until full secondary QC has been carried out	-666
The data are of poor quality and excluded from the data product.	-777
The data appear of good quality but their nature, being from shallow depths, coastal regions, without crossovers or similar, prohibits full secondary QC	-888
No data exist for this variable for the cruise in question	-999

<sup>a</sup>The value of 0 is used for variables with additive adjustments (salinity, TCO<sub>2</sub>, TAlk, pH) and 1 for variables with multiplicative adjustments (for oxygen, nutrients, CFCs). This is mathematically equivalent to 'no adjustment' in each case

Finally, several important information about flags are given in section 3.3.2 (Merging), but might be better placed in 3.1 (Data assembly and primary quality control) and 3.2 (Secondary quality control).

- **Changes made.** The information about WOCE flags has been added to Sect 3.1, as explained in response to Technical Correction #1, and information about the secondary QC flags has been added to paragraph 4.2, in response to Technical Correction #2

-I.45: The entire data product contains “measurements from more than 1.2 million water samples”. However, this number decreases significantly when the number of available core variables is considered. As an example, I found in the merged master file <0.5 million dissolved inorganic carbon (tco2) observations and <10.000 observations with all core variables being available (in both cases ignoring f and qc flags). To this end, readers might benefit from a more detailed description of the data set. Giving expected row numbers for a few exemplary combinations of subsetting conditions would be valuable

- **Changes made** We have included some illustrative examples in a new paragraph in Section 6: “The total number of data records are 1 275 558. Records with measurements for all 12 core variables, salinity, oxygen, nitrate, silicate, phosphate, TCO<sub>2</sub>, TAlk, pH, CFC-11, CFC-12, CFC-113, and CCl<sub>4</sub> are very rare; only 2026 records have measured data for all 12 in the merged product file (interpolated and calculated data excluded). Requiring only two measured seawater CO<sub>2</sub> chemistry variables in addition to all the other core variables brings the number of available records up to 9 230, so this is also very rare. A major limiting factor is simultaneous availability of data for all four freon species, only 26 277 records have measurements of CFC-11, CFC-12, CFC-113, and CCl<sub>4</sub> while 400 587 have data for at least one of these (not considering availability of other core variables). A total of 398 757 records have measured data for two out of the three CO<sub>2</sub> chemistry core variables. The number of measured fCO<sub>2</sub> data are 33 924; note that these data were not subjected to quality control. The number of records with measured data for salinity, oxygen, and nutrients are 798 703, while the number of records with salinity and oxygen data are 1 077 859. All of these numbers are for measured data, not interpolated or calculated values.”

## References

Jackett, D. R. and McDougall, T. J.: A neutral density variable for the world's oceans, *J Phys Oceanogr*, 27, 237-263, 1997.

# An updated version of the global interior ocean biogeochemical data product, **GLODAPv2.2020**

Are Olsen<sup>1</sup>, Nico Lange<sup>2</sup>, Robert M. Key<sup>3</sup>, Toste Tanhua<sup>2</sup>, Henry C. Bittig<sup>4</sup>, Alex Kozyr<sup>5</sup>, Marta Álvarez<sup>6</sup>, Kumiko Azetsu-Scott<sup>7</sup>, Susan Becker<sup>8</sup>, Peter J. Brown<sup>9</sup>, Brendan R. Carter<sup>10,11</sup>, Leticia Cotrim da Cunha<sup>12</sup>, Richard A. Feely<sup>11</sup>, Steven van Heuven<sup>13</sup>, Mario Hoppema<sup>14</sup>, Masao Ishii<sup>15</sup>, Emil Jeansson<sup>16</sup>, Sara Jutterström<sup>17</sup>, Camilla S. Landa<sup>1</sup>, Siv K. Lauvset<sup>16</sup>, Patrick Michaelis<sup>2</sup>, Akihiko Murata<sup>18</sup>, Fiz F. Pérez<sup>19</sup>, Benjamin Pfeil<sup>1</sup>, Carsten Schirmick<sup>2</sup>, Reiner Steinfeldt<sup>20</sup>, Toru Suzuki<sup>21</sup>, Bronte Tilbrook<sup>22</sup>, Anton Velo<sup>19</sup>, Rik Wanninkhof<sup>23</sup>, Ryan J. Woosley<sup>24</sup>

<sup>1</sup> Geophysical Institute, University of Bergen and Bjerknes Centre for Climate Research, Bergen, Norway

<sup>2</sup> GEOMAR Helmholtz Centre for Ocean Research Kiel, Kiel, Germany

<sup>3</sup> Atmospheric and Oceanic Sciences, Princeton University, Princeton, NJ, 08540, USA

<sup>4</sup> Leibniz Institute for Baltic Sea Research Warnemünde, Rostock, Germany

<sup>5</sup> NOAA National Centers for Environmental Information, Silver Spring, MD, USA

<sup>6</sup> Instituto Español de Oceanografía, A Coruña, Spain

<sup>7</sup> Department of Fisheries and Oceans, Bedford Institute of Oceanography, Dartmouth, Nova Scotia, Canada

<sup>8</sup> UC San Diego, Scripps Institution of Oceanography, San Diego CA 92093, USA

<sup>9</sup> National Oceanography Centre, Southampton, UK

<sup>10</sup> Cooperative Institute for Climate, Ocean and Ecosystem Studies, University Washington, Seattle, Washington, USA

<sup>11</sup> Pacific Marine Environmental Laboratory, National Oceanic and Atmospheric Administration, Seattle, Washington, USA

<sup>12</sup> Faculdade de Oceanografia, Universidade do Estado do Rio de Janeiro, Rio de Janeiro (RJ), Brazil

<sup>13</sup> Centre for Isotope Research, Faculty of Science and Engineering, University of Groningen, Groningen, the Netherlands

<sup>14</sup> Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research, Bremerhaven, Germany

<sup>15</sup> Oceanography and Geochemistry Research Department, Meteorological Research Institute, Japan Meteorological Agency, Tsukuba, Japan

<sup>16</sup> NORCE Norwegian Research Centre, Bjerknes Centre for Climate Research, Bergen, Norway

<sup>17</sup> IVL Swedish Environmental Research Institute, Gothenburg, Sweden

<sup>18</sup> Research Institute for Global Change, Japan Agency for Marine-Earth Science and Technology, Yokosuka, Japan

<sup>19</sup> Instituto de Investigaciones Marinas, IIM – CSIC, Vigo, Spain

<sup>20</sup> University of Bremen, Institute of Environmental Physics, Bremen, Germany

<sup>21</sup> Marine Information Research Center, Japan Hydrographic Association, Tokyo, Japan

<sup>22</sup> CSIRO Oceans and Atmosphere and Antarctic Climate and Ecosystems Co-operative Research Centre, University of Tasmania, Hobart, Australia

<sup>23</sup> Atlantic Oceanographic and Meteorological Laboratory, National Oceanic and Atmospheric Administration, Miami, USA.

<sup>24</sup> Center for Global Change Science, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

Correspondence to: Are Olsen (are.olsen@uib.no)

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**Abstract.** The Global Ocean Data Analysis Project (GLODAP) is a synthesis effort providing regular compilations of surface-to-bottom ocean biogeochemical data, with an emphasis on seawater inorganic carbon chemistry and related variables determined through chemical analysis of seawater samples. GLODAPv2.2020 is an update of the previous version, GLODAPv2.2019. The major changes are: data from 106 new cruises added, extension of time coverage to 2019, and the inclusion of available (also for historical cruises) discrete fugacity of CO<sub>2</sub> (*f*CO<sub>2</sub>) values in the merged product files. GLODAPv2.2020 now includes measurements from more than 1.2 million water samples from the global oceans collected on 946 cruises. The data for the 12 GLODAP core variables (salinity, oxygen, nitrate, silicate, phosphate, dissolved inorganic carbon, total alkalinity, pH, CFC-11, CFC-12, CFC-113, and CCl<sub>4</sub>) have undergone extensive quality control with a focus on systematic evaluation of bias. The data are available in two formats: (i) as submitted by the data originator but updated to WOCE exchange format and (ii) as a merged data product with adjustments applied to minimize bias. These adjustments were derived by comparing the data from the 106 new cruises with the data from the 840 quality-controlled cruises of the GLODAPv2.2019 data product using crossover analysis. Comparisons to empirical algorithm estimates provided additional context for adjustment decisions, this is new to this version. The adjustments are intended to remove potential biases from errors related to measurement, calibration, and data handling practices without removing known or likely time trends or variations in the variables evaluated. The compiled and adjusted data product is believed to be consistent to better than 0.005 in salinity, 1 % in oxygen, 2 % in nitrate, 2 % in silicate, 2 % in phosphate, 4 μmol kg<sup>-1</sup> in dissolved inorganic carbon, 4 μmol kg<sup>-1</sup> in total alkalinity, 0.01–0.02 in pH (depending on region), and 5 % in the halogenated transient tracers. The other variables included in the compilation, such as isotopic tracers and discrete *f*CO<sub>2</sub>, were not subjected to bias comparison or adjustments.

The original data, their documentation and doi codes are available at the Ocean Carbon Data System of NOAA NCEI ([https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2\\_2020/](https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2_2020/), last access: 20 June 2020). This site also provides access to the merged data product, which is provided as a single global file and as four regional ones – the Arctic, Atlantic, Indian, and Pacific oceans – under <https://doi.org/10.25921/2c8h-sa89> (Olsen et al., 2020). These bias-adjusted product files also include significant ancillary and approximated data. These were obtained by interpolation of, or calculation from, measured data. This living data update documents the GLODAPv2.2020 methods and provides a broad overview of the secondary quality control procedures and results.

## 1 Introduction

The oceans mitigate climate change by absorbing both atmospheric CO<sub>2</sub> corresponding to a significant fraction of anthropogenic CO<sub>2</sub> emissions (Friedlingstein et al., 2019; Gruber et al., 2019) and most of the excess heat in the Earth System caused by the enhanced greenhouse effect (Cheng et al., 2020; Cheng et al., 2017). The objective of GLODAP (Global Ocean Data Analysis Project, [www.glodap.info](http://www.glodap.info), last access: 25 May 2020) is to ensure provision of high quality and bias-corrected water column bottle data from the ocean surface to bottom that document the state and the evolving changes in physical and chemical ocean properties, e.g., the inventory of the excess CO<sub>2</sub> in the ocean, natural oceanic carbon, ocean acidification, ventilation rates, oxygen levels, and vertical nutrient transports. The core quality-controlled and bias-adjusted variables, are salinity, dissolved oxygen, inorganic macronutrients (nitrate, silicate, and phosphate), seawater CO<sub>2</sub> chemistry variables (dissolved inorganic carbon – TCO<sub>2</sub>, total alkalinity – TALK, and pH on the total H<sup>+</sup> scale), and the halogenated transient tracers chlorofluorocarbon-11 (CFC-11), CFC-12, CFC-113, and CCl<sub>4</sub>.

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Other chemical tracers are usually measured on the cruises included in GLODAP. A subset of these data is distributed as part of the product but has not been extensively quality controlled or checked for measurement biases in this effort. For some of these variables, better sources of data may exist, for example the product by Jenkins et al. (2019) for helium isotope and tritium data. GLODAP also includes derived variables to facilitate interpretation, such as potential density anomalies and apparent oxygen utilization (AOU). A full list of variables included in the product is provided in Table 1.

The oceanographic community largely adheres to principles and practices for ensuring open access to research data, such as the FAIR (Findable, Accessible, Interoperable, Reusable) initiative (Wilkinson et al., 2016), but the plethora of file formats and different levels of documentation, combined with the need to retrieve data on a per cruise basis from different access points, limits the realization of their full scientific potential. For biogeochemical data there is the added complexity of different levels of standardization and calibration, and even different units used for the same variable, such that the comparability between data sets is often poor. Standard operating procedures have been developed for some variables (Dickson et al., 2007; Hood et al., 2010; Hydes et al., 2012) and certified reference materials (CRM) exist for seawater TCO<sub>2</sub> and TALK measurements (Dickson et al., 2003) and for nutrients in seawater (CRMNS; Aoyama et al., 2012; Ota et al., 2010). Despite this, biases in data still occur. These can arise from poor sampling and preservation practices, calibration procedures, instrument design, and inaccurate calculations. The use of CRMs does not by itself ensure accurate measurements of seawater CO<sub>2</sub> chemistry (Bockmon and Dickson, 2015), and the CRMNS have only become available recently and are not universally used. For salinity and oxygen, lack of calibration of the data from conductivity-temperature-depth (CTD) profiler mounted sensors is an additional and widespread problem, particularly for oxygen (Olsen et al., 2016). For halogenated transient tracers, uncertainties in standard gas composition, extracted water volume, and purge efficiency typically provide the largest sources of uncertainty. In addition to bias, occasional outliers occur. In rare cases poor precision - many multiples worse than that expected with current measurement techniques - can render a set of data of limited use. GLODAP deals with these issues by presenting the data in a uniform format, including any meta data, either publicly-available or submitted by the data originator, and by subjecting the data to primary and secondary quality control assessments, focusing on precision and consistency, respectively. The secondary quality control focuses on deep data, where natural variability is minimal. Adjustments are applied to the data to minimize cases of bias that could be confidently established relative to the measurement precision for the variables and cruises considered.

