An updated version of the global interior ocean biogeochemical data product, GLODAPv2.2021~~0~~

Siv K. Lauvset [1], Nico Lange [2], Toste Tanhua [2], Henry C. Bittig [3], Are Olsen [4], Alex Kozyr [5], Marta Álvarez [6], Susan Becker [7], Peter J. Brown [8], Brendan R. Carter [9,10], Leticia Cotrim da Cunha [11], Richard A. Feely [10], Steven van Heuven [12], Mario Hoppema [13], Masao Ishii [14], Emil Jeansson [1], Sara Jutterström [15], Steve D. Jones [4], Maren K. Karlsen [4], Claire Lo Monaco [16], Patrick Michaelis [2], Akihiko Murata [17], Fiz F. Pérez [18], Benjamin Pfeil [15], Carsten Schirnick [2], Reiner Steinfeldt [19], Toru Suzuki [20], Bronte Tilbrook [21], Anton Velo [18], Rik Wanninkhof [22], Ryan J. Woosley [23], and Robert M. Key [24]

[1] NORCE Norwegian Research Centre, Bjerknes Centre for Climate Research, Bergen, Norway
[2] GEOMAR Helmholtz Centre for Ocean Research Kiel, Kiel, Germany
[3] Leibniz Institute for Baltic Sea Research Warnemünde, Rostock, Germany
[4] Geophysical Institute, University of Bergen and Bjerknes Centre for Climate Research, Bergen, Norway
[5] NOAA National Centers for Environmental Information, Silver Spring, MD, USA
[6] Instituto Español de Oceanografía, IEO-CSIC, A Coruña, Spain
[7] UC San Diego, Scripps Institution of Oceanography, San Diego CA 92093, USA
[8] National Oceanography Centre, Southampton, UK
[9] Cooperative Institute for Climate Ocean and Ecosystem Studies, University Washington, Seattle, Washington, USA
[10] Pacific Marine Environmental Laboratory, National Oceanic and Atmospheric Administration, Seattle, Washington, USA
[11] Faculdade de Oceanografia/PPG-Oceanografia, Universidade do Estado do Rio de Janeiro, Rio de Janeiro (RJ), Brazil
[12] Centre for Isotope Research, Faculty of Science and Engineering, University of Groningen, Groningen, the Netherlands
[13] Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research, Bremerhaven, Germany
[14] Meteorological Research Institute, Japan Meteorological Agency, Tsukuba, Japan
[15] IVL Swedish Environmental Research Institute, Gothenburg, Sweden
[16] LOCEAN, Sorbonne Université, Paris, France
[17] Research Institute for Global Change, Japan Agency for Marine-Earth Science and Technology, Yokosuka, Japan
[18] Instituto de Investigaciones Marinas, IIM – CSIC, Vigo, Spain
[19] University of Bremen, Institute of Environmental Physics, Bremen, Germany
[20] Marine Information Research Center, Japan Hydrographic Association, Tokyo, Japan
[21] CSIRO Oceans and Atmosphere and Australian Antarctic Program Partnership, University of Tasmania, Hobart, Australia
[22] Atlantic Oceanographic and Meteorological Laboratory, National Oceanic and Atmospheric Administration, Miami, USA.
[23] Center for Global Change Science, Massachusetts Institute for Technology, Cambridge, Massachusetts, USA
[24] Atmospheric and Oceanic Sciences, Princeton University, Princeton, NJ, 08540, USA

Correspondence to: siv.lauvset@norceresearch.no

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

~~[1] Geophysical Institute, University of Bergen and Bjerknes Centre for Climate Research, Bergen, Norway~~
~~[2] GEOMAR Helmholtz Centre for Ocean Research Kiel, Kiel, Germany~~
~~[3] Atmospheric and Oceanic Sciences, Princeton University, Princeton, NJ, 08540, USA~~

[4] Leibniz Institute for Baltic Sea Research Warnemünde, Rostock, Germany

[5] NOAA National Centers for Environmental Information, Silver Spring, MD, USA

[6] Instituto Español de Oceanografía, A Coruña, Spain

[7] Departement of Fisheries and Oceans, Bedford Institute of Oceanography, Dartmouth, Nova Scotia, Canada

