GLODAPv2.2020 – the second update of GLODAPv2

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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 water samples. GLODAPv2.2020 is an update of the previous version, GLODAPv2.2019. The major changes are: data from 106 more cruises added, extension of time coverage until 2019, and the inclusion of available discrete fugacity of CO_2 (fCO_2) values in the merged product files. GLODAPv2.2020 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_4) have undergone extensive quality control, especially 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. They correct for errors related to measurement, calibration, and data handling practices, while taking into account any 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^{-1} in dissolved inorganic carbon, 4 µmol kg^{-1} in total alkalinity, 0.01–0.02, depending on region, in pH, and 5 % in the halogenated transient tracers. The other variables included in the compilation, such as isotopic tracers and discrete fCO_2 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/, 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). The bias corrected 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 atmospheric CO_2 corresponding to a significant fraction of anthropogenic CO_2 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, 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_2 in the ocean, natural oceanic carbon, ocean acidification, ventilation rates, oxygen levels, and vertical nutrient transports. The GLODAP core variables, which are quality controlled and bias corrected are salinity, dissolved oxygen, inorganic macronutrients (nitrate, silicate, and phosphate), seawater CO_2 chemistry variables (dissolved inorganic carbon – TCO_2, total alkalinity – TAlk, and pH on the total H^+ scale), and the halogenated transient tracers CFC-11, CFC-12, CFC-113, and CCl_4. Other chemical tracers are usually also 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)

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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$_2$ and TAlk measurements (Dickson et al., 2003) and for nutrients in seawater (CRMNS; Aoyama et al., 2012; Ota et al., 2010). Still biases in data occur. These can arise from poor sampling and general operation practices, calibration procedures, instrument design, and inaccurate calculations. The use of CRMs does not by itself ensure accurate measurements of seawater CO$_2$ chemistry (Bockmon and Dickson, 2015), and the CRMNS have only become available recently and are not universally used. For salinity and oxygen, lack of – or improper – conductivity-temperature-depth (CTD) sensor calibration is an additional and widespread problem (Olsen et al., 2016). For halogenated transient tracers, uncertainties in the 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 can render a set of data unusable. GLODAP deals with these issues by presenting the data in a uniform format, by including any documentation that was either submitted by the data originator or could be attained, and by subjecting the data to primary and secondary quality control assessments, focusing on precision and consistency, respectively. Adjustments are applied on the data to minimize severe cases of bias.

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 also included data from important "historical" cruises, 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 particular 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 CLIVAR 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 format of "living data format" of *Earth System Science Data* to document significant additions and changes to the dataset. This is the second regular update and adds data from 106 new cruises to the last update GLODAPv2.2019 (Olsen et al., 2019).

2 Key features of the update

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

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provided in Table A1 in the Appendix. Their sampling locations are shown alongside those of GLODAPv2.2019 in Fig. 1, while the coverage in time is shown in Fig. 2. The added cruises are from the years 2004-2019 with most 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). The data collected across the Davis Strait 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) is another important addition. Other cruises from the Atlantic include those carried out on the RV *Maria S. Merian* and RV *Meteor*, with transient tracer but not nutrients or seawater CO_2 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 RSS *James Cook* (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*, which has measurements for stable isotopes of carbon and oxygen (δ^{13}C and δ^{18}O) off the Iberian Peninsula (Voelker et al., 2015) but no data for nutrients, seawater CO_2 chemistry, or transient tracers. Two new cruises are included for the Indian Ocean, both 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 sole addition for the Arctic. Finally, the 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 previously, aiming to ensure the consistency of the data from the 106 new cruises to the previous release of this data product (the GLODAPv2.2019 adjusted data product). 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). The aim is to conduct a full analysis (i.e., 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). 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 added.

3 Methods

3.1 Data assembly and primary quality control

The data for the 106 new cruises were retrieved from data centers (typically CCHDO, NCEI, PANGAEA) or submitted directly to us. Each cruise is identified by an EXPOCODE. The EXPOCODE 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 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 person/group 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 and 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 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. Exchange file preparation entailed units conversion in some cases, most frequently from milliliters per liter (mL L^{-1}; oxygen) or micromoles per liter (µmol L^{-1}; nutrients) to micromoles per kilogram of seawater (µmol kg^{-1}). The default 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 milliliter to micromole conversion, while for the per liter to per kilogram conversion density based on reported salinity and draw temperatures was preferred, but draw temperature was frequently not reported and potential density was used instead. The potential errors introduced by any of these procedures are insignificant. Missing numbers are indicated by -999, with trailing zeros to comply with the number format for the variable in question, as specified in Swift and Diggs (2008).

Each data column (except temperature and pressure, which are assumed "good" if they exist) has an associated column of data flags. For the exchange files, these flags conform to the WOCE definitions for water sample bottles and are listed in Table 2. If no such WOCE flags were submitted with the data, they were assigned by us. In any case, 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 as such. In some cases, outliers were detected during the secondary QC; the consequential flag changes have then also been applied in the original cruise data files.

3.2 Secondary quality control

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 magnitude of the offset, factors such as its precision, 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 for. A guiding principle for these considerations was to not apply an adjustment whenever in doubt. Conversly, 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

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variable and cruise, i.e., an underlying assumption is that cruises suffer from either no or a single and constant measurement bias. Except where explicitly noted (Sect. 3.3.1), adjustments were not changed for data previously included in GLODAPv2.2019.

Crossover comparisons, multi-linear regressions (MLRs), and comparison of deep-water averages were used to identify offsets for salinity, oxygen, nutrients, TCO_2, 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_2 chemistry variables was not used for the evaluation of pH (Sect. 3.2.4). New to the present version is the more extensive use of CANYON-B and CONTENT predictions for the evaluation of offsets in nutrients and seawater CO_2 chemistry data (Section 3.2.5). For the halogenated transient tracers, examination of surface saturation levels and the relationship among the tracers were used to assess the data 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

Salinity and oxygen data can be obtained either by analysis of water samples (bottle data) and/or directly from the CTD sensor pack. These two 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 of the upcast when 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, where the fourth (see below) never occurred during our analyses, but is included to maintain consistency with GLODAPv2:

1. No data are available: no action needed.
2. No bottle values: use CTD values.
3. No CTD values: use bottle values.
4. Too few data of both types for comparison and more than 80 % of the records have bottle values: use 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 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

The crossover analyses were conducted with the MATLAB toolbox prepared by Lauvset and Tanhua (2015) and with the GLODAPv2.2019 data product as reference. In areas where a strong trend in salinity was present, the TAlk and TCO_2 data were salinity normalized before crossover analysis, following Friis et al. (2003).

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 larger influence on the comparison than data with more scatter. Whether the scatter reflects actual variability or data

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precision is irrelevant in this context as increased scatter regardless decreases the confidence in the comparison. Stations that are compared must be within 2° arc distance (~ 200 km) of each other, and only deep data are used. This minimizes effects of natural variability. As default, we used 1500 dbar as the upper depth limit, but in regions where deep mixing or convection occurs (such as the Nordic, Labrador, and Irminger seas) a more conservative limit of 2000 dbar was applied. The deeper limit was also applied to the majority of the northern Pacific cruises on the RV *Keifu Maru II* and RV *Ryofu Maru III* due the great abundance of deep data of the new- and reference cruises. As an example, the crossover for TCO_2 measured on the two cruises 49UP20160109 and 49UP20160703 is shown in Fig. 3. For TCO_2 the offset is determined as the difference. This is also the case for salinity, TAlk, and pH. For the nutrients, oxygen, and the halogenated transient tracers, ratios are used. This in accordance with the procedures followed for GLODAPv2. The TCO_2 values from 49UP20160109 are higher, with a weighed mean offset of 3.62 ± 2.67 μmol kg^{-1}, compared to those measured at 49UP20160703.

For each of the 106 new cruises, such a crossover comparison was conducted against all cruises possible 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_2 at 49UP20160109 is shown in Fig. 4. The TCO_2 data measured at this cruise are high when compared to the data measured at all nearby cruises included in GLODAPv2.2019, by 3.68 ± 0.83 μmol kg^{-1}. This is slightly less than the initial minimum adjustment limit for TCO_2 of 4 μmol kg^{-1} (Table 3), but the offset is present against all cruises and there is no obvious time trend (particularly important for TCO_2), and as such qualifies for an adjustment of the data in the merged data product. In this case -3 μmol kg^{-1} was applied, in order to bring the TCO_2 data from 49UP20160109 into consistency with GLODAPv2.2019.

Two exceptions to the above-described procedure exist: In the Japanese Sea six new cruises were added. In this region, there are only data from two cruises 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 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).

3.2.3 Other consistency analyses

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_2, and TAlk data, namely MLR analyses and deep water averages, broadly following Jutterström et al. (2010). For the MLRs, the presence of bias in the data for the cruise in question was identified by comparing the MLR generated with the measured values. These methods were useful in the data-sparse Arctic and Southern oceans. 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_2 were allowed), with the exact selection determined based on the statistical robustness of the fit, as evaluated using the coefficient of determination (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

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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 any crossover and CANYON-B and CONTENT results that existed, to determine whether or not to apply an adjustment.