GLODAPv2.2020 builds on earlier synthesis efforts for biogeochemical data obtained from research cruises, GLODAPv1.1 (Key et al., 2004; Sabine et al., 2005), Carbon dioxide in the Atlantic Ocean (CARINA) (Key et al., 2010), Pacific Ocean Interior Carbon (PACIFICA) (Suzuki et al., 2013), and notably GLODAPv2 (Olsen et al., 2016). GLODAPv1.1 combined data from 115 cruises with biogeochemical measurements from the global ocean. The vast majority of these were the sections covered during the World Ocean Circulation Experiment and the Joint Global Ocean Flux Study (WOCE/JGOFS) in the 1990s, but data from important "historical" cruises were also included, such as from the Geochemical Ocean Sections Study (GEOSECS), Transient Traces in the Ocean (TTO), and South Atlantic Ventilation Experiment (SAVE). GLODAPv2 was released in 2016 with data from 724 scientific cruises, including those from GLODAPv1.1, CARINA, PACIFICA, and data from 168 additional cruises. A particularly important source of data were the cruises executed within the framework of the "repeat hydrography" program (Talley et al., 2016), instigated in the early 2000s as part of the Climate and Ocean: Variability, Predictability and Change (CLIVAR) program and since 2007 organized as the Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP) (Sloyan et al., 2019). GLODAPv2 is now updated regularly using the "living data format" of Earth System Science Data to document significant additions and changes to the dataset.

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160 Within this there are two types of GLODAP updates: full and intermediate. Full updates involve a reanalysis, notably  
crossover and inversion, of the entire dataset (both historical and new cruises) and all adjustments are subject to change.  
This was carried out for GLODAPv2. For intermediate updates, recently-available data are added following quality  
165 control procedures to ensure their consistency with the cruises included in the latest GLODAP release. Except for obvious  
outliers and similar types of errors (Sect. 3.3.1), the data included in previous releases are not changed during  
intermediate updates. Additionally, the GLODAP mapped climatologies (Lauvset et al., 2016) are not updated for these  
intermediate products appended. The exact version number and release year (if appended) of the product used should  
always be reported in studies, rather than making a generic reference to GLODAP.  
170 Creating and interpreting inversions, and other checks of the full data set needed for full updates are too demanding in  
terms of time and resources to be preformed every year or two-years (including an inversion) again after the third GO-  
SHIP survey has been completed. This completion is currently scheduled for 2023, and we anticipate that GLODAPv3  
will become available a few years thereafter. In the intermin. presented here is the second intermediate update, which  
adds data from 106 new cruises to the last update, GLODAPv2.2019 (Olsen et al., 2019).

## 2 Key features of the update

175 GLODAPv2.2020 (Olsen et al., 2020) contains data from 946 cruises, covering the global ocean from 1972 to 2019,  
compared to 840 for the period 1972-2017 for GLODAPv2.2019. Information on the 106 cruises added to this version is  
provided in Table A1 in the Appendix. Cruise sampling locations are shown alongside those of GLODAPv2.2019 in Fig.  
1, while the coverage in time is shown in Fig. 2. Not all cruises have data for all of the above-mentioned 12 core  
180 variables; for example, cruises with only seawater CO<sub>2</sub> chemistry or transient tracer data are still included even without  
accompanying nutrient data due to their value towards computation of, for example, carbon inventories. In some other  
cases, cruises without any of these properties measured were included – this was because they did contain data for other  
carbon related tracers such as carbon isotopes, with the main intention of ensuring their wider availability. The added  
cruises are from the years 2004-2019, with most being more recent than 2010. The majority of the new data were  
obtained from the two vessels RV *Keifu Maru II* and RV *Ryofu Maru III*, which are operated by the Japan Meteorological  
Agency in the western North Pacific (Oka et al., 2018; Oka et al., 2017). Another important addition is the data collected  
185 across the Davis Strait between Canada and Greenland, from 10 cruises between 2004-2015 through a collaboration  
between the Bedford Institute of Oceanography, Canada and the University of Washington, USA (Azetsu-Scott et al.,  
2012). Other cruises from the Atlantic include those carried out on the RV *Maria S. Merian* and RV *Meteor*, with  
transient tracer data but not nutrients or seawater CO<sub>2</sub> chemistry data; the 2016 occupation of the OVIDE line (Pérez et  
al., 2018); the 2019 occupation of A17 onboard RV *Hesperides*; the 2018 occupation of A9.5 onboard RRS *James Cook*  
190 (King et al., 2019); and A02 on the RV *Celtic Explorer* in 2017 (McGrath et al., 2019). Two older North Atlantic cruises  
that did not find their way into GLODAPv2 have been added, a 2008 occupation of AR07W including more extensive  
subpolar NA sampling (35TH20080825) and a 2007 RV *Pelagia* cruise (64PE20071026) covering the Northeast Atlantic.  
The final Atlantic cruise is 29GD20120910 onboard RV *Garcia del Cid*, with measurements for stable isotopes of carbon  
and oxygen ( $\delta^{13}\text{C}$  and  $\delta^{18}\text{O}$ ) off the Iberian Peninsula (Voelker et al., 2015) but no data for nutrients, seawater CO<sub>2</sub>  
195 chemistry, or transient tracers. Two new Indian Ocean cruises are included, both took place in the far south, in the Indian  
sector of the Southern Ocean: an Argo deployment cruise south and west of Kerguelen Island onboard the RV *S. A.*  
*Agulhas I*, and the 2018 occupation of GO-SHIP line SR03 onboard the RV *Investigator*. The JOIS cruise in 2015 is the

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sole addition for the Arctic. Finally, new data along the US West Coast are from two cruises conducted on board the RVs *Wecoma* (WCOA2011, 32WC20110812) and *Ronald H. Brown* (WCOA2016, 33RO20160505) as part of NOAA’s ocean acidification program.

All new cruises were subjected to primary (Sect. 3.1) and secondary (Sect. 3.2) quality control (QC). These procedures are essentially the same as for GLODAPv2.2019, aiming to ensure the consistency of the data from the 106 new cruises with the previous release of this data product (in this case, the GLODAPv2.2019 adjusted data product). The aim is to conduct a full analysis (i.e., A naming convention has been introduced to distinguish intermediate from full product updates. For the latter the version number will change, while for the former the year of release is

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### 3 Methods

#### 3.1 Data assembly and primary quality control

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The data from the 106 new cruises were submitted directly to us or retrieved from data centers: typically the CLIVAR and Carbon Hydrographic Data Office (<https://cchdo.ucsd.edu>, last access: 20 October 2020), National Center for Environmental Information (<https://www.ncei.noaa.gov>, last access 20 October 2020), and PANGAEA (<https://pangaea.de>, last access 20 October 2020). Each cruise is identified by an expedition code (EXPCODE). The EXPCODE is guaranteed to be unique and constructed by combining the country code and platform code with the date of departure in the format YYYYMMDD. The country and platform codes were taken from the ICES (International Council for the Exploration of the Sea) library (<https://vocab.ices.dk/>, last access: 20 June 2020).

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The individual cruise data files were converted to the WOCE exchange format: a comma delimited ASCII format for CTD and bottle data from hydrographic cruises. GLODAP deals only with bottle data and CTD data at bottle trip depths, and their exchange format is briefly reviewed here with full details provided in Swift and Diggs (2008). The first line of each exchange file specifies the data type, in the case of GLODAP this is “BOTTLE”, followed by a date and time stamp and identification of the group and person, who prepared the file, e.g., “PRINUNIVRMK” is Princeton University, Robert M. Key. Next follows the README section: this provides brief cruise specific information, such as dates, ship, region, method plus quality notes for each variable measured, citation information, and references to any papers that used or presented the data. The README information was typically assembled from the information contained in the metadata submitted by the data originator. In some cases, issues noted during the primary QC and other information such as file update notes are included. The only rule for the README section is that it must be concise and informative. The README is followed by data column headers, units, and then the data. The headers and units are standardized and provided in Table 1 for the variables included in GLODAP. Exchange file preparation required unit conversion in some cases, most frequently from milliliters per liter (mL L<sup>-1</sup>; oxygen) or micromoles per liter (μmol L<sup>-1</sup>; nutrients) to micromoles per kilogram of seawater (μmol kg<sup>-1</sup>). The default conversion procedure for nutrients was to use seawater density at reported salinity, an assumed measurement-temperature of 22 °C, and pressure of 1 atm. For oxygen, the factor 44.66 was used for the “milliliters of oxygen” to “micromoles of oxygen” conversion, while the density required for the “per liter” to “per kilogram” conversion was calculated from the reported salinity and draw temperatures whenever possible. However, potential density was used instead when draw temperature was not reported. The potential errors introduced by any of these procedures are insignificant. Missing numbers are indicated by -999.

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Each data column (except temperature and pressure, which are assumed “good” if they exist) has an associated column of data flags. For the original data exchange files, these flags conform to the WOCE definitions for water samples, and are

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305 listed in Table 2. For the merged and adjusted product files these flags are simplified: questionable (WOCE flag 3) and bad (WOCE flag 4) data are removed and their flags are set to 9. The same procedure is applied to data flagged 8 (very few such data exist); WOCE flags 1 (Data not received) and 5 (Data not reported) are also set to 9, while flags of 6 (Mean of replicate measurements) and 7 (Manual chromatographic peak measurement) are set to 2, if the data appear good. Also, in the merged product files a flag of 0 is used to indicate a value that could be measured but is somehow approximated: for salinity, oxygen, phosphate, nitrate, and silicate, the approximation is conducted using vertical interpolation; for seawater CO<sub>2</sub> chemistry variables (TCO<sub>2</sub>, TALK, pH, and fCO<sub>2</sub>), the approximation is conducted using calculation from two measured CO<sub>2</sub> chemistry variables (Sect 3.2.2). Importantly, interpolation of CO<sub>2</sub> chemistry variables is never performed and thus a flag value of 0 has a unique interpretation.

310 If no WOCE flags were submitted with the data, then they were assigned by us. Regardless, all incoming files were subjected to primary QC to detect questionable or bad data - this was carried out following Sabine et al. (2005) and Tanhua et al. (2010), primarily by inspecting property-property plots. Outliers showing up in two or more different such plots were generally defined as questionable and flagged. In some cases, outliers were detected during the secondary QC; the consequent flag changes have then also been applied in the GLODAP versions of the original cruise data files.

### 3.2 Secondary quality control

320 The aim of the secondary QC was to identify and correct any significant biases in the data from the 106 new cruises relative to GLODAPv2.2019, while retaining any signal due to temporal changes. To this end, secondary QC in the form of consistency analyses was conducted to identify offsets in the data. All identified offsets were scrutinized by the GLODAP reference group through a series of teleconferences during March and April 2020 in order to decide the adjustments to be applied to correct for the offset (if any). To guide this process, a set of initial minimum adjustment limits was used (Table 3). These are set according to the expected measurement precision for each variable, and are the same as those used for GLODAPv2.2019. In addition to the average magnitude of the offsets, factors such as the precision of the offsets, persistence towards the various cruises used in the comparison, regional dynamics, and the occurrence of time trends or other variations were considered. Thus, not all offsets larger than the initial minimum limits have been adjusted. A guiding principle for these considerations was to not apply an adjustment whenever in doubt. Conversely, in some cases where data and offsets were very precise and the cruise had been conducted in a region where variability is expected to be small, adjustments lower than the minimum limits were applied. Any adjustment was applied uniformly to all values for a variable and cruise, i.e., an underlying assumption is that cruises suffer from either no or a single and constant measurement bias. Adjustments for salinity, TCO<sub>2</sub>, TALK and pH are always additive, while adjustments for oxygen, nutrients and the halogenated transient tracers are always multiplicative. Except where explicitly noted (Sect. 3.3.1), adjustments were not changed for data previously included in GLODAPv2.2019.