[8] UC San Diego, Scripps Institution of Oceanography, San Diego CA 92093, USA

[9] National Oceanography Centre, Southampton, UK

[10] Cooperative Institute for Climate Ocean and Ecosystem Studies, University Washington, Seattle, Washington, USA

[11] Pacific Marine Environmental Laboratory, National Oceanic and Atmospheric Administration, Seattle, Washington, USA

[12] Faculdade de Oceanografia, Universidade do Estado do Rio de Janeiro, Rio de Janeiro (RJ), Brazil

[13] Centre for Isotope Research, Faculty of Science and Engineering, University of Groningen, Groningen, the Netherlands

[14] Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research, Bremerhaven, Germany

[15] Oceanography and Geochemistry Research Department, Meteorological Research Institute, Japan Meteorological Agency, Tsukuba, Japan

[16] NORCE Norwegian Research Centre, Bjerknes Centre for Climate Research, Bergen, Norway

[17] IVL Swedish Environmental Research Institute, Gothenburg, Sweden

[18] Research Institute for Global Change, Japan Agency for Marine-Earth Science and Technology, Yokosuka, Japan

[19] Instituto de Investigaciones Marinas, IIM – CSIC, Vigo, Spain

[20] University of Bremen, Institute of Environmental Physics, Bremen, Germany

[21] Marine Information Research Center, Japan Hydrographic Association, Tokyo, Japan

[22] CSIRO Oceans and Atmosphere and Antarctic Climate and Ecosystems Co-operative Research Centre, University of Tasmania, Hobart, Australia

[23] Atlantic Oceanographic and Meteorological Laboratory, National Oceanic and Atmospheric Administration, Miami, USA.

[24] Center for Global Change Science, Massachusetts Institute for Technology, Cambridge, Massachusetts, USA

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

Abstract. The Global Ocean Data Analysis Project (GLODAP) is a synthesis effort providing regular compilations of surface-to-bottom ocean biogeochemical data, with an emphasis on seawater inorganic carbon chemistry and related variables determined through chemical analysis of seawater samples. GLODAPv2.2021 is an update of the previous version, GLODAPv2.2020. The major changes are: data from 43 new cruises were added, data coverage extended until 2020, removal of all data with missing temperatures, and the inclusion of a digital object identifier (doi) for each cruise in the product files. In addition, a number of minor corrections to GLODAPv2.2020 data were performed. GLODAPv2.2021 includes measurements from more than 1.3 million water samples from the global oceans collected on 989 cruises. ~~GLODAPv2.2020 is an update of the previous version, GLODAPv2.2019. The major changes are: data from 106 new cruises added, extension of time coverage to 2019, and the inclusion of available (also for historical cruises) discrete fugacity of CO_2 ($f$$CO_2$) values in the merged product files. GLODAPv2.2020 now includes measurements from more than 1.2 million water samples from the global oceans collected on 946 cruises.~~ The data for the 12 GLODAP core variables (salinity, oxygen, nitrate, silicate, phosphate, dissolved inorganic carbon, total alkalinity, pH, CFC-11, CFC-12, CFC-113, and CCl_4) have undergone extensive quality control with a focus on systematic evaluation of bias. The data are available in two formats: (i) as submitted by the data originator but updated to WOCE exchange format and (ii) as a merged data product with adjustments applied to minimize bias. . For this annual update, adjustments for the 43 new cruises were derived by comparing those data with the data from the 946 quality-controlled cruises in the GLODAPv2.2020 ~~These adjustments were derived by comparing the data from the 106 new cruises with the data from the 840 quality controlled cruises of the GLODAPv2.2019~~ data product using crossover analysis. Comparisons to empirical algorithm estimates provided additional context for adjustment decisions, this is new to this version. The adjustments are intended to remove potential biases from errors related to measurement, calibration, and data handling practices without removing known or likely time trends or variations in the variables evaluated. The compiled and adjusted data product is believed to be consistent to better than 0.005 in salinity, 1 % in oxygen, 2 % in nitrate, 2 % in silicate, 2 % in phosphate, 4 μmol kg^{-1} in dissolved inorganic carbon, 4 μmol kg^{-1} in total alkalinity, 0.01–0.02 in pH (depending on region), and 5 % in the halogenated transient tracers. The other variables included in the compilation, such as isotopic tracers and discrete $f$$CO_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.ncei.noaa.gov/access/ocean-carbon-data-system/oceans/GLODAPv2_2021/, last access: 07 July 2021). ~~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/ttgq-n825 (Lauvset et al., 2021)~~https://doi.org/10.25921/2c8h-sa89 (Olsen et al., 2020)~~. These bias-adjusted product files also include significant ancillary and approximated data, and can be accessed via www.glodap.info (last access: 29 June 2021).. These were obtained by interpolation of, or calculation from, measured data. This living data update documents the GLODAPv2.2021~~0~~ methods and provides a broad overview of the secondary quality control procedures and results.