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3.2.4 pH scale conversion and quality control

Altogether 82 of the 106 new cruises included 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. This is sufficiently accurate for scale-temperature-pressure conversions. 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 Uppström (1974). These procedures are the same as used for GLODAPv2.2019 (Olsen et al., 2019)

Internal consistency of CO_2 system variables were not used for the secondary quality control of the pH data of the 106 new cruises, but only crossover analysis supplemented by CONTENT and CANYON-B (Sect. 3.2.5). This avoids uncertainties in the quality control owing to incomplete understanding of the thermodynamic constants, major ion concentrations, measurement biases, and potential contribution of organic compounds to alkalinity (Álvarez et al., 2020; Takeshita et al., 2020). However, this applies only to the new cruises. The pH data of 840 of the 936 cruises in GLODAPv2.2020 were QC'd for GLODAPv2 and GLODAPv2.2019, and for these earlier products internal consistency of CO_2 system was used for secondary QC of pH. Therefore the level of consistency between these 936 cruises remains at 0.01 to 0.02 pH units, as more thoroughly discussed in Olsen et al. (2019)

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Deleted: 77 of the 116 new cruises included pH data. For about 30 % of these, the pH data were not supplied on the total scale, and at 25°C and 0 dbar pressure, which is the GLODAP standard. These data were converted to total pH scale and temperature and pressure of 25°C and 0 dbar. The conversions were conducted by 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). Whenever TAlk data were missing, these values were approximated as 67 times salinity. The proportionality (67) is the mean ratio of TAlk to salinity in the GLODAPv2 data. This is sufficiently accurate for scale-temperature-pressure conversions. 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 Uppström (1974). These procedures are the same as used for GLODAPv2 (Olsen et al., 2016), except for the CANYON-B estimation of phosphate and silicate. ... [39]

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) from the analyses described above. CANYON-B is a neural network for estimating nutrients and seawater CO_2 chemistry variables from temperature, salinity, and oxygen. CONTENT additionally considers the consistency among the estimated CO_2 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. Of course, we kept in mind that this relies on the accuracies of the T, S and O_2 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. 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_2 values revealed in the crossover comparisons discussed in Sect. 3.2.2. The magnitude of the inconsistencies for the CANYON-B estimate was 3.4 μmol kg^{-1}, i.e., slightly less than that the weighted mean crossover offset of 3.7 μmol kg^{-1}, while the CONTENT estimate gave an inconsistency of 2.7 μmol kg^{-1}. 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_2 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 by considering the each data point in it self, primary QC issues has been revealed and corrected for some of the cruises.

3.2.6 Halogenated transient tracers

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For the halogenated transient tracers (CFC-11, CFC-12, CFC-113, and CCl_4; 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 deep-water concentrations. 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.

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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_6 and CCl_4 were replaced with new ones received from the Principal Investigator, and recently published data for $\delta^{13}C$ and $\Delta^{14}C$ 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 $\delta^{13}C$ 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 $\delta^{13}C$ value of station 21 cast 3 bottle 4 was found bad and has been removed.
- For 74JC20100319 the $\delta^{13}C$ value at station 37 bottle 7 was found bad and has been removed.

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- All δ^{13}C values from the large volume Gerard barrels (identified by bottle number greater than 80) were removed from the product files as these 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 ^{o}C.
- For cruises 33RO20110926, 33RO20150525, and 33RO20150410, δ^{13}C and Δ^{14}C data have become available and 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^{-1} is now applied to the TCO_2 values.
- Additional primary QC have been applied to the cruises with *Keifu Maru II* and *Ryofu Maru III* that were included in GLODAPv2.2019.
- Discrete fugacity of CO_2 (fCO_2) data are now included in the product files whenever available. Discrete fCO_2 is one of the four variables that describes seawater CO_2 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 for GLODAPv1.1 (Sabine et al., 2005). However, for some cruises fCO_2 data were included indirectly in both GLODAPv1.1 and GLODAPv2 as they had been used to calculate TAlk, in combination with TCO_2. These calculated TAlk values were, however, not included in v2.2019. We have now chosen to include the discrete fCO_2 values in the product files. This increases transparency and traceability of the product; the fCO_2 data are also highly relevant for ongoing efforts toward resolving recently identified inconsistencies in our understanding of the relationships among the four seawater CO_2 chemistry variables (Carter et al., 2018; Fong and Dickson, 2019; Takeshita et al., 2020; Àlvarez et al., 2020). A total of 33924 discrete fCO_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 CO_2 (pCO_2) to fCO_2 for the 20 cruises where pCO_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 fCO_2 data have not been subjected to secondary QC. The inclusion of discrete fCO_2 data has led to some changes in the calculations of missing seawater 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., 2016), and GLODAPv2.2019 (Olsen et al., 2019), with some modifications:

- Data from the 106 new cruises were merged and sorted according to EXPOCODE, 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.

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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), and GLODAPv2 (Olsen et al., 2016), but with minor changes:

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- 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 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.
- Missing sampling pressures or depths were calculated following UNESCO (1981).
- For both oxygen and salinity, CTD and bottle values were merged following procedures summarized in Sect. 3.2.1.
- 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 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. For each of these variables the data product also has separate columns of secondary QC flags, indicating by cruise and variable whether (“1”) or not (“0”) data successfully received secondary QC. A 0 flag here 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.
- 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 Sérazin (2011). Apparent oxygen utilization was determined using the combined fit in Garcia and Gordon (1992).
- Partial pressures for CFC-11, CFC-12, CFC-113, CCl_4, and SF_6 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_2 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_2 chemistry variables gives more degrees of freedom in this respect, e.g., a particular record may have measured data for TCO_2, TAlk, and pH, and then a choice needs to be made with regard to which pair to use for the calculation of $f\mathrm{CO}_2$. We followed two simple principles. First, TCO_2 and TAlk was the preferred pair to calculate pH and $f\mathrm{CO}_2$, because we have higher confidence in the TCO_2 and TAlk data

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than pH (given the issues summarized in Sect. 3.2.4) and $f\mathrm{CO}_2$ (because it was not subjected to secondary QC). Second, if either TCO_2 or TAlk was missing and both pH and $f\mathrm{CO}_2$ data existed, pH was preferred (because $f\mathrm{CO}_2$ has not been subjected to secondary QC). All other options 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_2, TAlk, and pH, if the number of measured values for a specific cruise were less than half the number of calculated, then all measured values were replaced by calculated values. Such replacements were not done for calculations involving $f\mathrm{CO}_2$, as this would tend to overwrite all measured $f\mathrm{CO}_2$ values or would entail replacing a measured variable that has been subjected to secondary QC (i.e., TCO_2, TAlk, or pH) with one calculated from a variable that has not been subjected to secondary QC (i.e., $f\mathrm{CO}_2$). Calculated values have been assigned WOCE flag 0.

– 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 at 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. 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.

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_2 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_2 data are not included in the product.

4.2 Adjustment summary

The secondary QC actions for the 12 core variables and distribution of adjustments applied are summarized in Table 5 and Fig. 6, respectively. A very small fraction of the data is adjusted for most variables. None of the salinity data are adjusted, for oxygen and nitrate 1% of the data are adjusted, 2 % for TCO_2, 5 % for TAlk, 7 % for phosphate, and 9 % for silicate. For the CFCs, data from one of 16 cruises with CFC-11 is adjusted, while the fractions are two of 21 for CFC-12, and one out of three for CFC-113. The adjustments for the variables are also fairly small, overall. Thus the tendency observed during the production of GLODAPv2.2019 remains, namely, that the data collected at the large majority of recent cruises are consistent with earlier releases of this product.

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The quality control of pH data proved challenging for this version. The large majority had been collected in the northwestern Pacific, at the 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 units, which 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 that are being added are comparatively many (~ 70 cruises vs. ~ 130 already included 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 (by 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|) and include the rest of the data as is. This is the reason that the number of adjusted cruises for pH is zero (Table 5). 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. This might result in re-inclusion of these data, the formal decision for these are therefore "suspend" (Table 5). For now, some caution should be exercised if looking at trends in ocean pH in that region using these data.

For the nutrients, the 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 it 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 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 6. The data for CFCs were omitted for previously discussed reasons (Sect. 3.2.6). Globally, the improvement is modest. Considering the initial data quality, this result was expected, but 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 TCO_2, and Pacific Ocean pH data all show considerable improvements.

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) For several variables improvement is evident over time. Most TCO_2 and TAlk data from the 1970s needed an adjustment, but this fraction steadily declines until only a small percentage is adjusted. 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; however, there remains issues with the pH adjustments and this a topic for future development in GLODAP, with the support from the OCB Carbonate System Intercomparison Forum (CSIF, 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

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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

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/ (last access: 22 June 2020). The data are available as comma-separated ascii files (*.csv) and as binary MATLAB files (*.mat). 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 EXPOCODE of a cruise with GLODAP cruise number is provided with the data files. In the MATLAB files this information is also 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.

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/ (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.

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 principle investigator names are provided in the CST. Contacting principle 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.

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

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6 Summary

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. 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.

Except for salinity and oxygen, the core data were collected exclusively through chemical analyses of individually collected water samples. The data of 12 core variables: salinity, oxygen, nitrate, silicate, phosphate, TCO$_2$, TAlk, pH, CFC-11, CFC-12, CFC-113, and CCl$_4$ 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.

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 natural variability or anthropogenic trends 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 considers data below 500 dbar. Data consistency for cruises with exclusively shallow sampling was not examined.

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 δ^{13}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. 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 TCO$_2$, TAlk, pH, and fCO$_2$ any data flagged 0 are calculated from two measured seawater 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.