335 Crossover comparisons, multi-linear regressions (MLRs), and comparison of deep-water averages were used to identify offsets for salinity, oxygen, nutrients, TCO<sub>2</sub>, TALK, and pH (Sect. 3.2.2 and 3.2.3). In contrast to GLODAPv2 and GLODAPv2.2019, evaluation of the internal consistency of the seawater CO<sub>2</sub> chemistry variables was not used for the evaluation of pH (Sect. 3.2.4). New to the present version is more extensive use of two predictions from two empirical algorithms—"Carbonate system And Nutrients concentration from hydrological properties and Oxygen using a Neural-network version B" (CANYON-B) and "CONsisTency EstimatioN and amount" (CONTENT), (Bittig et al., 2018)—for the evaluation of offsets in nutrients and seawater CO<sub>2</sub> chemistry data (Section 3.2.5). For the halogenated transient tracers, comparisons of surface saturation levels and the relationships among the tracers were used to assess the data

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355 consistency (Sect. 3.2.6). For salinity and oxygen, CTD and bottle values were merged into a “hybrid” variable prior to  
the consistency analyses (Sect. 3.2.1).

### 3.2.1 Merging of sensor and bottle data

360 Salinity and oxygen data can be obtained by analysis of water samples (bottle data) and/or directly from the CTD sensor  
pack. These two measurement types are merged and presented as a single variable in the product. The merging was  
conducted prior to the consistency checks, ensuring their internal calibration in the product. The merging procedures were  
only applied to the bottle data files, which commonly include values recorded by the CTD at the pressures where the  
water samples are collected. Whenever both CTD and bottle data were present in a data file, the merging step considered  
the deviation between the two and calibrated the CTD values if required and possible. Altogether seven scenarios are  
possible for each of the CTD-O<sub>2</sub> sensor properties individually, where the fourth (see below) never occurred during our  
365 analyses, but is included to maintain consistency with GLODAPv2:

1. No data are available: no action needed.
2. No bottle values are available: use CTD values.
3. No CTD values are available: use bottle values.
4. Too few data of both types are available for comparison and more than 80 % of the records have bottle values: use  
370 bottle values.
5. The CTD values do not deviate significantly from bottle values: replace missing bottle values with CTD values.
6. The CTD values deviate significantly from bottle values: calibrate CTD values using linear fit with respect to bottle  
data and replace missing bottle values with the so-calibrated CTD values.
7. The CTD values deviate significantly from bottle values, and no good linear fit can be obtained for the cruise: use  
375 bottle values and discard CTD values.

The number of cases encountered for each scenario is summarized in Sect. 4.1.

### 3.2.2 Crossover analyses

380 The crossover analyses were conducted with the MATLAB toolbox prepared by Lauvset and Tanhua (2015) and with the  
GLODAPv2.2019 data product as the reference data product. The toolbox implements the ‘running-cluster’ crossover  
analysis first described by Tanhua et al. (2010). This analysis compares data from two cruises on a station-by-station  
basis and calculates a weighted mean offset between the two and its weighted standard deviation. The weighting is based  
on the scatter in the data such that data that have less scatter have a larger influence on the comparison than data with  
more scatter. Whether the scatter reflects actual variability or data precision is irrelevant in this context as increased  
scatter nevertheless decreases the confidence in the comparison. Stations are compared when they are within 2° arc  
385 distance (~ 200 km) of each other. Only deep data are used to minimize the effects of natural variability. Either the 1500  
or 2000 dbar depth surface was used as upper bound, depending on the number of available data, their variation at  
different depths, and the region in question. This was evaluated on a case-by-case basis by comparing crossovers with  
both depth limits and using the one that provided the most clear and robust information. In regions where deep mixing or  
convection occurs, such as the Nordic, Irminger and Labrador seas, the upper bound was always placed at 2000 dbar,  
390 while winter mixing in the first two regions is normally not deeper than this (Brakstad et al., 2019; Frøb et al., 2016).  
convection beyond this limit has occasionally been observed in the Labrador Sea (Yashayaev and Loder, 2016). However,  
using an upper depth limit deeper than 2000 dbar will quickly give too few data for robust analysis. In addition, even

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below the deepest winter mixed layers properties do change over the time periods considered (e.g., Falck and Olsen, 2010), so this limit does not guarantee steady conditions. In the Southern Ocean deep convection beyond 2000 dbar seldom occurs, an exception being the processes accompanying the formation of the Weddell Polynya in the 1970s (Gordon, 1978). Deep and bottom water formation usually occurs along the Antarctic coasts, where relatively thin nascent dense water plumes flow down the continental slope. We cautiously avoid such cases, which are easily recognizable. In order to avoid removing persistent temporal trends, all crossover results are also evaluated as a function of time (see below).

As an example of crossover analysis, the crossover for TCO<sub>2</sub> measured on the two cruises 49UP20160109, which is new to this version, and 49UP20160703, which was included in GLODAPv2.2019, is shown in Fig. 3. For TCO<sub>2</sub> the offset is determined as the difference, as is the case for salinity, TALK, and pH. For the nutrients, oxygen, and the halogenated transient tracers, ratios are used. This is in accordance with the procedures followed for GLODAPv2. The TCO<sub>2</sub> values from 49UP20160109 are higher, with a weighed mean offset of  $3.62 \pm 2.67 \mu\text{mol kg}^{-1}$  compared to those measured on 49UP20160703.

For each of the 106 new cruises, such a crossover comparison was conducted against all possible cruises in GLODAPv2.2019, i.e., all cruises that had stations closer than 2° arc distance to any station for the cruise in question.

The summary figure for TCO<sub>2</sub> on 49UP20160109 is shown in Fig. 4. The TCO<sub>2</sub> data measured on this cruise are high by  $3.68 \pm 0.83 \mu\text{mol kg}^{-1}$  when compared to the data measured on nearby cruises included in GLODAPv2.2019. This is slightly less than the initial minimum adjustment limit for TCO<sub>2</sub> of  $4 \mu\text{mol kg}^{-1}$  (Table 3), but the offset is present against

all cruises and there is no obvious time trend (particularly important for TCO<sub>2</sub>), and as such qualifies for an adjustment of the data in the merged data product. In this case  $-3 \mu\text{mol kg}^{-1}$  was applied: this is somewhat less than indicated by the

crossover analysis, but a smaller adjustment is supported by the CANYON-B and CONTENT results (Sect. 3.2.5). Adjustments are typically round numbers relative to the precision of the variable being considered (e.g.,  $-3$  not  $-3.4$  for TCO<sub>2</sub> and  $0.005$  not  $0.0047$  for pH) to avoid the communicating that the ideal adjustments are known to high precision.

One exception to the above-described procedure exists, namely in the Sea of Japan where six new cruises were added. In this region, only two other cruises were included in GLODAPv2.2019. Therefore, all eight cruises were compared against

each other and strong outliers were adjusted accordingly, instead of adjusting the six new cruises towards the existing two.

### 3.2.3 Other consistency analyses

MLR analyses and deep water averages, broadly following Jutterström et al. (2010), were also used for the secondary QC of salinity, oxygen, nutrients, TCO<sub>2</sub>, and TALK data. These approaches are particularly valuable when a cruise has either very few or no valid crossovers with GLODAPv2, but are used more generally to provide more insight on the consistency of the data. The latter was the case for the 106 new cruises; i.e., no adjustment decisions were reached on the basis of

MLR and deep water average analyses alone. For the MLRs, the presence of bias in the data was identified by comparing the MLR-generated values with the measured values. Both analyses were conducted on samples collected deeper than the

1500 or 2000 dbar pressure level to minimize the effects of natural variations, and both used available GLODAPv2.2019 data from within 2° of the cruise in question to generate the MLR or deep water average. The lower depth limit was set to the deepest sample for the cruise in question. For the MLRs, all of the above-mentioned variables could be included among the independent variables (e.g., for a TALK MLR, salinity, oxygen, nutrients, and TCO<sub>2</sub> were allowed), with the

exact selection determined based on the statistical robustness of the fit, as evaluated using the coefficient of determination

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( $r^2$ ) and root mean square error (RMSE). MLRs based on variables that were suspect for the cruise in question were avoided (e.g., if oxygen appeared biased it was not included as an independent variable). The MLRs could be based on 10 to 500 samples, and the robustness of the fit ( $r^2$ , RMSE) and quantity of fitting data were considered when using the results to guide whether to apply a correction. The same applies for the deep-water averages (i.e., the standard deviation of the mean). MLR and deep-water average results showing offsets above the minimum adjustment limits were carefully scrutinized, along with [available](#), crossover [values](#) and CANYON-B and CONTENT [estimates](#), to determine whether or not to apply an adjustment.

### 3.2.4 pH scale conversion and quality control

Altogether 82 of the 106 new cruises included [measured](#) pH data. For one of these, the pH data were not supplied on the total scale or at 25 °C and 0 dbar pressure, which is the GLODAP standard, and were thus converted. The conversion was conducted using CO2SYS (Lewis and Wallace, 1998) for MATLAB (van Heuven et al., 2011) with reported pH and TALK as inputs, and generating pH output values at total scale at 25 °C and 0 dbar of pressure (named phts25p0 in the product). Missing TALK data were approximated as 67 times salinity. The proportionality (67) is the mean ratio of TALK to salinity in GLODAPv2 data. [The uncertainties introduced with this approximation are negligible \(order  \$10^{-7}\$  pH units\) for the scale conversions and order  \$10^{-3}\$  pH units for the temperature and pressure conversion \(evaluated by repeating conversions with 2 times the standard deviation of the ratio, i.e.,  \$67 \pm 4.1\$ \). This is sufficiently accurate relative to other sources of uncertainty, which are discussed below.](#) Data for phosphate and silicate are also needed, and were, whenever missing, determined using CANYON-B (Bittig et al., 2018). The conversion was conducted with the carbonate dissociation constants of Lueker et al. (2000), the bisulfate dissociation constant of Dickson (1990), and the borate-to-salinity ratio of Upström (1974). These procedures are the same as used for GLODAPv2.2019 (Olsen et al., 2019). [In contrast to past GLODAP pH QC, evaluation of the internal consistency of CO<sub>2</sub> system variables was not used for the secondary quality control of the pH data of the 106 new cruises, only crossover analysis was used, supplemented by CONTENT and CANYON-B \(Sect. 3.2.5\). Recent literature has demonstrated that internal consistency evaluation procedures are subject to errors, owing to incomplete understanding of the thermodynamic constants, major ion concentrations, measurement biases, and potential contribution of organic compounds or other unknown protolytes to alkalinity \(Takeshita et al., 2020\), which lead to pH dependent offsets in calculated pH \(Álvarez et al., 2020; Carter et al., 2018\); these may be interpreted as biases and generate false corrections. The offsets are particularly strong at pH levels below 7.7, when calculated and measured pH are different by on average between 0.01 and 0.02 units. For the North Pacific, this is a problem as pH values below 7.7 can occur at the depths interrogated during the QC \(>1500 dbar for this region, Olsen et al., 2016\). Since any corrections, which may thus be an artifact, are applied to the full profiles, we assign an uncertainty of 0.02 to the North Pacific pH data in the merged product files. Elsewhere, the uncertainties that have arisen are smaller, since deep pH is typically larger than 7.7 \(Lauvset et al., 2020\), and at such levels the difference between calculated and measured pH is less than 0.01 on average \(Álvarez et al., 2020; Carter et al., 2018\). Outside the North Pacific, we believe, therefore that the pH data are consistent to 0.01. Avoiding interconsistency considerations for these intermediate products helps to reduce the problem, but since the reference data set \(also as used for the generation of the CANYON-B and CONTENT algorithms\) has these issues, a full re-evaluation, envisioned for GLODAPv3, is needed to address the problem satisfactorily.](#)

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### 3.2.5 CANYON-B and CONTENT analyses

CANYON-B and CONTENT (Bittig et al., 2018) were used to support decisions regarding application of adjustments (or not). CANYON-B is a neural network for estimating nutrients and seawater CO<sub>2</sub> chemistry variables from temperature, salinity, and oxygen. CONTENT additionally considers the consistency among the estimated CO<sub>2</sub> chemistry variables to further refine them. These approaches were developed using the data included in the GLODAPv2 data product. Their advantage compared to crossover analyses for evaluating consistency among cruise data is that effects of water mass changes on ocean properties are represented in the non-linear relationships in the underlying neural network. For example, if elevated nutrient values are measured on a cruise but are not due to a measurement bias but actual aging of the water mass(es) that have been sampled and as such accompanied by a decrease in oxygen concentrations, the measured values and the CANYON-B estimates will be similar. Vice-versa, if the nutrient values are biased, the measured values and CANYON-B predictions will be dissimilar.