1 Introduction

The oceans mitigate climate change by absorbing both atmospheric CO_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~~03 June 2021) 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

125 oceanic carbon, ocean acidification, ventilation rates, oxygen levels, and vertical nutrient transports (Tanhua et al., 2021). The core quality-controlled and bias-adjusted variables 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 chlorofluorocarbon-11 (CFC-11), CFC-12, CFC-113, and CCl_4.

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

135 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. In addition, the manual data retrieval is time consuming and prone to data handling errors (Tanhua et al., 2021). For biogeochemical data there is the added complexity

140 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). Despite this, biases in data still occur. These can arise from poor sampling and preservation practices,

145 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 calibration of the data from conductivity-temperature-depth (CTD) profiler mounted sensors is an additional and widespread problem, particularly for oxygen (Olsen et al., 2016). For halogenated transient tracers, uncertainties in standard gas composition, extracted water volume,

150 and purge efficiency typically provide the largest sources of uncertainty. In addition to bias, occasional outliers occur. In rare cases poor precision - many multiples worse than that expected with current measurement techniques - can render a set of data of limited use. GLODAP deals with these issues by presenting the data in a uniform format, including any meta data either publicly-available or submitted by the data originator, and by subjecting the data to primary and secondary quality control assessments, focusing on precision and consistency, respectively. The secondary quality control

155 focuses on deep data, where natural variability is minimal. Adjustments are applied to the data to minimize cases of bias that could be confidently established relative to the measurement precision for the variables and cruises considered. Key metadata is provided in the header of each data file, and full cruise reports submitted by the data providers are accessible through the GLODAPv2 cruise summary table (https://www.ncei.noaa.gov/access/ocean-carbon-data-system/oceans/GLODAPv2_2021/cruise_table_v2021.html, last access: 07 July 2021).

160 GLODAPv2.2021~~0~~ builds on earlier synthesis efforts for biogeochemical data obtained from research cruises, GLODAPv1.1 (Key et al., 2004; Sabine et al., 2005), Carbon dioxide in the Atlantic Ocean (CARINA) (Key et al., 2010),

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

Within this there are two types of GLODAP updates: full and intermediate. Full updates involve a reanalysis, notably crossover and inversion, of the entire dataset (both historical and new cruises) and all adjustments are subject to change. This was carried out for GLODAPv2. For intermediate updates, recently-available data are added following quality control procedures to ensure their consistency with the cruises included in the latest GLODAP release. Except for obvious outliers and similar types of errors (Sect. 3.3.1), the data included in previous releases are not changed during intermediate updates. Additionally, the GLODAP mapped climatologies (Lauvset et al., 2016) are not updated for these intermediate products. A naming convention has been introduced to distinguish intermediate from full product updates. For the latter the version number will change, while for the former the year of release is appended. The exact version number and release year (if appended) of the product used should always be reported in studies, rather than making a generic reference to GLODAP.

Creating and interpreting inversions, and other checks of the full data set needed for full updates are too demanding in terms of time and resources to be p~~re~~rformed every year or two -years. The aim is to conduct a full analysis (i.e., including an inversion) again after the third GO-SHIP survey has been completed. This completion is currently scheduled for 2023, and we anticipate that GLODAPv3 will become available a few years thereafter. In the interim~~rmin~~, the third intermediate update is presented here, which adds data from 43 new cruises to the last update, GLODAPv2.2020 (Olsen et al., 2020).