Based on the initial minimum adjustment limits and the improvement of the consistency from the adjustments (Table 6), 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 µmol kg^{-1} in TCO$_2$, 4 µmol 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.

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7 Author contributions.

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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

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The authors declare that they have no competing interests.

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[a]**	**2nd QC flag name[b]**	**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 botttle 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	$kg\ m^{-3}$	sigma0	(salinityf)		
Potential density anomaly, ref 1000 dbar	$kg\ m^{-3}$	sigma1	(salinityf)		
Potential density anomaly, ref 2000 dbar	$kg\ m^{-3}$	sigma2	(salinityf)		
Potential density anomaly, ref 3000 dbar	$kg\ m^{-3}$	sigma3	(salinityf)		
Potential density anomaly, ref 4000 dbar	$kg\ m^{-3}$	sigma4	(salinityf)		
Neutral density anomaly	$kg\ m^{-3}$	gamma	(salinityf)		
Oxygen	$\mu mol\ kg^{-1}$	oxygen	oxygenf	oxygenqc	CTDOXY/OXYGEN
Apparent oxygen utilization	$\mu mol\ kg^{-1}$	aou	aouf		
Nitrate	$\mu mol\ kg^{-1}$	nitrate	nitratef	nitrateqc	NITRAT
Nitrite	$\mu mol\ kg^{-1}$	nitrite	nitritef		NITRIT
Silicate	$\mu mol\ kg^{-1}$	silicate	silicatef	silicateqc	SILCAT
Phosphate	$\mu mol\ kg^{-1}$	phosphate	phosphatef	phosphateqc	PHSPHT
TCO_2	$\mu mol\ kg^{-1}$	tco2	tco2f	tco2qc	TCARBON
TAlk	$\mu mol\ kg^{-1}$	talk	talkf	talkqc	ALKALI
pH on total scale, 25° C and 0 dbar of pressure		phts25p0	phts25p0f	phtsqc	PH_TOT

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pH on total scale, in situ temperature and pressure		phtsinsitutp	phtsinsitutpf	phtsqc	
fCO$_2$ at 20° C and 0 dbar of pressure	µatm	fco2	fco2f		FCO2/PCO2
fCO$_2$ temperature[c]	°C	fco2temp	(fco2f)		FCO2_TMP/PCO2_TMP
CFC-11	pmol kg^{-1}	cfc11	cfc11f	cfc11qc	CFC-11
pCFC-11	ppt	pcfc11	(cfc11f)		
CFC-12	pmol kg^{-1}	cfc12	cfc12f	cfc12qc	CFC-12
pCFC-12	ppt	pcfc12	(cfc12f)		
CFC-113	pmol kg^{-1}	cfc113	cfc113f	cfc113qc	CFC-113
pCFC-113	ppt	pcfc113	(cfc113f)		
CCl$_4$	pmol kg^{-1}	ccl4	ccl4f	ccl4qc	CCL4
pCCl$_4$	ppt	pccl4	(ccl4f)		
SF$_6$	fmol kg^{-1}	sf6	sf6f		SF6
pSF6	ppt	psf6	(sf6f)		
δ^{13}C	‰	c13	c13f	c13qc	DELC13
Δ^{14}C	‰	c14	c14f		DELC14
Δ^{14}C counting error	‰	c14err			C14ERR
^{3}H	TU	h3	h3f		TRITIUM
^{3}H counting error	TU	h3err			TRITER
δ^{3}He	%	he3	he3f		DELHE3
^{3}He counting error	%	he3err			DELHER
He	nmol kg^{-1}	he	hef		HELIUM
He counting error	nmol kg^{-1}	heerr			HELIER
Ne	nmol kg^{-1}	neon	neonf		NEON
Ne counting error	nmol kg^{-1}	neonerr			NEONER
δ^{18}O	‰	o18	o18f		DELO18
Total organic carbon	µmol L^{-1} [d]	toc	tocf		TOC
Dissolved organic carbon	µmol L^{-1} [d]	doc	docf		DOC
Dissolved organic nitrogen	µmol L^{-1} [d]	don	donf		DON
Dissolved total nitrogen	µmol L^{-1} [d]	tdn	tdnf		TDN
Chlorophyll *a*	µg kg^{-1} [d]	chla	chlaf		CHLORA

[a] 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. [b] Secondary QC flags indicate whether data have been subjected to full secondary QC (1) or not (0), as described in Sect. 3. [c] Included for clarity, is 20 °C for all occurences. [d] 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 and product files.

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

[a] Flag set to 9 in product files

[b] Data are not included in the GLODAPv2.2020 product files and their flags set to 9.

[c] 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_2	4 µmol kg^{-1}
TAlk	4 µmol 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 present: use CTD derived values.	20	5
3	No CTD values present: use bottle data.	0	67
4	Too few data of both types for comparison and >80% of 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 these 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. Summary of secondary QC results for the 106 new cruises, in number of cruises per result and per variable.

	Sal.	Oxy.	NO_3	Si	PO_4	TCO_2	TAlk	pH	CFC-11	CFC-12	CFC-113	CCl_4
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[a]	89	85	82	73	75	68	67	65	12	17	2	0
Adjusted[b]	0	1	1	9	7	2	6	0	1	2	0	0
-888[c]	17	14	14	14	14	22	23	12	2	2	1	0
-666[d]	0	0	0	0	0	0	0	5	0	0	0	0
-777[e]	0	1	0	1	1	0	0	0	1	0	0	0

[a] The data are included in the data product file as is, with a secondary QC flag of 1.

[b] The adjusted data are included in the data product file with a secondary QC flag of 1.

[c] 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.

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

[e] Data are of poor quality and excluded from the data product.

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Table 6.

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.

	ARCTIC			ATLANTIC			INDIAN			PACIFIC			GLOBAL		
	Unadj		Adj	Unadj		Adj	Unadj		Adj	Unadj		Adj	Unadj		Adj
Sal (x1000)	1.7	=>	1.7	5.6	=>	5.6	4.0	=>	4.0	1.9	=>	1.9	2.4	=>	2.4
Oxy (%)	0.8	=>	0.8	0.7	=>	0.7	0.5	=>	0.5	0.5	=>	0.5	0.5	=>	0.5
NO_3 (%)	0.9	=>	0.9	1.6	=>	1.5	0.6	=>	0.6	0.5	=>	0.5	0.5	=>	0.5
Si (%)	3.6	=>	3.6	2.5	=>	2.4	1.9	=>	1.1	1.0	=>	0.8	1.0	=>	0.8
PO_4 (%)	5.0	=>	2.6	2.2	=>	2.0	0.8	=>	0.8	0.8	=>	0.7	0.8	=>	0.8
TCO_2 (µmol/kg)	3.4	=>	3.4	2.6	=>	2.6	1.9	=>	1.9	2.1	=>	1.8	2.2	=>	1.9
TAlk (µmol/kg)	2.9	=>	2.9	1.7	=>	1.7	2.4	=>	1.6	2.5	=>	2.1	2.4	=>	2.1
pH (x1000)	NA	=>	NA	8.5	=>	8.5	NA	=>	NA	8.3	=>	7.4	8.3	=>	7.5

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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.nodc.noaa.gov/ocads/oceans/GLODAPv2_2020/cruise_table_v20202.html