Used in the correct way and with caution this tool is a powerful supplement to the traditional crossover analyses.

Specifically, we gave no weight to comparisons where the crossover analyses had suggested that the S and/or O<sub>2</sub> data were biased as this would lead to error in the predicted values. We also considered the uncertainties of the CANYON-B and CONTENT estimates. These uncertainties are determined for each predicted value, and for each comparison the ratio of the difference (between measured and predicted values) to the local uncertainty was used to gauge the comparability.

As an example, the CANYON-B/CONTENT analyses of the data obtained at 49UP20160109 are presented in Fig. 5. The CANYON-B and CONTENT results confirmed the positive offset in the TCO<sub>2</sub> values revealed in the crossover comparisons discussed in Sect. 3.2.2. The magnitude of the inconsistency for the CANYON-B estimate was 3.4 μmol kg<sup>-1</sup>, i.e., slightly less than that the weighted mean crossover offset of 3.7 μmol kg<sup>-1</sup>, while the CONTENT estimate gave an inconsistency of 2.7 μmol kg<sup>-1</sup>. The differences between these consistency estimates owes to differences in the actual approach, the weighting across stations, stations considered (i.e., crossover comparisons use only stations within ~200 km of each other, while CANYON-B and CONTENT considers all stations where necessary variables are sampled, and depth range considered (> 500 dbar for CANYON-B and CONTENT vs. >1500/2000 dbar for crossovers). The specific difference between the CANYON-B and CONTENT estimates is a result of the seawater CO<sub>2</sub> chemistry considerations by the latter. For the other variables, the inconsistencies are low and agree with the crossover results (not shown here but results can be accessed through the Adjustment Table) with the exception of pH. The pH results are further discussed in Sect. 4.2.

Another advantage of CANYON-B and CONTENT is that these procedures provide estimates at the level of individual data points, e.g., pH values are determined for every sampling location and depth where T, S, and O<sub>2</sub> data are available. Cases of strong differences between measured and estimated values are always examined. This has helped to identify primary QC issues for some variables and cruises, for example a case of an inverted pH profile at cruise 32PO20130829, which has been amended.

### 3.2.6 Halogenated transient tracers

For the halogenated transient tracers (CFC-11, CFC-12, CFC-113, and CCl<sub>4</sub>; CFCs for short) inspection of surface saturation levels and evaluation of relationships between the tracers for each cruise were used to identify biases, rather than crossover analyses. Crossover analysis is of limited value for these variables given their transient nature and low concentrations at depth. As for GLODAPv2, the procedures were the same as those applied for CARINA (Jeansson et al., 2010; Steinfeldt et al., 2010).

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### 3.3 Merged product generation

The merged product file for GLODAPv2.2020 was created by correcting known issues in the GLODAPv2.2019 merged file, and then appending a merged and bias-corrected file containing the 106 new cruises to this error-corrected GLODAPv2.2019 file.

#### 3.3.1 Updates and corrections for GLODAPv2.2019

Several minor omissions and errors have been identified in the GLODAPv2 and v2.2019 data products since their release in 2016 and 2019, respectively. Most of these have been corrected in this release. In addition, some recently available data have been added for a few cruises. The changes are:

- For cruise 33RR20160208, the CFC-113 data of station 31 were found to be bad and have been removed. Additionally, the flags for CFC-11, CFC-12, SF<sub>6</sub> and CCl<sub>4</sub> were replaced with new ones received from the Principal Investigator, and recently published data for δ<sup>13</sup>C and Δ<sup>14</sup>C have been added to the product file.
- For 18HU20150504, the pH data measured at stations 196, 200, and 203 were found offset by approximately +0.1 units, because such large offset points to general data quality problems, these data have been removed.
- For 32PO20130829, pH values of station 133 cast 1 were in the wrong order in the file. This has been amended. Additionally, pH values from cast 2 at this station were deemed questionable and have been removed.
- For 33RR20050109, the δ<sup>13</sup>C values of station 7 bottle 32 and station 16 bottle 22 were found bad (values were less than -6 ‰) and have been removed from the product file.
- For 35MF19850224, the δ<sup>13</sup>C value of station 21 cast 3 bottle 4 was found bad and has been removed.
- For 74JC20100319 the δ<sup>13</sup>C value at station 37 bottle 7 was found bad and has been removed.
- All δ<sup>13</sup>C values from the large volume Gerard barrels (identified by bottle number greater than 80) were removed from the product files as these [values](#) often have poor precision and accuracy related to gas extraction procedures.
- For 33HQ20150809, temperatures of station 52 cast 1 were found bad (less than -2 °C) and have been removed, hence all other samples were removed for this cast as well (the same depths and variables were sampled at the other casts, however). Temperatures for casts 2 and 8 were replaced with updated values; these changes are very minor, on the order of 0.001 °C.
- For cruises 33RO20110926, 33RO20150525, and 33RO20150410, δ<sup>13</sup>C and Δ<sup>14</sup>C data have become available and [were](#) added to the product.
- Ship code for all RV *Maria S. Merian* cruises have been changed from MM to M2.
- For cruises 49SH20081021 and 49UF20121024, an adjustment of + 6 μmol kg<sup>-1</sup> is now applied to the TCO<sub>2</sub> values.
- Additional primary QC have been applied to the cruises with *Keifu Maru II* and *Ryofu Maru III* that were included in GLODAPv2.2019.
- [Neutral density values in GLODAPv2 and GLODAPv2.2019 had been calculated using the polynomial approximation of Sérazin \(2011\). All of these values were replaced with neutral density calculated following Jackett and McDougall \(1997\).](#)
- Discrete *f*CO<sub>2</sub> data are now included in the product files whenever available. Discrete *f*CO<sub>2</sub> is one of the variables that [describe](#) seawater CO<sub>2</sub> chemistry, but is rarely measured and has not been included in GLODAP product files before, in particular as a result of apparent quality issues that were not fully understood during the secondary QC

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655 | for GLODAPv1.1 (Sabine et al., 2005). However, for some cruises  $f\text{CO}_2$  data were included indirectly in both  
GLODAPv1.1 and GLODAPv2 as they had been used in combination with  $\text{TCO}_2$  to calculate TALK. We have now  
chosen to include the discrete  $f\text{CO}_2$  values in the product files. This increases transparency and traceability of the  
product; the  $f\text{CO}_2$  data are also highly relevant for ongoing efforts toward resolving recently identified  
inconsistencies in our understanding of the relationships among the seawater  $\text{CO}_2$  chemistry variables (Carter et  
660 | al., 2018; Fong and Dickson, 2019; Takeshita et al., 2020; Álvarez et al., 2020). A total of 33 924 discrete  $f\text{CO}_2$   
measurements from 34 cruises conducted between 1983-2014 are now included. All values were converted to 20°  
C and 0 dbar pressure using CO2SYS for MATLAB (van Heuven et al., 2011). This was also used for the  
conversion of partial pressure of  $\text{CO}_2$  ( $p\text{CO}_2$ ) to  $f\text{CO}_2$  for the 20 cruises where  $p\text{CO}_2$  was reported. The procedures  
for these conversions, in terms of dissociation constants and approximation of missing variables, were the same as  
for the pH conversions (Sect. 3.2.4). These  $f\text{CO}_2$  data have not been subjected to secondary QC. The inclusion of  
665 | discrete  $f\text{CO}_2$  data has led to some changes in the calculations of missing seawater  $\text{CO}_2$  chemistry variables; these  
are described towards the end of the next section.

### 3.3.2 Merging

The new data were merged into a bias-minimized product file following the procedures used for GLODAPv1.1 (Key et  
al., 2004; Sabine et al., 2005), CARINA (Key et al., 2010), PACIFICA (Suzuki et al., 2013), GLODAPv2 (Olsen et al.,  
670 | 2016), and GLODAPv2.2019 (Olsen et al., 2019), with some modifications:

- Data from the 106 new cruises were merged and sorted according to EXPCODE, station, and pressure. GLODAP cruise numbers were assigned consecutively, starting from 2001, so they can be distinguished from the GLODAPv2.2019 cruises that ended at 1116.
- For some cruises the combined concentration of nitrate and nitrite was reported instead of nitrate. If explicit nitrite concentrations were also given, these were subtracted to get the nitrate values. If not, the combined concentration was renamed to nitrate. As nitrite concentrations are very low in the open ocean, this has no practical implications.
- When bottom depths were not given, they were approximated as the deepest sample pressure +10 dbar or extracted from ETOPO1 (Amante and Eakins, 2009), whichever was greater. For GLODAPv2, bottom depths were extracted from the Terrain Base (National Geophysical Data Center/NESDIS/NOAA/U.S. Department of Commerce, 1995). The intended use of this variable is only drawing approximate bottom topography for sections.
- Whenever temperature was missing in the original data file, all data for that record were removed and their flags set to 9. The same was done when both pressure and depth were missing. For all surface samples collected using buckets or similar, the bottle number was set to zero. There are some exceptions to this, in particular for cruises that also used Gerard barrels for sampling. These may have valuable tracer data that are not accompanied by a temperature, so such data have been retained.
- All data with WOCE quality flags 3, 4, 5, or 8 were excluded from the product files and their flags set to 9. Hence, in the product files a flag 9 can indicate not measured (as is also the case for the original exchange formatted data files) or excluded from the product; in any case, no data value appears. All flags 6 (replicate measurement) and 7 (manual chromatographic peak measurement) were set to 2, provided the data appeared good.
- Missing sampling pressures (depths) were calculated from depths (pressures) following UNESCO (1981).
- For both oxygen and salinity, CTD and bottle values were merged following procedures summarized in Sect. 3.2.1.

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- Missing salinity, oxygen, nitrate, silicate, and phosphate values were vertically interpolated whenever practical, using a quasi-Hermetian piecewise polynomial. “Whenever practical” means that interpolation was limited to the vertical data separation distances given in Table 4 in Key et al. (2010). Interpolated salinity, oxygen, and nutrient values have been assigned a WOCE quality flag 0.
- The data for the 12 core variables were corrected for bias using the adjustments determined during the secondary QC.
- Values for potential temperature and potential density anomalies (referenced to 0, 1000, 2000, 3000, and 4000 dbar) were calculated using Fofonoff (1977) and Bryden (1973). Neutral density was calculated using Jackett and McDougall (1997), thus neutral density for all 946 cruises are calculated using this procedure
- Apparent oxygen utilization was determined using the combined fit in Garcia and Gordon (1992).
- Partial pressures for CFC-11, CFC-12, CFC-113, CCl<sub>4</sub>, and SF<sub>6</sub> were calculated using the solubilities by Warner and Weiss (1985), Bu and Warner (1995), Bullister and Wisegarver (1998), and Bullister et al. (2002).
- Missing seawater CO<sub>2</sub> chemistry variables were calculated, whenever possible. The procedures for these calculations have been slightly altered as the product now contains four such variables; earlier versions of GLODAPv2 (Olsen et al., 2016; Olsen et al., 2019) included only three, so whenever two were included the one to calculate was unequivocal. Four CO<sub>2</sub> chemistry variables gives more degrees of freedom in this respect, e.g., a particular record may have measured data for TCO<sub>2</sub>, TAlk, and pH, and then a choice needs to be made with regard to which pair to use for the calculation of *f*CO<sub>2</sub>. We followed two simple principles. First, TCO<sub>2</sub> and TAlk was the preferred pair to calculate pH and *f*CO<sub>2</sub>, because we have higher confidence in the TCO<sub>2</sub> and TAlk data than pH (given the issues summarized in Sect. 3.2.4) and *f*CO<sub>2</sub> (because it was not subjected to secondary QC). Second, if either TCO<sub>2</sub> or TAlk was missing and both pH and *f*CO<sub>2</sub> data existed, pH was preferred (because *f*CO<sub>2</sub> has not been subjected to secondary QC). All other combinations, involve only two measured variables. The calculations were conducted using CO2SYS (Lewis and Wallace, 1998) for MATLAB (van Heuven et al., 2011), with the constants set as for the pH conversions (Sect. 3.2.4). For calculations involving TCO<sub>2</sub>, TAlk, and pH, if less than a third of the total number of values, measured and calculated combined, for a specific cruise were measured, then all these were replaced by calculated values. The reason for this is that secondary QC of the few measured values was often not possible in such cases, for example due to a limited number of deep data available. Such replacements were not done for calculations involving *f*CO<sub>2</sub>, as this would either overwrite all measured *f*CO<sub>2</sub> values or would entail replacing a measured variable that has been subjected to secondary QC (i.e., TCO<sub>2</sub>, TAlk, or pH) with one calculated from a variable that has not been subjected to secondary QC (i.e., *f*CO<sub>2</sub>). Calculated seawater CO<sub>2</sub> chemistry values have been assigned WOCE flag 0. Seawater CO<sub>2</sub> chemistry values have not been interpolated, so the interpretation of the 0 flag is unique.
- The resulting merged file for the 106 new cruises was appended to the merged product file for GLODAPv2.2019.

