

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 CO₂ 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 fCO₂" 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:

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- 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.