No	EXPOCODE	Region	Alias	Start	End	Ship
2001	06M220120625	Atlantic	MSM21/2	20120625	20120724	*Maria S. Merian*
2002	06M220130419	Atlantic	MSM27	20130419	20130506	*Maria S. Merian*
2003	06M220130509	Atlantic	MSM28	20130509	20130620	*Maria S. Merian*
2004	06M220140507	Atlantic	MSM38	20140507	20140605	*Maria S. Merian*
2005	06M220150502	Atlantic	MSM42	20150502	20150522	*Maria S. Merian*
2006	06M220150525	Atlantic	MSM43	20150525	20150627	*Maria S. Merian*
2007	06M320100804	Atlantic	M82/2	20100804	20100901	*Meteor*
2008	096U20180111	Indian	SR03.2018	20180111	20180222	*Investigator*
2009	18HU20050904	Atlantic	Davis Strait 2005	20050904	20050922	*Hudson*
2010	18SN20150920	Arctic	JOIS2015	20150920	20151016	*Louis S. St-Laurent*
2011	29AH20160617	Atlantic	OVIDE-16, A25, A01W	20160617	20160731	*Sarmiento de Gamboa*
2012	29GD20120910	Atlantic	EUROFLEETS	20120910	20120915	*Garcia del Cid*
2013	29HE20190406	Atlantic	FICARAM_XIX, A17	20190406	20190518	*Hesperides*
2014	316N20040922	Atlantic	Davis Strait 2004, KN179-05	20040922	20041004	*Knorr*
2015	316N20061001	Atlantic	Davis Strait 2006, KN187-02	20061001	20061004	*Knorr*
2016	316N20071003	Atlantic	Davis Strait 2007, DKN192-02	20071003	20071021	*Knorr*
2017	316N20080901	Atlantic	Davis Strait 2008, KN194-02	20080901	20080922	*Knorr*
2018	316N20091006	Atlantic	Davis Strait 2009, KN196-02	20091006	20091028	*Knorr*
2019	316N20100804	Atlantic	Davis Strait 2010	20100804	20100929	*Knorr*
2020	316N20101015	Atlantic	KN199-04, GEOTRACES-2010	20101015	20101105	*Knorr*
2021	316N20111002	Atlantic	Davis Strait 2011, KN203-04	20111002	20111021	*Knorr*
2022	316N20130914	Atlantic	Davis Strait 2013, KN213-02	20130914	20131003	*Knorr*
2023	316N20150906	Atlantic	Davis Strait 2015	20150906	20150924	*Knorr*
2024	32WC20110812	Pacific	WCOA2011	20110812	20110830	*Wecoma*
2025	33RO20160505	Pacific	WCOA2016	20160505	20160606	*Ronald H. Brown*
2026	35TH20080825	Atlantic	SUBPOLAR08	20080825	20080915	*Thalassa*
2027	45CE20170427	Atlantic	CE17007, A02	20170427	20170522	*Celtic Explorer*
2028	49UF20101002	Pacific	ks201007	20101002	20101104	*Keifu Maru II*
2029	49UF20101109	Pacific	ks201008	20101109	20101126	*Keifu Maru II*
2030	49UF20101203	Pacific	ks201009	20101203	20101222	*Keifu Maru II*
2031	49UF20111004	Pacific	ks201109	20111004	20111127	*Keifu Maru II*
2032	49UF20111205	Pacific	ks201110	20111205	20111221	*Keifu Maru II*
2033	49UF20120410	Pacific	ks201203	20120410	20120424	*Keifu Maru II*
2034	49UF20120602	Pacific	ks201205	20120602	20120614	*Keifu Maru II*
2035	49UF20131006	Pacific	ks201307	20131006	20131022	*Keifu Maru II*
2036	49UF20131029	Pacific	ks201308	20131029	20131210	*Keifu Maru II*
2037	49UF20140107	Pacific	ks201401	20140107	20140125	*Keifu Maru II*
2038	49UF20140206	Pacific	ks201402	20140206	20140326	*Keifu Maru II*
2039	49UF20140410	Pacific	ks201403	20140410	20140505	*Keifu Maru II*
2040	49UF20140512	Pacific	ks201404	20140512	20140617	*Keifu Maru II*
2041	49UF20140623	Pacific	ks201405, P09, P13	20140623	20140826	*Keifu Maru II*
2042	49UF20140904	Pacific	ks201406	20140904	20141019	*Keifu Maru II*
2043	49UF20150107	Pacific	ks201501	20150107	20150126	*Keifu Maru II*

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2044	49UF20150202	Pacific	ks201502	20150202	20150306	*Keifu Maru II*
2045	49UF20150415	Pacific	ks201504	20150415	20150504	*Keifu Maru II*
2046	49UF20150511	Pacific	ks201505	20150511	20150611	*Keifu Maru II*
2047	49UF20150620	Pacific	ks201506, P09, P13	20150620	20150823	*Keifu Maru II*
2048	49UF20151021	Pacific	ks201508	20151021	20151202	*Keifu Maru II*
2049	49UF20160107	Pacific	ks201601	20160107	20160126	*Keifu Maru II*
2050	49UF20160201	Pacific	ks201602	20160201	20160310	*Keifu Maru II*
2051	49UF20160407	Pacific	ks201604	20160407	20160507	*Keifu Maru II*
2052	49UF20160512	Pacific	ks201605	20160512	20160610	*Keifu Maru II*
2053	49UF20160618	Pacific	ks201606	20160618	20160723	*Keifu Maru II*
2054	49UF20160730	Pacific	ks201607	20160730	20160912	*Keifu Maru II*
2055	49UF20160917	Pacific	ks201608	20160917	20161007	*Keifu Maru II*
2056	49UF20161116	Pacific	ks201609	20161116	20161219	*Keifu Maru II*
2057	49UF20170110	Pacific	ks201701, P09, P10	20170110	20170223	*Keifu Maru II*
2058	49UF20170228	Pacific	ks201702	20170228	20170326	*Keifu Maru II*
2059	49UF20170408	Pacific	ks201703	20170408	20170426	*Keifu Maru II*
2060	49UF20170502	Pacific	ks201704	20170502	20170606	*Keifu Maru II*
2061	49UF20170612	Pacific	ks201705	20170612	20170713	*Keifu Maru II*
2062	49UF20170719	Pacific	ks201706, P09, P10	20170719	20170907	*Keifu Maru II*
2063	49UF20171107	Pacific	ks201708	20171107	20171208	*Keifu Maru II*
2064	49UF20180129	Pacific	ks201802	20180129	20180309	*Keifu Maru II*
2065	49UF20180406	Pacific	ks201804	20180406	20180512	*Keifu Maru II*
2066	49UF20180518	Pacific	ks201805	20180518	20180703	*Keifu Maru II*
2067	49UF20180709	Pacific	ks201806	20180709	20180829	*Keifu Maru II*
2068	49UF20180927	Pacific	ks201808	20180927	20181021	*Keifu Maru II*
2069	49UP20110912	Pacific	rf201109	20110912	20110929	*Ryofu Maru III*
2070	49UP20120306	Pacific	rf201202	20120306	20120325	*Ryofu Maru III*
2071	49UP20121116	Pacific	rf201208	20121116	20121218	*Ryofu Maru III*
2072	49UP20130307	Pacific	rf201302	20130307	20130327	*Ryofu Maru III*
2073	49UP20130426	Pacific	rf201304	20130426	20130527	*Ryofu Maru III*
2074	49UP20131128	Pacific	rf201310	20131128	20131223	*Ryofu Maru III*
2075	49UP20140108	Pacific	rf201401, P09, P10	20140108	20140301	*Ryofu Maru III*
2076	49UP20140307	Pacific	rf201402	20140307	20140326	*Ryofu Maru III*
2077	49UP20140429	Pacific	rf201404	20140429	20140530	*Ryofu Maru III*
2078	49UP20140609	Pacific	rf201405	20140609	20140629	*Ryofu Maru III*
2079	49UP20141112	Pacific	rf201409	20141112	20141202	*Ryofu Maru III*
2080	49UP20150110	Pacific	rf201501	20150110	20150223	*Ryofu Maru III*
2081	49UP20150228	Pacific	rf201502	20150228	20150326	*Ryofu Maru III*
2082	49UP20150408	Pacific	rf201503	20150408	20150419	*Ryofu Maru III*
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2084	49UP20150604	Pacific	rf201505	20150604	20150623	*Ryofu Maru III*
2085	49UP20150627	Pacific	rf201506	20150627	20150716	*Ryofu Maru III*
2086	49UP20151115	Pacific	rf201509	20151115	20151216	*Ryofu Maru III*
2087	49UP20160109	Pacific	rf201601, P09, P10	20160109	20160222	*Ryofu Maru III*
2088	49UP20160227	Pacific	rf201602	20160227	20160324	*Ryofu Maru III*
2089	49UP20160408	Pacific	rf201603	20160408	20160421	*Ryofu Maru III*
2090	49UP20160427	Pacific	rf201604	20160427	20160601	*Ryofu Maru III*
2091	49UP20160608	Pacific	rf201605	20160608	20160628	*Ryofu Maru III*
2092	49UP20161021	Pacific	rf201608	20161021	20161206	*Ryofu Maru III*

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

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Figure Captions

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.

Figure 3. Example crossover figure, for TCO_2 for cruises 49UP20160109 (blue) and 49UP20160703 (red), as it was generated during the crossover analysis. Panels **(a)** and **(b)** show the station positions. Panel **(d)** shows the data below the upper depth limit (in this case 2000 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 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)**.

Figure 4. Example summary figure, for TCO_2 crossovers for 49UP20160109 versus the cruises in GLODAPv2.2019 (with cruise EXPOCODE 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. The weighted mean and standard deviation of all these offsets are shown in the red lines and are 3.68 ± 0.83 µmol kg^{-1}. The black dashed line is the reference line for a +4 µmol kg^{-1} offset (the corresponding line for – 4 µmol kg^{-1} offset is right on top of x-axis and not visible).

Figure 5. Example summary figure for CONTENT and CANYON-B 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 CO_2 chemistry variables (Note, different abbreviations for TCO_2 (CT) and TAlk (AT)). Black dots 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. A value below 1 indicates a good match between the two 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 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.

Figure 6. Distribution of applied adjustments for each core variable that received secondary QC. 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 5 for these numbers).

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

Figure 8. Distribution of applied adjustments per decade for the 946 cruises included in GLODAPv2.2020. Dark blue: not adjusted; light blue: absolute adjustment is smaller than initial minimum adjustment limit (Table 3); orange: absolute adjustment is between limit and 2 times the limit, red: absolute adjustment is larger than 2 times the limit.

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 north of 45° N (red), north of equator to 45° N (orange), equator to 45° S (light blue), and south of 45° S (dark blue).