#### 4 Secondary quality control results and adjustments

All material produced during the secondary QC is available via the online GLODAP Adjustment Table hosted by GEOMAR, Kiel, Germany at <https://glodapv2-2020.geomar.de/> (last access: 18 June 2020), and which can also be accessed through [www.glodap.info](http://www.glodap.info). This is similar in form and function to the GLODAPv2 Adjustment Table (Olsen et al., 2016) and includes a brief written justification for any adjustments applied.

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#### 4.1 Sensor and bottle data merge for salinity and oxygen

Table 4 summarizes the actions taken for the merging of the CTD and bottle data for salinity and oxygen. For 81 % of the 106 cruises added with this update, both CTD and bottle data were included for salinity in the original cruise data files and for all these cruises the two data types were found to be consistent. This is similar to the GLODAPv2.2019 results. For oxygen, only 25 % of the cruises included both CTD O<sub>2</sub> and bottle values; this is much less than for GLODAPv2.2019 where 50 % of the cruises included both. Having both CTD and bottle values in the data files is highly preferred as the information is valuable for quality control (bottle mistrips, leaking Niskin bottles, and oxygen sensor drift are among the issues that can be revealed). The extent to which the bottle data (i.e., OXYGEN in the individual cruise exchange files) in reality is mislabeled CTD data (i.e., should be CTDOXY) is uncertain. Regardless, the large majority of the CTD and bottle oxygen were consistent and did not need any further calibration of the CTD values (23 out of 25 cruises), while for two cruises no good fit could be obtained and their CTD O<sub>2</sub> data are not included in the product.

#### 4.2 Adjustment summary

The secondary QC has 5 different outcomes, provided there are data. These are summarized in Table 5, along with the corresponding codes that appear in the online Adjustment Table and that are also occasionally used as shorthand for decisions in the coming text. The level of secondary QC varies among the cruises. Specifically, in some cases data were too shallow or geographically too isolated for full and conclusive consistency analyses. A secondary QC flag has been included in the merged product files to enable their identification, with “0” used for variables and cruises not subjected to full secondary QC (corresponding to code -888 in Table 5) and “1” for variables and cruises that were subjected to full secondary QC. The secondary QC flags are assigned per cruise and variable, not for individual data points and are independent of—and included in addition to—the primary (WOCE) QC flag. For example, interpolated (salinity, oxygen, nutrients) or calculated (TCO<sub>2</sub>, TALK, pH) values, which have a primary QC flag 0, may have a secondary QC flag of 1 if the measured data these values are based on have been subjected to full secondary QC. Conversely, individual data points may have a secondary QC flag of 0, even if their primary QC flag is 2 (good data). A 0 flag means that data were too shallow or geographically too isolated for consistency analyses or that these analyses were inconclusive, but that we have no reasons to believe that the data in question are of poor quality. Prominent examples for this version are the 10 new Davis Strait cruises: no data were available in this region in GLODAPv2.2019, which, combined with complex hydrography and differences in sampling locations, rendered conclusive secondary QC impossible. As a consequence, most, but not all, of these data (some being excluded because of poor precision after consultation with the PI) are included with a secondary QC flag of 0.

The secondary QC actions for the 12 core variables and the distribution of applied adjustments are summarized in Table 6, and Fig. 6, respectively. For most variables, only a very small fraction of the data are adjusted: no salinity data, 1 % of oxygen and nitrate data, 2 % of TCO<sub>2</sub> data, 5 % of TALK data, 7 % of phosphate data, and 9 % of silicate data are adjusted. For the CFCs, data from one of 16 cruises with CFC-11 are adjusted, while for CFC-12 and CFC-113 the fractions are two of 21 cruises and one of three cruises respectively. The magnitudes of the various adjustments applied are also small, overall. Thus, the tendency observed during the production of GLODAPv2.2019 remains, namely, that the large majority of recent cruises are consistent with earlier releases of this product.

For the Sea of Japan cruises, (where two existed in GLODAPv2.2019 and six were added in this version - Sect. 3.2.2), the crossover results showed biased TCO<sub>2</sub> data for one of the older cruises (49HS20081021, which is now adjusted up by 6

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umol kg<sup>-1</sup>), and biased TALK data for two of the presently added cruises (49UF20111004 and 49UF20121024, adjusted up by 5 and 6 umol kg<sup>-1</sup>, respectively)

The quality control of pH data proved challenging for this version. The large majority of new pH data had been collected in the northwestern Pacific on cruises conducted by the Japan Meteorological Agency. Figure 7 shows the distribution of pH crossover offsets vs. GLODAPv2.2019. Most of the pH values are higher, some by up to 0.02 pH units; this is considerable, particularly as the data that are compared are from deeper than 2000 dbar where no changes due to ocean acidification are expected. The challenging aspect lies in the fact that the data added are comparatively many (~ 70 cruises vs. ~ 130 already included in this region in v2.2019) and also are more recent (2010-2018 vs. 1993-2016). As such they might be of higher quality given advances in pH measurement techniques over the years. Adjusting a large fraction of the new cruises down (following the adjustment limit of 0.01) is not advisable. We therefore chose to not adjust any pH data, but to exclude the most serious outliers from the product file (using a limit of |0.015|, which led to exclusion of pH data from five cruises), and include the rest of the data without adjustments. We expect that a crossover and inversion analysis of all pH data in the northwestern Pacific will provide more information on the consistency among the cruises, and such an analysis will be conducted for the next update. For now, some caution should be exercised if looking at trends in ocean pH in the northwestern Pacific using GLODAPv2.2020. The crossover and inversion might also result in re-inclusion of the excluded data. The formal decision for the excluded outliers is therefore to “suspend” them (Table 6).

For the nutrients, adjustments were applied to maintain consistency with data included in GLODAPv2 and GLODAPv2.2019. An alternative goal for the adjustments would be maintaining consistency with data from cruises that employed CRMNS to ensure accuracy of nutrient analyses. Such a strategy was adopted by Aoyama (2020) for preparation of the Global Nutrients Dataset 2013 (GND13), and is being considered for GLODAP as well. However, as this would require a re-evaluation of the entire data set, this will not occur until the next full update of GLODAP, i.e., GLODAPv3. For now, we note the overall agreement between the adjustments applied in these two efforts (Aoyama, 2020), and that most disagreements appear to be related to cases where no adjustments were applied in GLODAP. This can be related to the strategy followed for nutrients for GLODAPv2, where data from GO-SHIP lines were considered a priori more accurate than other data. CRMNS are used for nutrients on most GO-SHIP lines.

The improvement in data consistency due to the secondary QC process is evaluated by comparing the weighted mean of the absolute offsets for all crossovers before and after the adjustments have been applied. This “consistency improvement” for core variables is presented in Table 7. The data for CFCs were omitted from these analyses for previously discussed reasons (Sect. 3.2.6). Globally, the improvement is modest. Considering the initial data quality, this result was expected. However, this does not imply that the data initially were consistent everywhere. Rather, for some regions and variables there are substantial improvements when the adjustments are applied. For example, Arctic Ocean phosphate, Indian Ocean silicate and TALK, and Pacific Ocean pH data all show considerable improvements. For the latter, the improvement is a result of exclusion of data and not application of adjustments, as discussed above.

The various iterations of GLODAP provide insight into initial data quality covering more than 4 decades. Figure 8 summarizes the applied absolute adjustment magnitude per decade. These distributions are broadly unchanged compared to GLODAPv2.2019 (Fig. 6 in Olsen et al., 2019). Most TCO<sub>2</sub> and TALK data from the 1970s needed an adjustment, but this fraction steadily declines until only a small percentage is adjusted in recent years. This is encouraging and demonstrates the value of standardizing sampling and measurement practices (Dickson et al., 2007), the widespread use of CRMs (Dickson et al., 2003), and instrument automation. The pH adjustment frequency also has a downward trend;

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880 however, there remain issues with the pH adjustments and this is a topic for future development in GLODAP, with the support from the OCB Ocean Carbonate System Intercomparison Forum (OCSIF, <https://www.us-ocb.org/ocean-carbonate-system-intercomparison-forum/>, last accessed: 20 June 2020) working group (Álvarez et al., 2020). For the nutrients and oxygen, only the phosphate adjustment frequency decreases from decade to decade. However, we do note that the more recent data from the 2010s receive the fewest adjustments. This may reflect recent increased attention that seawater nutrient measurements have received through an operation manual (Becker et al., 2019; Hydes et al., 2012) availability of CRMNS (Aoyama et al., 2012; Ota et al., 2010), and the SCOR working group #147, Towards comparability of global oceanic nutrient data (COMPONUT). For silicate, the fraction of cruises receiving adjustments peaks in the 1990s and 2000s. This is related to the 2 % offset between US and Japanese cruises in the Pacific Ocean that was revealed during production of GLODAPv2 and discussed in Olsen et al. (2016). For salinity and the halogenated transient tracers, the number of adjusted cruises is small in every decade.

## 5 Data availability

890 The GLODAPv2.2020 merged and adjusted data product is archived at NOAA NCEI under <https://doi.org/10.25921/2c8h-sa89> (Olsen et al., 2020). These data and ancillary information are also available via our web pages <https://www.glodap.info> and [https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2\\_2020/](https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2_2020/) (last access: 22 June 2020). The data are available as comma-separated ascii files (\*.csv) and as binary MATLAB files (\*.mat) that use the open-source Hierarchical Data Format version 5 (HDF5) data format. Regional subsets are available for the Arctic, Atlantic, Pacific, and Indian oceans. There are no data overlaps between regional subsets and each cruise exists in only one basin file even if data from that cruise crosses basin boundaries. The station locations in each basin file are shown in Fig. 9. The product file variables are listed in Table 1. A lookup table for matching the EXPCODE of a cruise with GLODAP cruise number is provided with the data files. In the MATLAB files this information is available as a cell array. A “known issues document” accompanies the data files and provides an overview of known errors and omissions in the data product files. It is regularly updated, and users are encouraged to inform us whenever any new issues are identified. It is critical that users consult this document whenever the data products are used.

900 The original cruise files are available through the GLODAPv2.2020 cruise summary table (CST) hosted by NOAA NCEI: [https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2\\_2020/](https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2_2020/) (Last access: 22 June 2020). Each of these files has been assigned a doi, but these are not listed here. The CST also provides brief information on each cruise and access to metadata, cruise reports, and its Adjustment Table entry.

905 While GLODAPv2.2020 is made available without any restrictions, users of the data should adhere to the fair data use principles:

For investigations that rely on a particular (set of) cruise(s), recognize the contribution of GLODAP data contributors by at least citing the articles where the data are described and, preferably, contacting principal investigators for exploring opportunities for collaboration and co-authorship. To this end, relevant articles and principal investigator names are provided in the cruise summary table. Contacting principal investigators comes with the additional benefit that the principal investigators often possess expert insight into the data and/or particular region under investigation. This can improve scientific quality and promote data sharing.

910 This paper should be cited in any scientific publications that result from usage of the product. Citations provide the most efficient means to track use, which is important for attracting funding to enable the preparation of future updates.