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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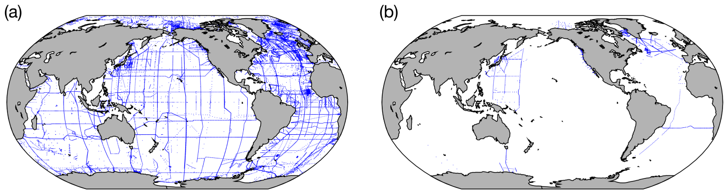

Figure 1

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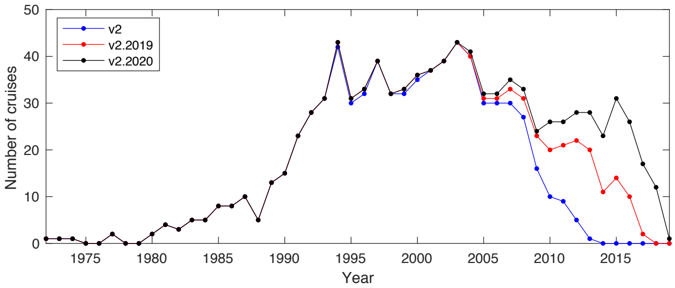

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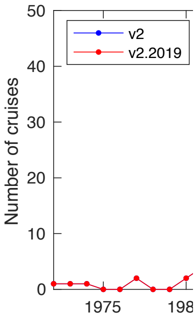

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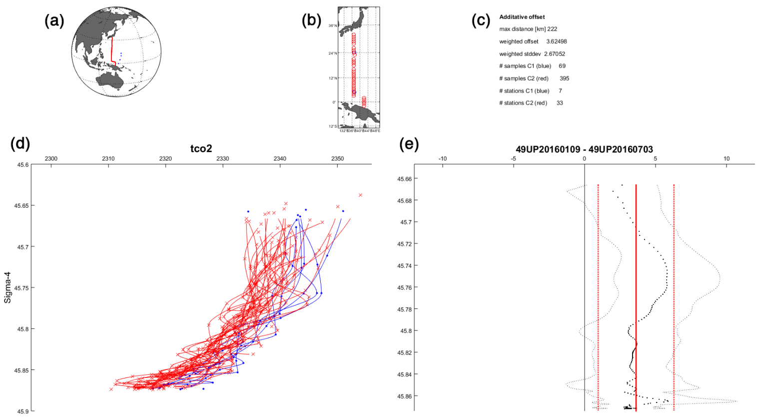

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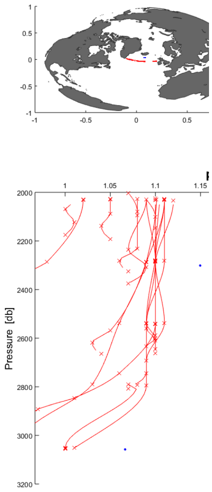

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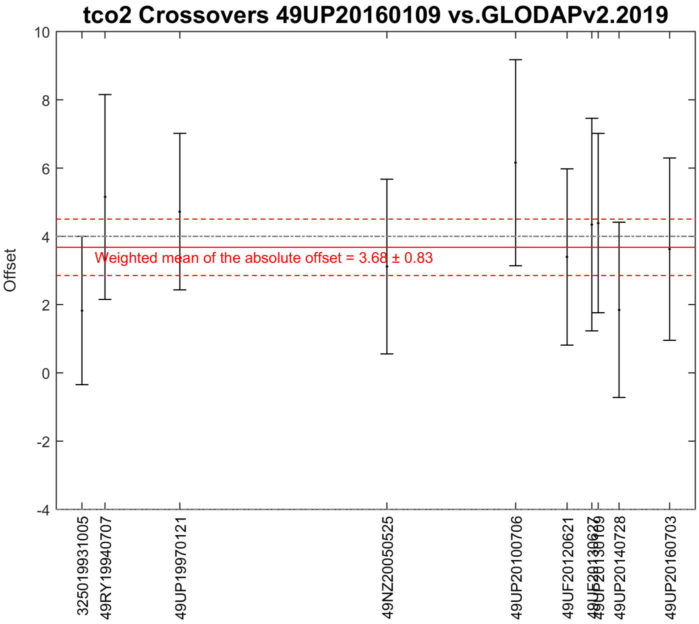

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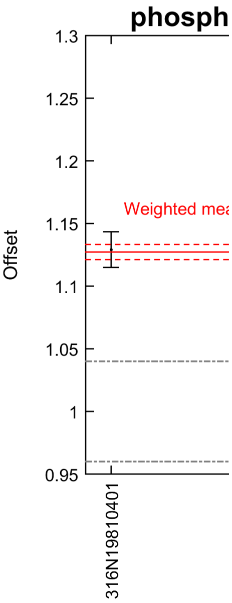

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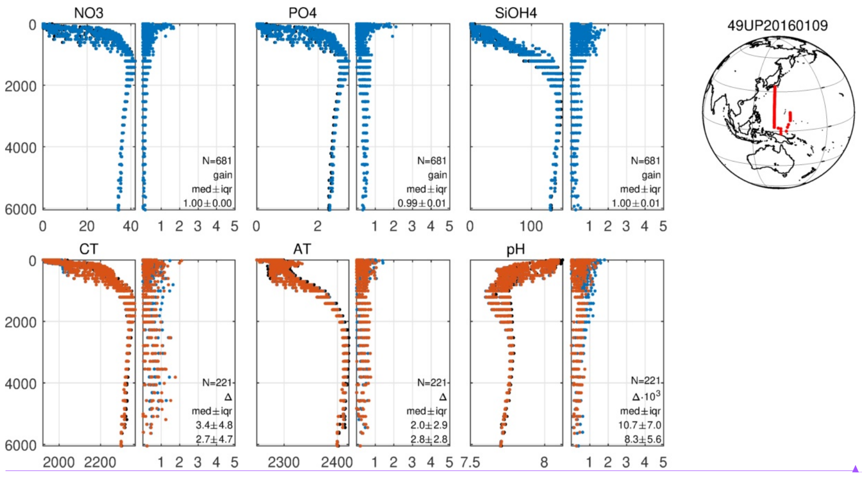

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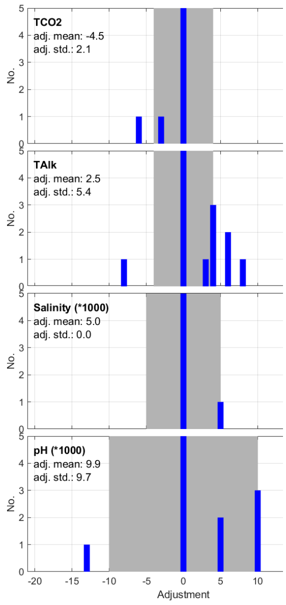

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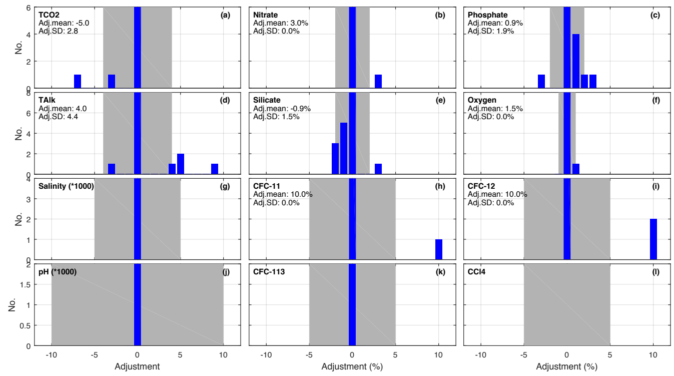

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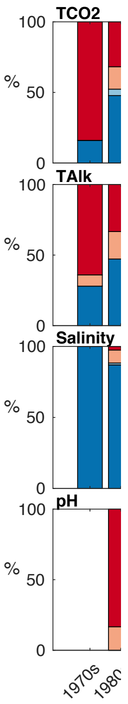

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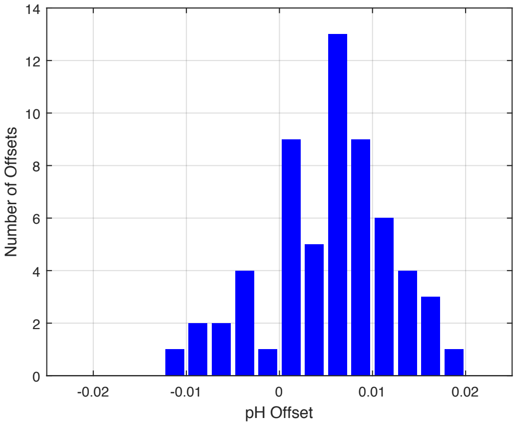

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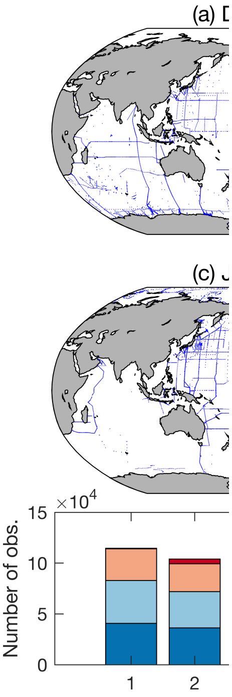

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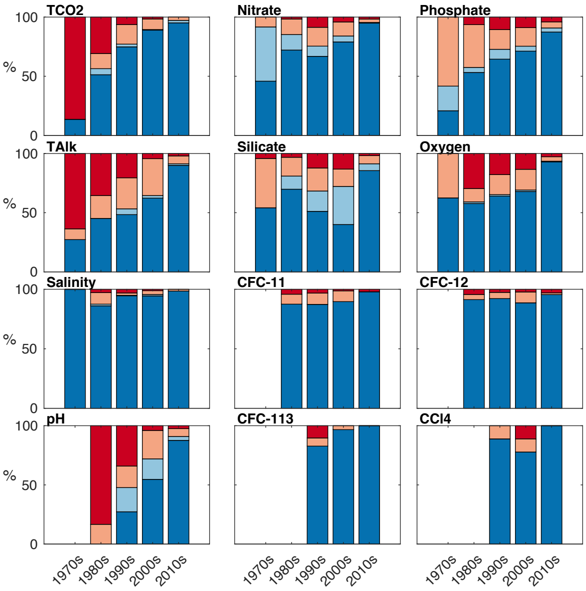

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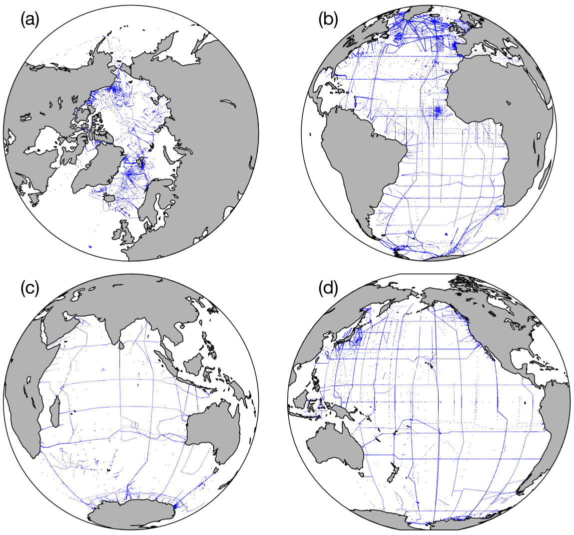

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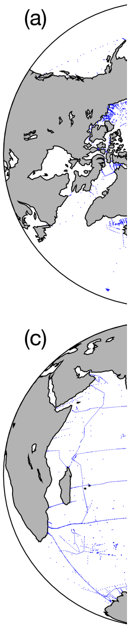

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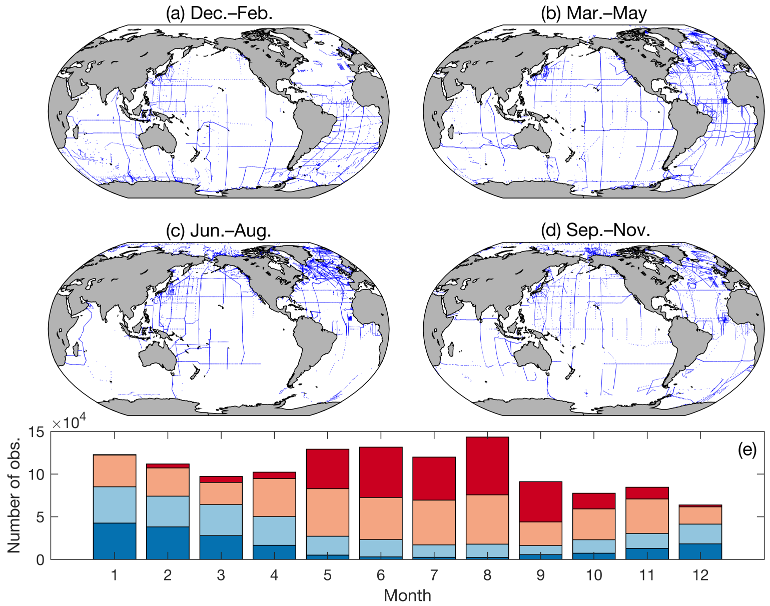

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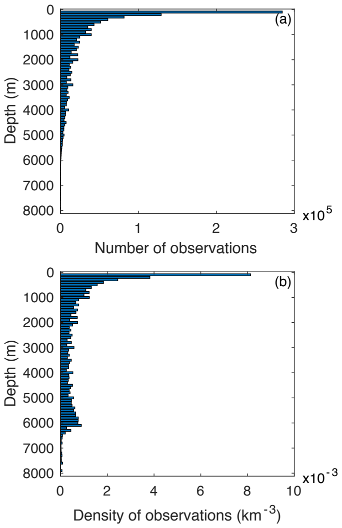

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Figure 11

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[15] NOAA National Centers for Environmental Information, Silver Spring, MD, USA
[16] LOCEAN, CNRS, Sorbonne Université, Paris, France

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[21] International Ocean Carbon Coordination Project, Institute of Oceanology of Polish Academy of Sciences, Sopot, Poland
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CO_2 corresponding to a significant fraction of anthropogenic CO_2 emissions (Gruber et al., 2019; Le Quéré et al., 2018) and most of the excess heat in the Earth System caused by the enhanced greenhouse effect resulting from the fraction of CO_2 and other greenhouse gases remaining in the atmosphere (Cheng et al., 2017). The objective of GLODAP (Global Ocean Data Analysis Project, www.glodap.info, last access: 17 September 2019

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Examples include stable isotopes of carbon and oxygen ($\delta^{13}C$ and $\delta^{18}O$), radioisotopes (^{14}C, ^{3}H, ^{3}He), noble gases (He, Ne), and organic material including total organic carbon (TOC), dissolved organic carbon (DOC), total dissolved nitrogen (TDN), and chlorophyll *a* (Chl *a*).

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The first version of GLODAP, GLODAPv1.1, was released in 2005 (Key et al., 2004; Sabine et al., 2005). It contains data from 115 cruises with biogeochemical measurements from the global ocean. The vast majority of these are 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). The second version of GLODAP, GLODAPv2, was released in 2016 (Key et al., 2015; Lauvset et al., 2016; Olsen et al., 2016) with data from 724 scientific cruises: those included in GLODAPv1.1, those amassed for the Carbon in the Atlantic Ocean (CARINA) data synthesis (Key et al., 2010), those amassed for the Pacific Ocean Interior Carbon

(PACIFICA) synthesis (Suzuki et al., 2013), and data from 168 additional cruises. The additional cruises include many collected within the framework of the "repeat hydrography" program (Talley et al., 2016), instigated in the early 2000s as part of CLIVAR and since 2007 organized as the Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP). Both GLODAPv1.1 and GLODAPv2 data were released in three formats: (i) as submitted by the data originator but reformatted to WOCE exchange format (Swift and Diggs, 2008) and subjected to primary quality control to flag outliers, (ii) as a merged data product with bias minimization adjustments applied, and (iii) as globally mapped climatological distributions. We refer to the first as the original data, to the second as the data product, and to the third as the mapped product.

The GLODAP products have been widely used. The first version formed the basis for the first data-based estimate of the global ocean inventory of anthropogenic carbon (Sabine et al., 2004), and the descriptive paper on GLODAPv1.1 (Key et al., 2004) has been cited more than 800 times according to Web of Science (Clarivate Analytics). For GLODAPv2, we have registered more than 120 applications. Examples include model evaluation (Beadling et al., 2018; Goris et al., 2018; Tjiputra et al., 2018; Ward et al., 2018), model initialization (Orr et al., 2017), water mass analyses (Jeansson et al., 2017; Peters et al., 2018; Rae and Broecker, 2018), ocean acidification (Fassbender et al., 2017; García-Ibáñez et al., 2016; Perez et al., 2018), calibration of Argo biogeochemical sensor measurements (Bushinsky et al., 2017; Johnson et al., 2017), calibration of multiple linear regression (MLR) and neural-network-based methods for biogeochemical data estimation (Bittig et al., 2018; Carter et al., 2018; Fry et al., 2016; Sauzède et al., 2017), contextualization of paleo-oceanographic data (Glock et al., 2018; Sessford et al., 2018), and calculation of inventory, transport, and variability of ocean carbon (DeVries et al., 2017; Fröb et al., 2018; Fröb et al., 2016; Gruber et al., 2019; Panassa et al., 2018; Pardo et al., 2017; Quay et al., 2017). A full list of GLODAPv2 citations is provided at https://www.glodap.info/index.php/glodap-impact/ (last access: 17 September 2019).

Principles

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(FAIR) principles (Wilkinson et al., 2016), and are largely adhered to by the oceanographic community. Data are routinely made available on a per cruise basis through national and international data centers. However,

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variable units, such that the comparability between many data sets is 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_2 and TAlk measurements (Dickson et al., 2003) and for nutrients in seawater (CRMNS; (Aoyama et al., 2012; Ota et al., 2010).

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A total of twelve years separated the release of the two versions of GLODAP. The urgency and complexity of modern climate change issues necessitate more frequent updates. Ocean carbon uptake responds quickly to annual-to-decadal changes in ocean circulation (Fröb et al., 2016; Landschützer et al., 2015), ocean acidification is progressing at unprecedented rates and already causing carbonate mineral undersaturation in some regions (Feely et al., 2008; Qi et al., 2017), oxygen minimum zones are rapidly expanding (Breitburg et al., 2018), and declining nutrient supply to the euphotic zone is potentially changing phytoplankton composition in certain large ocean regions (Rousseaux and Gregg, 2015). In addition, improvements in data management practices and increased computational resources are transforming approaches to, and expectations for, integrated data products. The Surface Ocean CO_2 Atlas (SOCAT) is a prominent example in this regard with annual releases and rapid use in global carbon budgets (Bakker et al., 2016; Bakker et al., 2014; Le Quéré et al., 2018; Pfeil et al., 2013). GLODAP is also becoming an important source of calibration and validation data for the biogeochemical sensors that are now deployed on autonomous platforms. Altogether, regular and rapid updates are important.

This contribution documents the first such regular update of GLODAP, which adds data from 116 new cruises to the 724 included in GLODAPv2 and corrects errors and omissions in GLODAPv2. It also forms the basis for the documentation of future updates, adopting the *Earth System Science Data* "living data" format for evolving data sets.