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## 6 Summary

930 GLODAPv2.2020 is an update of GLODAPv2.2019. Data from 106 new cruises have been added to supplement the earlier release and extend temporal coverage by 2 years. GLODAP now includes 47 years, 1972–2019, of global interior ocean biogeochemical data from 946 cruises.

935 The total number of data records are 1 275 558. Records with measurements for all 12 core variables, salinity, oxygen, nitrate, silicate, phosphate, TCO<sub>2</sub>, TAlk, pH, CFC-11, CFC-12, CFC-113, and CCl<sub>4</sub> are very rare; only 2026 records have measured data for all 12 in the merged product file (interpolated and calculated data excluded). Requiring only two measured seawater CO<sub>2</sub> chemistry variables in addition to all the other core variables brings the number of available records up to 9 230, so this is also very rare. A major limiting factor is simultaneous availability of data for all four freon species, only 26 277 records have measurements of CFC-11, CFC-12, CFC-113, and CCl<sub>4</sub> while 400 587 have data for at least one of these (not considering availability of other core variables). A total of 398 757 records have measured data for two out of the three CO<sub>2</sub> chemistry core variables. The number of measured fCO<sub>2</sub> data are 33 924; note that these data were not subjected to quality control. The number of records with measured data for salinity, oxygen, and nutrients are 940 798 703, while the number of records with salinity and oxygen data are 1 077 859. All of these numbers are for measured data, not interpolated or calculated values.

945 Figure 10 illustrates the seasonal distribution of the data. As for previous versions there is a bias around summertime in the data in both hemispheres; most data are collected during April through November in the Northern Hemisphere while most data are collected during November through April in the Southern Hemisphere. These tendencies are strongest for the poleward regions and reflect the harsh conditions during winter months, which make fieldwork difficult. Figure 11 illustrates the distribution of data with depth. The upper 100 m is the best sampled part of the global ocean, both in terms of number (Fig. 11a) and density (Fig. 11b) of observations. The number of observations steadily declines with depth. In part, this is caused by the reduction of ocean volume towards greater depths. Below 1000 m the density of observations stabilizes and even increases between 5000 and 6000 m; the latter is a zone where the volume of each depth surface decreases sharply (Weatherall et al., 2015). In the deep trenches, i.e., areas deeper than ~ 6000 m, both number and density of observations are low.

955 Except for salinity and oxygen, the core data were collected exclusively through chemical analyses of individually collected water samples. The data of the 12 core variables, were subjected to primary quality control to identify questionable or bad data points (outliers) and secondary quality control to identify systematic measurement biases. The data are provided in two ways: as a set of individual exchange-formatted original cruise data files with assigned WOCE flags, and as globally and regionally merged data product files with adjustments applied to the data according to the outcome of the consistency analyses. Importantly, no adjustments were applied to data in the individual cruise files while primary-QC changes were applied.

960 The consistency analyses were conducted by comparing the data from the 106 new cruises to GLODAPv2.2019. Adjustments were only applied when the offsets were believed to reflect biases relative to the earlier data product release related to measurement, calibration, and/or data handling practices, and not to natural variability or anthropogenic trends.

965 The Adjustment Table at <https://glodapv2-2020.geomar.de/> (last access: 18 June 2020) lists all applied adjustments and provides a brief justification for each. The consistency analyses rely on deep ocean data (>1500 or 2000 dbar depending on region), but supplementary CANYON-B and CONTENT analyses consider data below 500 dbar. Data consistency for cruises with exclusively shallow sampling was not examined. No pH data were adjusted for this version, but we note that

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975 this is largely a consequence of problems in establishing a reasonable pH baseline level in the deep northwest Pacific  
(Sect. 4.2). A comprehensive analysis of all available pH data in that region should be conducted for the next update.

Secondary QC flags are included for the 12 core variables in the product files. These flags indicate whether (1) or not (0) the data successfully received secondary QC. A secondary QC flag of 0 does not by itself imply that the data are of lower quality than those with a flag of 1. It means these data have not been as thoroughly checked. For  $\delta^{13}\text{C}$ , the QC results by Becker et al. (2016) for the North Atlantic were applied, and a secondary QC flag was therefore added to this variable.

980 The primary WOCE QC flags in the product files are simplified (e.g., all questionable and bad data were removed). For salinity, oxygen, and the nutrients, any data flagged 0 are interpolated rather than measured. For  $\text{TCO}_2$ , TALK, pH, and  $f\text{CO}_2$  any data flags of 0 indicate that the values were calculated from two other measured seawater  $\text{CO}_2$  variables. Finally, while questionable (WOCE flag =3) and bad (WOCE flag =4) data have been excluded from the product files, some may have gone unnoticed through our analyses. Users are encouraged to report on any data that appear suspicious.

985 Based on the initial minimum adjustment limits and the improvement of the consistency resulting from the adjustments (Table 7), the data subjected to consistency analyses are believed to be consistent to better than 0.005 in salinity, 1 % in oxygen, 2 % in nitrate, 2 % in silicate, 2 % in phosphate, 4  $\mu\text{mol kg}^{-1}$  in  $\text{TCO}_2$ , 4  $\mu\text{mol kg}^{-1}$  in TALK, and 5 % for the halogenated transient tracers. For pH, the consistency among all data is estimated as 0.01–0.02, depending on region. As mentioned above, the included  $f\text{CO}_2$  data have not been subjected to quality control, therefore no uncertainty estimate is given for this variable. This should be conducted in future efforts.

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## 7 Author contributions.

AO and TT led the team that produced this update. RMK, AK, and BP compiled the original data files. NL conducted the secondary QC analyses. HCB conducted the CANYON-B and CONTENT analyses. CS manages the Adjustment Table e-infrastructure. AK maintains the GLODAPv2 webpages at NCEI/OCADS while CSL maintains www.glodap.info. PM prepared PYTHON scripts for the merging of the data. All authors contributed to the interpretation of the secondary QC results and decisions on whether to apply actual adjustments. Many conducted ancillary QC analyses. AO wrote the manuscript with input from all authors.

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## 8 Competing interests

The authors declare that they have no competing interests.

## 1000 9 Acknowledgements

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**Table 1.** Variables in the GLODAPv2.2020 comma separated (csv) product files, their units, short and flag names, and corresponding names in the individual cruise exchange files. In the MATLAB product files that are also supplied a "G2" has been added to every variable name.

Variable	Units	Product file name	WOCE flag name <sup>a</sup>	2nd QC flag name <sup>b</sup>	Exchange file name
Assigned sequential cruise number		cruise			
Station		station			STANBR
Cast		cast			CASTNO
Year		year			DATE
Month		month			DATE
Day		day			DATE
Hour		hour			TIME
Minute		minute			TIME
Latitude		latitude			LATITUDE
Longitude		longitude			LONGITUDE
Bottom depth	m	bottomdepth			
Pressure of the deepest sample	dbar	maxsampdepth			DEPTH
Niskin bottle number		bottle			BTLNBR
Sampling pressure	dbar	pressure			CTDPRS
Sampling depth	m	depth			
Temperature	°C	temperature			CTDTMP
potential temperature	°C	theta			
Salinity		salinity	salinityf	salinityqc	CTDSAL/SALNTY
Potential density anomaly	kg m <sup>-3</sup>	sigma0	(salinityf)		
Potential density anomaly, ref 1000 dbar	kg m <sup>-3</sup>	sigma1	(salinityf)		
Potential density anomaly, ref 2000 dbar	kg m <sup>-3</sup>	sigma2	(salinityf)		
Potential density anomaly, ref 3000 dbar	kg m <sup>-3</sup>	sigma3	(salinityf)		
Potential density anomaly, ref 4000 dbar	kg m <sup>-3</sup>	sigma4	(salinityf)		
Neutral density anomaly	kg m <sup>-3</sup>	gamma	(salinityf)		
Oxygen	μmol kg <sup>-1</sup>	oxygen	oxygenf	oxygenqc	CTDOXY/OXYGEN
Apparent oxygen utilization	μmol kg <sup>-1</sup>	aou	aouf		
Nitrate	μmol kg <sup>-1</sup>	nitrate	nitratef	nitrateqc	NITRAT
Nitrite	μmol kg <sup>-1</sup>	nitrite	nitritef		NITRIT
Silicate	μmol kg <sup>-1</sup>	silicate	silicatef	silicateqc	SILCAT
Phosphate	μmol kg <sup>-1</sup>	phosphate	phosphatef	phosphateqc	PHSPHT
TCO <sub>2</sub>	μmol kg <sup>-1</sup>	tco2	tco2f	tco2qc	TCARBON
TAlk	μmol kg <sup>-1</sup>	talk	talkf	talkqc	ALKALI
pH on total scale, 25° C and 0 dbar of pressure		phts25p0	phts25p0f	phtsqc	PH_TOT

Variable	Units	Product file name	WOCE flag name <sup>a</sup>	2nd QC flag name <sup>b</sup>	Exchange file name
pH on total scale, in situ temperature and pressure		phtsinsitup	phtsinsitupf	phtsqc	
$f_{\text{CO}_2}$ at 20° C and 0 dbar of pressure	µatm	fco2	fco2f		FCO2/PCO2
$f_{\text{CO}_2}$ temperature <sup>c</sup>	°C	fco2temp	(fco2f)		FCO2_TMP/PCO2_TMP
CFC-11	pmol kg <sup>-1</sup>	cfc11	cfc11f	cfc11qc	CFC-11
pCFC-11	ppt	pcfc11	(cfc11f)		
CFC-12	pmol kg <sup>-1</sup>	cfc12	cfc12f	cfc12qc	CFC-12
pCFC-12	ppt	pcfc12	(cfc12f)		
CFC-113	pmol kg <sup>-1</sup>	cfc113	cfc113f	cfc113qc	CFC-113
pCFC-113	ppt	pcfc113	(cfc113f)		
CCl <sub>4</sub>	pmol kg <sup>-1</sup>	ccl4	ccl4f	ccl4qc	CCL4
pCCl <sub>4</sub>	ppt	pccl4	(ccl4f)		
SF <sub>6</sub>	fmol kg <sup>-1</sup>	sf6	sf6f		SF6
psF6	ppt	psf6	(sf6f)		
δ <sup>13</sup> C	‰	c13	c13f	c13qc	DELC13
Δ <sup>14</sup> C	‰	c14	c14f		DELC14
Δ <sup>14</sup> C counting error	‰	c14err			C14ERR
<sup>3</sup> H	TU	h3	h3f		TRITIUM
<sup>3</sup> H counting error	TU	h3err			TRITER
δ <sup>3</sup> He	‰	he3	he3f		DELHE3
<sup>3</sup> He counting error	‰	he3err			DELHER
He	nmol kg <sup>-1</sup>	he	hef		HELIUM
He counting error	nmol kg <sup>-1</sup>	heerr			HELIER
Ne	nmol kg <sup>-1</sup>	neon	neonf		NEON
Ne counting error	nmol kg <sup>-1</sup>	neonerr			NEONER
δ <sup>18</sup> O	‰	o18	o18f		DELO18
Total organic carbon	µmol L <sup>-1 d</sup>	toc	tocf		TOC
Dissolved organic carbon	µmol L <sup>-1 d</sup>	doc	docf		DOC
Dissolved organic nitrogen	µmol L <sup>-1 d</sup>	don	donf		DON
Dissolved total nitrogen	µmol L <sup>-1 d</sup>	tdn	tdnf		TDN
Chlorophyll <i>a</i>	µg kg <sup>-1 d</sup>	chl <sub>a</sub>	chl <sub>a</sub> f		CHLORA

1220 <sup>a</sup>The only derived variable assigned a separate WOCE flag is AOU as it depends strongly on both temperature and oxygen (and less strongly on salinity). For the other derived variables, the applicable WOCE flag is given in parenthesis. <sup>b</sup>Secondary QC flags indicate whether data have been subjected to full secondary QC (1) or not (0), as described in Sect. 3. <sup>c</sup>Included for clarity, is 20 °C for all occurrences. <sup>d</sup>Units have not been checked; some values in micromoles per kilogram (for TOC, DOC, DON, TDN) or microgram per liter (for Chl *a*) are probable.

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**Table 2.** WOCE flags in GLODAPv2.2020 exchange format original data files ([briefly; for full details see Swift, 2010](#)) and the simplified scheme used in the merged product files.