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GLODAPv2.2019 (Olsen et al., 2019) contains data from 840 cruises, covering the global ocean from 1972 to 2017. The sampling locations of the 116 cruises added in this update are shown alongside those of GLODAPv2 in Fig. 1, while the coverage in time is shown in Fig. 2. Compared to GLODAPv2, the added data are mostly repeat observations and extend the coverage in time. Information on cruises added to this version is provided in Table A1 in the Appendix.

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The crossover analyses were conducted with the Matlab toolbox prepared by Lauvset and Tanhua (2015) and with the GLODAPv2 data product as reference. In areas where a strong trend in salinity was present, the TAlk and TCO_2 data were salinity normalized following Friis et al. (2003), before crossover analysis.
The toolbox implements the 'running-cluster' crossover analysis first described by Tanhua et al. (2010).

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Jutterström et al. (2010).

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77 of the 116 new cruises included pH data. For about 30 % of these, the pH data were not supplied on the total scale, and at 25°C and 0 dbar pressure, which is the GLODAP standard. These data were converted to total pH scale and temperature and pressure of 25°C and 0 dbar. The conversions were conducted by 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). Whenever TAlk data were missing, these values were approximated as 67 times salinity. The proportionality (67) is the mean ratio of TAlk to salinity in the GLODAPv2 data. This is sufficiently accurate for scale-temperature-pressure conversions. 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 Uppström (1974). These procedures are the same as used for GLODAPv2 (Olsen et al., 2016), except for the CANYON-B estimation of phosphate and silicate.

The secondary quality control of the pH data also followed previous procedures, using a combination of crossovers and internal consistency calculations. The latter were conducted when a cruise had data for TCO_2 and TAlk, in addition to pH. Note that internal consistency was only considered for the secondary

QC of pH, and not for the secondary QC of TCO_2 and TAlk. Hence, the adjustments applied for pH are not only a bias correction but also a seawater CO_2 chemistry consistency correction. This is one factor that makes the secondary quality control of pH data problematic, in particular with regard to the application of a uniform correction for an entire cruise or leg based on offsets in deep data. pH dependent offsets between pH determined spectrophotometrically with purified dyes and pH calculated from TCO_2 and TAlk have recently been found. For example, at a pH of 7.6 the calculated pH is higher by ~ 0.01 than measured pH (Carter et al., 2018). The causes of these discrepancies are not entirely clear, suggestions include deficiencies in dissociation constants used for the seawater CO_2 chemistry calculations, errors in the total boron-to-salinity ratio, and unknown protolytes affecting the TAlk (Carter et al., 2018; Fong and Dickson, 2019). Such low pH values exist only in the deep North Pacific Ocean. Here, application of pH corrections based on seawater CO_2 consistency considerations could impact the correction. Broadly speaking, the pH data in GLODAP have been obtained using a variety of methods (e.g. potentiometric measurements, and spectrophotometric measurements with purified or impure dyes). The pH values produced by these different approaches have documented pH-dependent offsets from one another (Carter et al., 2013; Liu et al., 2011; Patsavas et al., 2015; Yao et al., 2007) that challenge the viability of the uniform adjustments applied (Carter et al., 2018). While we have continued to apply such uniform offsets for this update, we have chosen the higher initial minimum adjustment limit of 0.01, which is twice that used for GLODAPv2 (0.005), to minimize the possibility of false corrections. The full ramifications and a revised strategy for identifying and minimizing bias in pH data is a topic for future development of the GLODAP data synthesis procedures. The full collection of pH values in GLODAPv2.2019 should only be considered to be consistent between cruises to 0.01 to 0.02 pH units.

3.2.5

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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 Sérazin (2011). Apparent oxygen utilization was determined using the combined fit in Garcia and Gordon (1992).

Partial pressures for CFC-11, CFC-12, CFC-113, CCl_4, and SF_6 were calculated using the solubilities by Warner and Weiss (1985), Bu and Warner (1995), Bullister and Wisegarver (1998), and Bullister et al. (2002).

Whenever only two seawater CO_2 chemistry variables were reported, the third was calculated 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). If this resulted in a mix of measured and calculated values for a certain CO_2 system variable for a specific cruise, and if the number of calculated values were equal to or exceeded twice the number of measured, then all measured were replaced by calculated values. Calculated values have been assigned WOCE flag 0.

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however, more than a third of these (38%) had uncalibrated CTD O_2 values. For comparison, half of the cruises in GLODAPv2 with both data types (50%) had uncalibrated CTD O_2 (Olsen et al., 2016); this fraction is therefore improving, but it is still too large. Our simple linear

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For data files that only contain bottle values for either or both variables, the tallies are somewhat uncertain, as some CTD values might have been be mislabeled by the data originators.

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1 % compared to 5 % for the 724 GLODAPv2 cruises), for the halogenated transient tracers (0 %–3 % adjusted, depending on variable, compared to 6 %– 10 % for GLODAPv2), and for TCO_2 (two cruises, i.e., 2 % compared to 1 7% for GLODAPv2).

The distributions of the magnitude of adjustments applied are presented in Fig. 5 and Table 6. For salinity, oxygen, and silicate, adjustments between 1 and 2 times the initial minimum adjustment limit are most prevalent. For nitrate, phosphate, CFC-11, and CFC-12, adjustments equal to or larger than 2 times the limit are most prevalent. For the salinity and oxygen this reflects that any biases in the data tends to be between 1 and 2 times the limit, while for CFC-11 and CFC-12 it also likely reflects limitations in our ability to confidently identify small biases. These limitations are related to the strongly transient nature of the CFCs. For TCO_2 and TAlk, none of the adjustments are larger than 2 times the adjustment limit, and for both properties half of the adjustments applied are below the limit. For TAlk, this distribution of adjustments supports the lowered minimum adjustment limit of 4 μmol kg^{-1} (instead of 6 μmol kg^{-1}); these data have sufficient precision to enable the identification of such small adjustments.

For TAlk, seven out of eight adjustments are positive (i.e., the data are biased low), for pH nine out of 10 adjustments are positive, and for oxygen six out of seven are positive. The adjustments for other variables were more distributed around zero. For TAlk, prevalence of a negative bias was also observed in the inter-laboratory comparison reported by Bockmon and Dickson (2015), who suggested the cause being the use of end point titrations rather than the (preferred) equivalence point titrations. However, 6 out of 7 of the negative bias cruises were Japanese. A tendency for bias in Japanese cruises to be negative was also identified in GLODAPv2 and may be due to the use of internal reference material. We note that the TAlk data from 23 out of 29 Japanese cruises with viable deep crossover checks had no apparent deep offset, so the majority of new TAlk data from Japan were consistent with GLODAPv2 even with the lowered threshold.

The prevalence of positive pH adjustments may relate to the fact that at low pH (as is common in the deeper waters where crossover analyses are done), measurements made with purified dyes tend to be lower than pH determined using electrodes, using impure spectrophotometric dyes with older dye coefficients (Clayton and Byrne, 1993), or calculated from TCO_2 and TAlk (Carter et al., 2018). The latter three types of pH data constitute the bulk of the reference data for the consistency checks, so the prevalence of a modern negative bias may be a consequence of limitations in the approaches used for the secondary quality control of the pH data in GLODAP. As mentioned above, refining these should be a priority in the future.

Here, we acknowledge the issue and believe that a realistic estimate of the consistency of the pH data in the product is approximately 0.01–0.02.

Crossover comparison is conducted on deep-water samples so atmospheric exchange during sample collection on the new cruises is not a viable explanation for the trend of positive oxygen adjustments. Atmospheric contamination would usually increase deep-water oxygen concentrations since deep oxygen levels are usually low. The data are not collected in any particular region, or associated with any specific laboratory, country, or method. Consequently, no particular explanation can be offered for the prevalence of positive adjustments.

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Ocean silicate for the adjusted data is 11.1 % and that for salinity is 10 ppm (i.e., a salinity of 0.01). This can be ascribed to two cruises, 58GS20130717 and 58GS20160802, conducted in the Greenland Sea where an increasing presence of Arctic sourced deep waters generates changes in these properties (Blindheim and Rey, 2004; Lauvset et al., 2018; Olafsson and Olsen, 2010; Olsen et al., 2009) that have not been corrected for. The impact of northern variability on the final consistency estimate can be determined for the Atlantic Ocean by excluding all data north of 50° N from the analysis. This gives a much better initial and final consistency, on par with that for the Indian and Pacific Oceans (Table 8).

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(Dickson et al., 2007), the widespread use of CRMs (Dickson et al., 2003), and instrument automation. pH adjustment frequency also has a downward trend; however, the situation is far from ideal and a topic for future development in GLODAP. For the nutrients and oxygen, only

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and 5 % for the halogenated transient tracers. For TAlk the stated consistency for GLODAPv2 is 6 μmol kg^{-1} (Olsen et al., 2016). We now believe this is better, 4 μmol kg^{-1}, not only for the 116 new cruises, but for all data in GLODAPv2 from 2016 as well. This is based on the global average absolute offset for TAlk in the adjusted GLODAPv2 data product of 2.8 μmol kg^{-1} (Table 5 in Olsen et al. (2016)) and the use of the initial minimum adjustment limit of 4 μmol kg^{-1} for the cruises added with the present version. For pH on the other hand, the consistency among all data is likely not better than 0.01–0.02

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Table 1. Variables in the GLODAPv2.2019

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actions per variable

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actions per variable

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Summary of the distribution of applied adjustments per variable, in number of adjustments applied for each variable.

	Adj.< limit	**Limit ≤ adj. < 2 x limit**	**2 x limit ≤ adj.**
Salinity	0	1	0
Oxygen	0	5	2

NO_3	0	2	4
Si	3	6	4
PO_4	1	4	5
TCO_2	1	1	0
TAlk	4	4	0
pH	2	6	2
CFC-11	0	0	1
CFC-12	0	1	2
CFC-113	0	0	0
CCl_4	0	0	0

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Table

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Table 8. Improvements resulting from the quality control of Atlantic cruises south of 50°N

	ATLANTIC		
	unadj		**adj**
Sal [x1000]	3.2	=>	3.1
Oxy [%]	0.8	=>	0.6
NO_3 [%]	2.1	=>	1.3
Si [%]	2.2	=>	1.7
PO_4 [%]	1.2	=>	0.9
TCO_2 [µmol/kg]	1.8	=>	1.8
TAlk [µmol/kg]	2.5	=>	1.7
pH [x1000]	9.7	=>	6.0

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2019

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2019

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2019

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1001	06AQ20110805	Arctic	ARK-XXVI/3	20110805	20111006	Polarstern
1002	06AQ20120107	Atlantic	ANT-XXVIII/3	20120107	20120311	Polarstern
1003	06AQ20120614	Arctic	ARK XXVII/1	20120614	20120715	Polarstern
1004 2001	06AQ20141202 06M220120625	Atlantic	PS89; ANT-XXXMSM21/2	2012062520 141202	201501312012 0724	Polarstern*Maria S. Merian*

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1005	06AQ20150817	Arctic	PS-94, ARK-XXIX/3	20150817	20151015	Polarstern
1006 2002	06M2200704140 6M220130419	Atlantic	MSM05-1MSM27	2007041420 130419	200705032013 0506	*Maria S. Merian*

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1010	06M320140530	Atlantic	M107	20140530	20140703	Meteor
1011	06M320150501	Atlantic	M116/1	20150501	20150603	Meteor

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2006

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20100804

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Indian

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Investigator

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Hudson

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Arctic

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Sarmiento de Gamboa

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1017	096U20150321	Indian	SOCCOM; IN2015_v01; IMOS	20150321	20150330	Investigator
1018	096U20160108	Indian	IN2016_v01, SOCCOM	20160108	20160227	Investigator
1019	096U20160314	Indian	IN2016_v02, SOCCOM	20160314	20160413	Investigator
1020	096U20160426	Pacific	IN2016_V03, P15S, SOCCOM	20160426	20160630	Investigator
1021	09AR19940101	Indian	09AR9407_1, AU9407, SR03	19940101	19940301	Aurora Australis
1022	09AR19950717	Indian	FORMEX, 09AR9501_1	19950717	19950902	Aurora Australis
1023	09AR19960119	Indian	S04I	19960119	19960323	Aurora Australis
1024	09AR20160111	Indian	SOCCOM; Kerguelen Axis (K-Axis) V3	20160111	20160315	Aurora Australis
1025	18HU20130507	Atlantic	AR07W_2013FICARAM_XIX, A17	2013050720	201305282019	*HesperidesHudson*
2013	29HE20190406			190406	0518	

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1034	317W20130803	Pacific	WCOA2013	20130803	20130829	Fairweather
1035	318M20130321	Pacific	GOSHIP_P02	20130321	20130501	Melville

1036	320620140320	Pacific	P16S_2014	20140320	20140505	Nathaniel B. Palmer
1037	320620151206	Pacific	OOISO; NBP15_11	20151206	20160102	Nathaniel B. Palmer
1038	325020131025	Pacific	TGT303, P21_2013	20131025	20131220	Thomas G. Thompson
1039	32P020130829	Pacific	WCOA2013	20130821	20130829	Point Sur
1040	33HQ20150809	Arctic	HLY1502, GN01, ARC01	20150809	20151013	Healy
1041	33RO201308033	Atlantic	A16N_Davis Strait 2013, KN213-02	2013080320	201310012013	Ronald H. Brown*Knorr*
2022	16N20130914			130914	1003	

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Pacific

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1045	33RO20161119	Pacific	RB1606, P18_2016, SOCCOM	20161119	20170203	Ronald H. Brown
1046	33RR20160208	Indian	I08S_2016	20160208	20160316	Roger Revelle
1047	35PK201405153	Atlantic	OVIDE_2014, A01W_2014,	2014051520	201406302008	*Thalassa*Pourquoi Pas?
2026	5TH20080825		A25_2014SUBPOLAR08	080825	0915	

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20111205

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20111221

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1054	49NZ20151223	Indian	MR15-05, I10_2015	20151223	20160108	Mirai
1055	49NZ201702084	Pacific	MR16-09, P17E, SOCCOMks201203	2012041020	201703052012	Mirai*Keifu Maru II*
2033	9UF20120410			170208	0424	

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1104	58GS20160802	Arctic	75N_2016	20160802	20160812	G.O. Sars
1105	58HJ20120807	Arctic	IMR, Arctic 2012	20120807	20120817	Helmer Hansen
1106	74DI201105206	Atlantic	EEL_2011_D365PE278	2011052020	201105312007	Discovery*Pelagia*
2104	4PE20071026			071026	1117	

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1107	74DI20110606	Atlantic	UKOA_D366	20110606	20110709	Discovery
1108	74DI20120731	Atlantic	EEL_2012, D379, AR07E_2012	20120731	20120817	Discovery
1109	74EQ20151206	Atlantic	A05_2015	20151206	20160122	Discovery
1110	74JC199903157	Atlantic	JR40, Albatross, A23JC159	1999031520	199904232018	*James* Clark Ross*Cook*
2105	40H20180228			180228	0410	

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1112	74JC20071231	Atlantic	JR177	20071231	20080216	James Clark Ross
1113	74JC20150110	Atlantic	JR306	20150110	20150122	James Clark Ross
1114	74JC20151217	Atlantic	JR15003	20151217	20151229	James Clark Ross
1115	74JC20161110	Atlantic	JR16002, SR1B	20161110	20161203	James Clark Ross
1116	77DN20070812	Arctic	LOMROG	20070812	20070919	Oden

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Figure 5.

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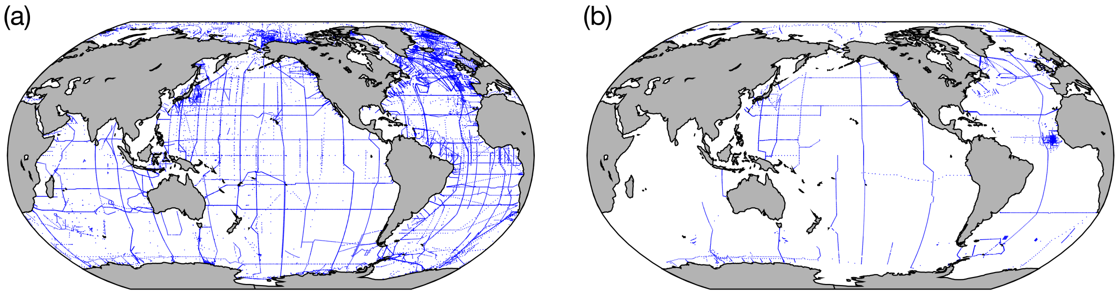
. Locations of stations included in the (a) Arctic, (b) Atlantic, (c) Indian, and (d) Pacific Ocean product files for the whole GLODAPv2.2019 dataset.



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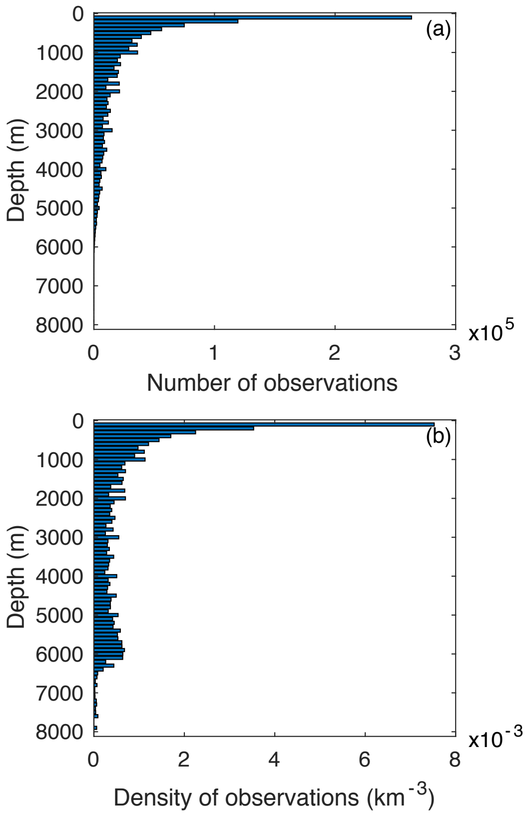
(a)
Depth (m)
0
1000
2000
3000
4000
5000
6000
7000
8000
0
1
2
3
x10^5
Number of observations
(b)
Depth (m)
0
1000
2000
3000
4000
5000
6000
7000
8000
0
2
4
6
8
x10^-3
Density of observations (km^-3)