WOCE Flag Value	Interpretation	
	Original data exchange files	Merged product files
0	Flag not used	Interpolated or calculated value
1	Data not received	Flag not used <sup>a</sup>
2	Acceptable	Acceptable
3	Questionable	Flag not used <sup>b</sup>
4	Bad	Flag not used <sup>b</sup>
5	Value not reported	Flag not used <sup>b</sup>
6	Average of replicate	Flag not used <sup>c</sup>
7	Manual chromatographic peak measurement	Flag not used <sup>c</sup>
8	Irregular digital peak measurement	Flag not used <sup>b</sup>
9	Sample not drawn	No data

<sup>a</sup>Flag set to 9 in product files

<sup>b</sup>Data are not included in the GLODAPv2.2020 product files and their flags set to 9.

<sup>c</sup>Data are included, but flag set to 2

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Table 3. Initial minimum adjustment limits.

Variable	Minimum Adjustment
Salinity	0.005
Oxygen	1 %
Nutrients	2 %
TCO <sub>2</sub>	4 $\mu\text{mol kg}^{-1}$
TAlk	4 $\mu\text{mol kg}^{-1}$
pH	0.01
CFCs	5 %

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**Table 4.** Summary of salinity and oxygen calibration needs and actions; number of cruises with each of the scenarios identified.

Case	Description	Salinity	Oxygen
1	No data are available: no action needed.	0	8
2	No bottle values <del>are available</del> ; use CTD values.	20	5
3	No CTD values <del>are available</del> ; use bottle values.	0	67
4	Too few data of both types <del>are available</del> for comparison and >80% of <del>the</del> records have bottle values: use bottle values.	0	0
5	The CTD values do not deviate significantly from bottle values: replace missing bottle values with CTD values.	86	23
6	The CTD values deviate significantly from bottle values: calibrate <del>CTD values</del> using linear fit and replace missing bottle values with calibrated CTD values.	0	1
7	The CTD values deviate significantly from bottle values, and no good linear fit can be obtained for the cruise: use bottle values and discard CTD values.	0	2

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**Table 5: Possible outcomes of the secondary QC and their codes in the online Adjustment Table**

<u>Secondary QC result</u>	<u>Code</u>
<u>The data are of good quality, consistent with the rest of the dataset and should not be adjusted.</u>	<u>0/1*</u>
<u>The data are of good quality but are biased: adjust by adding (for salinity, TCO<sub>2</sub>, TAlk, pH) or by multiplying (for oxygen, nutrients, CFCs) the adjustment value</u>	<u>Adjustment value</u>
<u>The data have not been QC'd, are of uncertain quality, and suspended until full secondary QC has been carried out</u>	<u>-666</u>
<u>The data are of poor quality and excluded from the data product.</u>	<u>-777</u>
<u>The data appear of good quality but their nature, being from shallow depths, coastal regions, without crossovers or similar, prohibits full secondary QC</u>	<u>-888</u>
<u>No data exist for this variable for the cruise in question</u>	<u>-999</u>
<u>*The value of 0 is used for variables with additive adjustments (salinity, TCO<sub>2</sub>, TAlk, pH) and 1 for variables with multiplicative adjustments (for oxygen, nutrients, CFCs). This is mathematically equivalent to 'no adjustment' in each case</u>	

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**Table 6.** Summary of secondary QC results for the 106 new cruises, in number of cruises per result and per variable.

	Sal.	Oxy.	NO <sub>3</sub>	Si	PO <sub>4</sub>	TCO <sub>2</sub>	TAlk	pH	CFC-11	CFC-12	CFC-113	CCl <sub>4</sub>
With data	106	101	97	97	97	92	96	82	16	21	3	0
No data	0	5	9	9	9	14	10	24	90	85	103	106
Unadjusted <sup>a</sup>	89	85	82	73	75	68	67	65	12	17	2	0
Adjusted <sup>b</sup>	0	1	1	9	7	2	6	0	1	2	0	0
-888 <sup>c</sup>	17	14	14	14	14	22	23	12	2	2	1	0
-666 <sup>d</sup>	0	0	0	0	0	0	0	5	0	0	0	0
-777 <sup>e</sup>	0	1	0	1	1	0	0	0	1	0	0	0

<sup>a</sup>The data are included in the data product file as is, with a secondary QC flag of 1.

<sup>b</sup>The adjusted data are included in the data product file with a secondary QC flag of 1.

<sup>c</sup>Data appear of good quality but have not been subjected to full secondary QC. They are included in data product with a secondary QC flag of 0.

<sup>d</sup>Data are of uncertain quality and suspended until full secondary QC has been carried out; they are excluded from the data product.

<sup>e</sup>Data are of poor quality and excluded from the data product.

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**Table 7.** Improvements resulting from quality control of the 106 new cruises, per basin and for the global data set. The numbers in the table are the weighted mean of the absolute offset of unadjusted and adjusted data versus GLODAPv2.2019. *n* is the total number of valid crossovers in the global ocean for the variable in question.

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	ARCTIC		ATLANTIC		INDIAN		PACIFIC		GLOBAL		<i>n</i> (global)
	Unadj	Adj	Unadj	Adj	Unadj	Adj	Unadj	Adj	Unadj	Adj	
<b>Sal ( x1000)</b>	1.7	=> 1.7	5.6	=> 5.6	4.0	=> 4.0	1.9	=> 1.9	2.4	=> 2.4	2841
<b>Oxy (%)</b>	0.8	=> 0.8	0.7	=> 0.7	0.5	=> 0.5	0.5	=> 0.5	0.5	=> 0.5	2462
<b>NO<sub>3</sub> (%)</b>	0.9	=> 0.9	1.6	=> 1.5	0.6	=> 0.6	0.5	=> 0.5	0.5	=> 0.5	2158
<b>Si (%)</b>	3.6	=> 3.6	2.5	=> 2.4	1.9	=> 1.1	1.0	=> 0.8	1.0	=> 0.8	1956
<b>PO<sub>4</sub> (%)</b>	5.0	=> 2.6	2.2	=> 2.0	0.8	=> 0.8	0.8	=> 0.7	0.8	=> 0.8	2047
<b>TCO<sub>2</sub> (μmol/kg)</b>	3.4	=> 3.4	2.6	=> 2.6	1.9	=> 1.9	2.1	=> 1.8	2.2	=> 1.9	512
<b>TAlk (μmol/kg)</b>	2.9	=> 2.9	1.7	=> 1.7	2.4	=> 1.6	2.5	=> 2.1	2.4	=> 2.1	521
<b>pH ( x1000)</b>	NA	=> NA	8.5	=> 8.5	NA	=> NA	8.3	=> 7.4	8.3	=> 7.5	458

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## Appendix A. Supplementary tables

**Table A1.** Cruises included in GLODAPv2.2020 that did not appear in GLODAPv2.2019. Complete information on each cruise, such as variables included, and chief scientist and principal investigator names is provided in the cruise summary table at [https://www.node.noaa.gov/ocads/oceans/GLODAPv2\\_2020/cruise\\_table\\_v2020.html](https://www.node.noaa.gov/ocads/oceans/GLODAPv2_2020/cruise_table_v2020.html)

No	EXPCODE	Region	Alias	Start	End	Ship
2001	06M220120625	Atlantic	MSM21/2	20120625	20120724	<i>Maria S. Merian</i>
2002	06M220130419	Atlantic	MSM27	20130419	20130506	<i>Maria S. Merian</i>
2003	06M220130509	Atlantic	MSM28	20130509	20130620	<i>Maria S. Merian</i>
2004	06M220140507	Atlantic	MSM38	20140507	20140605	<i>Maria S. Merian</i>
2005	06M220150502	Atlantic	MSM42	20150502	20150522	<i>Maria S. Merian</i>
2006	06M220150525	Atlantic	MSM43	20150525	20150627	<i>Maria S. Merian</i>
2007	06M320100804	Atlantic	M82/2	20100804	20100901	<i>Meteor</i>
2008	096U20180111	Indian	SR03.2018	20180111	20180222	<i>Investigator</i>
2009	18HU20050904	Atlantic	Davis Strait 2005	20050904	20050922	<i>Hudson</i>
2010	18SN20150920	Arctic	JOIS2015	20150920	20151016	<i>Louis S. St-Laurent</i>
2011	29AH20160617	Atlantic	OVIDE-16, A25, A01W	20160617	20160731	<i>Sarmiento de Gamboa</i>
2012	29GD20120910	Atlantic	EUROFLEETS	20120910	20120915	<i>Garcia del Cid</i>
2013	29HE20190406	Atlantic	FICARAM_XIX, A17	20190406	20190518	<i>Hesperides</i>
2014	316N20040922	Atlantic	Davis Strait 2004, KN179-05	20040922	20041004	<i>Knorr</i>
2015	316N20061001	Atlantic	Davis Strait 2006, KN187-02	20061001	20061004	<i>Knorr</i>
2016	316N20071003	Atlantic	Davis Strait 2007, DKN192-02	20071003	20071021	<i>Knorr</i>
2017	316N20080901	Atlantic	Davis Strait 2008, KN194-02	20080901	20080922	<i>Knorr</i>
2018	316N20091006	Atlantic	Davis Strait 2009, KN196-02	20091006	20091028	<i>Knorr</i>
2019	316N20100804	Atlantic	Davis Strait 2010	20100804	20100929	<i>Knorr</i>
2020	316N20101015	Atlantic	KN199-04, GEOTRACES-2010	20101015	20101105	<i>Knorr</i>
2021	316N20111002	Atlantic	Davis Strait 2011, KN203-04	20111002	20111021	<i>Knorr</i>
2022	316N20130914	Atlantic	Davis Strait 2013, KN213-02	20130914	20131003	<i>Knorr</i>
2023	316N20150906	Atlantic	Davis Strait 2015	20150906	20150924	<i>Knorr</i>
2024	32WC20110812	Pacific	WCOA2011	20110812	20110830	<i>Wecoma</i>
2025	33RO20160505	Pacific	WCOA2016	20160505	20160606	<i>Ronald H. Brown</i>
2026	35TH20080825	Atlantic	SUBPOLAR08	20080825	20080915	<i>Thalassa</i>
2027	45CE20170427	Atlantic	CE17007, A02	20170427	20170522	<i>Celtic Explorer</i>
2028	49UF20101002	Pacific	ks201007	20101002	20101104	<i>Keifu Maru II</i>
2029	49UF20101109	Pacific	ks201008	20101109	20101126	<i>Keifu Maru II</i>
2030	49UF20101203	Pacific	ks201009	20101203	20101222	<i>Keifu Maru II</i>
2031	49UF20111004	Pacific	ks201109	20111004	20111127	<i>Keifu Maru II</i>
2032	49UF20111205	Pacific	ks201110	20111205	20111221	<i>Keifu Maru II</i>
2033	49UF20120410	Pacific	ks201203	20120410	20120424	<i>Keifu Maru II</i>
2034	49UF20120602	Pacific	ks201205	20120602	20120614	<i>Keifu Maru II</i>
2035	49UF20131006	Pacific	ks201307	20131006	20131022	<i>Keifu Maru II</i>
2036	49UF20131029	Pacific	ks201308	20131029	20131210	<i>Keifu Maru II</i>
2037	49UF20140107	Pacific	ks201401	20140107	20140125	<i>Keifu Maru II</i>
2038	49UF20140206	Pacific	ks201402	20140206	20140326	<i>Keifu Maru II</i>
2039	49UF20140410	Pacific	ks201403	20140410	20140505	<i>Keifu Maru II</i>
2040	49UF20140512	Pacific	ks201404	20140512	20140617	<i>Keifu Maru II</i>
2041	49UF20140623	Pacific	ks201405, P09, P13	20140623	20140826	<i>Keifu Maru II</i>
2042	49UF20140904	Pacific	ks201406	20140904	20141019	<i>Keifu Maru II</i>

2043	49UF20150107	Pacific	ks201501	20150107	20150126	<i>Keifu Maru II</i>
2044	49UF20150202	Pacific	ks201502	20150202	20150306	<i>Keifu Maru II</i>
2045	49UF20150415	Pacific	ks201504	20150415	20150504	<i>Keifu Maru II</i>
2046	49UF20150511	Pacific	ks201505	20150511	20150611	<i>Keifu Maru II</i>
2047	49UF20150620	Pacific	ks201506, P09, P13	20150620	20150823	<i>Keifu Maru II</i>
2048	49UF20151021	Pacific	ks201508	20151021	20151202	<i>Keifu Maru II</i>
2049	49UF20160107	Pacific	ks201601	20160107	20160126	<i>Keifu Maru II</i>
2050	49UF20160201	Pacific	ks201602	20160201	20160310	<i>Keifu Maru II</i>
2051	49UF20160407	Pacific	ks201604	20160407	20160507	<i>Keifu Maru II</i>
2052	49UF20160512	Pacific	ks201605	20160512	20160610	<i>Keifu Maru II</i>
2053	49UF20160618	Pacific	ks201606	20160618	20160723	<i>Keifu Maru II</i>
2054	49UF20160730	Pacific	ks201607	20160730	20160912	<i>Keifu Maru II</i>
2055	49UF20160917	Pacific	ks201608	20160917	20161007	<i>Keifu Maru II</i>
2056	49UF20161116	Pacific	ks201609	20161116	20161219	<i>Keifu Maru II</i>
2057	49UF20170110	Pacific	ks201701, P09, P10	20170110	20170223	<i>Keifu Maru II</i>
2058	49UF20170228	Pacific	ks201702	20170228	20170326	<i>Keifu Maru II</i>
2059	49UF20170408	Pacific	ks201703	20170408	20170426	<i>Keifu Maru II</i>
2060	49UF20170502	Pacific	ks201704	20170502	20170606	<i>Keifu Maru II</i>
2061	49UF20170612	Pacific	ks201705	20170612	20170713	<i>Keifu Maru II</i>
2062	49UF20170719	Pacific	ks201706, P09, P10	20170719	20170907	<i>Keifu Maru II</i>
2063	49UF20171107	Pacific	ks201708	20171107	20171208	<i>Keifu Maru II</i>
2064	49UF20180129	Pacific	ks201802	20180129	20180309	<i>Keifu Maru II</i>
2065	49UF20180406	Pacific	ks201804	20180406	20180512	<i>Keifu Maru II</i>
2066	49UF20180518	Pacific	ks201805	20180518	20180703	<i>Keifu Maru II</i>
2067	49UF20180709	Pacific	ks201806	20180709	20180829	<i>Keifu Maru II</i>
2068	49UF20180927	Pacific	ks201808	20180927	20181021	<i>Keifu Maru II</i>
2069	49UP20110912	Pacific	rf201109	20110912	20110929	<i>Ryofu Maru III</i>
2070	49UP20120306	Pacific	rf201202	20120306	20120325	<i>Ryofu Maru III</i>
2071	49UP20121116	Pacific	rf201208	20121116	20121218	<i>Ryofu Maru III</i>
2072	49UP20130307	Pacific	rf201302	20130307	20130327	<i>Ryofu Maru III</i>
2073	49UP20130426	Pacific	rf201304	20130426	20130527	<i>Ryofu Maru III</i>
2074	49UP20131128	Pacific	rf201310	20131128	20131223	<i>Ryofu Maru III</i>
2075	49UP20140108	Pacific	rf201401, P09, P10	20140108	20140301	<i>Ryofu Maru III</i>
2076	49UP20140307	Pacific	rf201402	20140307	20140326	<i>Ryofu Maru III</i>
2077	49UP20140429	Pacific	rf201404	20140429	20140530	<i>Ryofu Maru III</i>
2078	49UP20140609	Pacific	rf201405	20140609	20140629	<i>Ryofu Maru III</i>
2079	49UP20141112	Pacific	rf201409	20141112	20141202	<i>Ryofu Maru III</i>
2080	49UP20150110	Pacific	rf201501	20150110	20150223	<i>Ryofu Maru III</i>
2081	49UP20150228	Pacific	rf201502	20150228	20150326	<i>Ryofu Maru III</i>
2082	49UP20150408	Pacific	rf201503	20150408	20150419	<i>Ryofu Maru III</i>
2083	49UP20150426	Pacific	rf201504	20150426	20150528	<i>Ryofu Maru III</i>
2084	49UP20150604	Pacific	rf201505	20150604	20150623	<i>Ryofu Maru III</i>
2085	49UP20150627	Pacific	rf201506	20150627	20150716	<i>Ryofu Maru III</i>
2086	49UP20151115	Pacific	rf201509	20151115	20151216	<i>Ryofu Maru III</i>
2087	49UP20160109	Pacific	rf201601, P09, P10	20160109	20160222	<i>Ryofu Maru III</i>
2088	49UP20160227	Pacific	rf201602	20160227	20160324	<i>Ryofu Maru III</i>
2089	49UP20160408	Pacific	rf201603	20160408	20160421	<i>Ryofu Maru III</i>
2090	49UP20160427	Pacific	rf201604	20160427	20160601	<i>Ryofu Maru III</i>



2091	49UP20160608	Pacific	rf201605	20160608	20160628	<i>Ryofu Maru III</i>
2092	49UP20161021	Pacific	rf201608	20161021	20161206	<i>Ryofu Maru III</i>
2093	49UP20170107	Pacific	rf201701	20170107	20170126	<i>Ryofu Maru III</i>
2094	49UP20170201	Pacific	rf201702	20170201	20170310	<i>Ryofu Maru III</i>
2095	49UP20170425	Pacific	rf201705	20170425	20170508	<i>Ryofu Maru III</i>
2096	49UP20170623	Pacific	rf201707	20170623	20170827	<i>Ryofu Maru III</i>
2097	49UP20170815	Pacific	rf201708	20170815	20171006	<i>Ryofu Maru III</i>
2098	49UP20171125	Pacific	rf201710	20171125	20171224	<i>Ryofu Maru III</i>
2099	49UP20180110	Pacific	rf201801	20180110	20180222	<i>Ryofu Maru III</i>
2100	49UP20180228	Pacific	rf201802	20180228	20180326	<i>Ryofu Maru III</i>
2101	49UP20180501	Pacific	rf201804	20180501	20180605	<i>Ryofu Maru III</i>
2102	49UP20180614	Pacific	rf201805	20180614	20180722	<i>Ryofu Maru III</i>
2103	49UP20180806	Pacific	rf201806, P13	20180806	20180927	<i>Ryofu Maru III</i>
2104	64PE20071026	Atlantic	PE278	20071026	20071117	<i>Pelagia</i>
2105	740H20180228	Atlantic	JC159	20180228	20180410	<i>James Cook</i>
2106	91AA20171209	Indian	NCAOR, SOE2017-18	20171209	20180204	<i>S.A. Agulhas I</i>

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## Figure Captions

1285 **Figure 1.** Location of stations in (a) GLODAPv2.2019 and for (b) the new data added in this update.

**Figure 2.** Number of cruises per year in GLODAPv2, GLODAPv2.2019, and GLODAPv2.2020.

1290 **Figure 3.** Example crossover figure, for  $\text{TCO}_2$  for cruises 49UP20160109 (blue) and 49UP20160703 (red), as it was generated during the crossover analysis. Panel (a) show all station positions for the two cruises and (b) show the specific stations used for the crossover analysis. Panel (d) shows the data of  $\text{TCO}_2$  ( $\mu\text{mol kg}^{-1}$ ) below the upper depth limit (in this case 2000 dbar) versus potential density anomaly referenced to 4000 dbar, as points and the interpolated profiles as lines. Non-interpolated data either did not meet minimum depth separation requirements (Table 4 in Key et al., 2010) or are the deepest sampling depth. The interpolation does not extrapolate. Panel (e) shows the mean  $\text{TCO}_2$  ( $\mu\text{mol kg}^{-1}$ ) difference profile (black, dots) with its standard deviation, and also the weighted mean offset (straight, red) and weighted standard deviation. Summary statistics are provided in (c).

1295 **Figure 4.** Example summary figure, for  $\text{TCO}_2$  crossovers for 49UP20160109 versus the cruises in GLODAPv2.2019 (with cruise EXPCODE listed on x-axis sorted according to year the cruise was conducted). The black dots and vertical error bars show the weighted mean offset and standard deviation for each crossover (in  $\mu\text{mol kg}^{-1}$ ). The weighted mean and standard deviation of all these offsets are shown in the red lines and are  $3.68 \pm 0.83 \mu\text{mol kg}^{-1}$ . The black dashed line is the reference line for a  $+4 \mu\text{mol kg}^{-1}$  offset (the corresponding line for  $-4 \mu\text{mol kg}^{-1}$  offset is right on top of x-axis and not visible).

1300 **Figure 5.** Example summary figure for CANYON-B and CONTENT analyses for 49UP20160109. Any data from regions where CONTENT and CANYON-B were not trained are excluded (in this case, the Sea of Japan). The top row shows the nutrients and the bottom row the seawater  $\text{CO}_2$  chemistry variables (Note, different abbreviations for  $\text{TCO}_2$  (CT) and TAlk (AT)). All are shown versus sampling pressure (dbar) and the unit is  $\mu\text{mol kg}^{-1}$  for all except pH, which is unitless. Black dots (which to a large extent are hidden by the predicted estimates) are the measured data, blue dots are CANYON-B estimates and red dots are the CONTENT estimates. Each variable has two figure panels. The left shows the depth profile while the right shows the absolute difference between measured and estimated values divided by the CANYON-B/CONTENT uncertainty estimate, which is determined for each estimated value. These values are used to gauge the comparability; a value below 1 indicates a good match, as it means that the difference between measured and estimated values is less than the uncertainty of the latter. The statistics in each panel are for all data deeper than 500 dbar and N is the number of samples; considered. A gain ratio and its interquartile range is given for the nutrients. For the seawater  $\text{CO}_2$  chemistry variables the numbers on each panel are the median difference between measured and predicted values for CANYON-B (upper) and CONTENT (lower). Both are given with their interquartile range.

1310 **Figure 6.** Distribution of applied adjustments for each core variable that received secondary QC, in  $\mu\text{mol kg}^{-1}$  for  $\text{TCO}_2$  and TAlk, unitless for salinity and pH (but multiplied with 1000 in both cases so a common x-axis can be used), while for the other properties adjustments are given in percent ((adjustment ratio-1)x100). Grey areas depict the initial minimum adjustment limits. The figure includes numbers for data subjected to secondary quality control only. Note also that the y-axis scale is set to render the number of adjustments to be visible, so the bar showing zero offset (the 0 bar) for each variable is cut off (see Table 6 for these numbers).

**Figure 7.** Distribution of pH offsets for the cruises from Japan Meteorological Agency added in GLODAPv2.2020.

**Figure 8.** Magnitude of applied adjustments relative to minimum adjustment limits (Table 3) per decade for the 946 cruises included in GLODAPv2.2020.

1320 **Figure 9.** Locations of stations included in the (a) Arctic, (b) Atlantic, (c) Indian, and (d) Pacific Ocean product files for the complete GLODAPv2.2020 dataset.

**Figure 10.** Distribution of data in GLODAPv2.2020 in (a) December–February, (b) March–May, (c) June–August, (d) September–November, and (e) number of observations for each month in four latitude bands.

1325 **Figure 11.** Number (a) and density (b) of observations in 100 m depth layers. The latter was calculated by dividing the number of observations in each layer by its global volume calculated from ETOPO2 (National Geophysical Data Center, 2006). For example, in the layer between 0 and 100 m there are on average 0.0075 observations per cubic kilometer. One observation is one water sampling point and has data for several variables.

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A full-blown consistency analysis of the entire GLODAPv2.2020 product (as done with the original GLODAPv2 product) has not been carried out, as it is too demanding in terms of time and resources to allow for frequent updates, particularly in terms of application of inversion results. The QC of GLODAPv2.2019 produced a sufficiently accurate data product that can serve as a reliable reference (this is in fact already done by some investigators to test their newly collected data; e.g. Panassa et al. 2018).

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including an inversion) again after the completion of the third GO-SHIP survey, currently scheduled for completion by 2023. Until that time, intermediate products like this are released regularly (every one or two years).

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was preferred, but draw temperature was frequently not reported and

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, with trailing zeros to comply with the number format for the variable in question, as specified in Swift and Diggs (2008).

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two existing. A similar approach was used for the 10 new Davis Strait cruises; in this region no data were available in GLODAPv2.2019. Due to the complex hydrography and differences in sampling locations it was very problematic to fully quality control these data, however, so most have been labeled -888, i.e., they are included in the product but with a secondary QC flag of 0 (Sect. 6).

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A few new cruises had no or very few valid crossovers with GLODAPv2 data. In that situation two other consistency analyses were carried out for salinity, oxygen, nutrients, TCO<sub>2</sub>, and TALK data, namely

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These methods were useful in the data-sparse Arctic and Southern oceans.