~~presented here is the second intermediate update, which adds data from 106 new cruises to the last update, GLODAPv2.2019 (Olsen et al., 2019).~~

2 Key features of the update

GLODAPv2.2021 contains data from 989 cruises covering the global ocean from 1972 to 2020, compared to 946 for the period 1972-2019 for GLODAPv2.2020 (Olsen et al., 2020). Information on the 43 cruises added to this version is provided in Table A1 in the Appendix. Cruise sampling locations are shown alongside those of GLODAPv2.2020 in Fig. 1, while the coverage in time is shown in Fig. 2. ~~GLODAPv2.2020 (Olsen et al., 2020) contains data from 946 cruises, covering the global ocean from 1972 to 2019, compared to 840 for the period 1972-2017 for GLODAPv2.2019. Information on the 106 cruises added to this version is provided in Table A1 in the Appendix. Cruise sampling locations are shown alongside those of GLODAPv2.2019 in Fig. 1, while the coverage in time is shown in Fig. 2.~~ Not all cruises have data for all of the above-mentioned 12 core variables; for example, cruises with only seawater CO_2 chemistry or

transient tracer data are still included even without accompanying nutrient data due to their value towards computation of, for example, carbon inventories. In some other cases, cruises without any of these properties measured were included – this was because they did contain data for other carbon related tracers such as carbon isotopes, with the main intention of ensuring their wider availability.

The added cruises are from the years 1982-2020, with most being more recent than 2014. In the Arctic Ocean there are seven cruises from the Canadian Basin carried out on RV *Louis S. St-Laurent* and one in the Nordic Seas carried out on RV *Johan Hjort*. In the Pacific Ocean the majority of added cruises are occupations of Line P carried out on RV *John P. Tully*, as well as a recent occupation of P06 (two legs with different expocodes) on RV *Nathaniel T. Palmer*. Note that for some Line P cruises only stations with seawater CO_2 chemistry data have been included in the product. Thus, all new Pacific Ocean cruises have seawater CO_2 chemistry data. Four out of six cruises added in the Atlantic Ocean (06M220140607 and 06M220160331 on RV *Maria S. Merian* and 06MT20180213 and 06MT20160828 on RV *Meteor*) do not have seawater CO_2 chemistry data, but are included for their transient tracer data. Five new Indian Ocean cruises are added, including the first occupation of GO-SHIP line I07N since 1995. All new cruises from the Indian Ocean include seawater CO_2 chemistry data, including pH on three of them, and transient tracers on all (with the exception of a 1982 cruise in the Red Sea onboard the RV *Marion Dufresne*). Finally, three new cruises are added from the Southern Ocean. All of these include seawater CO_2 chemistry.

All new cruises were subjected to primary (Sect. 3.1) and secondary (Sect. 3.2) quality control (QC). These procedures are the same as for GLODAPv2.2020, aiming to ensure the consistency of the data from the 43 new cruises with the previous release of this data product (in this case, the GLODAPv2.2020 adjusted data product).

For GLODAPv2.2021 we have also added a basin identifier to the product files, where 1 is the Atlantic Ocean, 4 is the Arctic Mediterranean Seas, 8 is the Pacific Ocean, and 16 is the Indian Ocean. These regions are abbreviated AO, AMS, PO, and IO respectively in the adjustment table. Data in the Mediterranean Sea are classified as AO. The basin identifier is now added to the product files to make it easier for users to identify in which ocean basin an individual cruise belongs, without having to use one of the four regional files. Note that there is no overlap between the regional files nor our basin identifiers, and cruises in the Southern Ocean are placed in the region where most of the data were collected. In this update we have also included the doi for each cruise in all product files, with the aim of easing access to the original data and metadata as well as improving the visibility of data providers.

The added cruises are from the years 2004-2019, with most being more recent than 2010. The majority of the new data were obtained from the two vessels RV *Keifu Maru II* and RV *Ryofu Maru III*, which are operated by the Japan Meteorological Agency in the western North Pacific (Oka et al., 2018; Oka et al., 2017). Another important addition is the data collected across the Davis Strait between Canada and Greenland, from 10 cruises between 2004-2015 through a collaboration between the Bedford Institute of Oceanography, Canada and the University of Washington, USA (Azetsu-Scott et al., 2012). Other cruises from the Atlantic include those carried out on the RV *Maria S. Merian* and RV *Meteor*, with transient tracer data but not nutrients or seawater CO_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 RRS *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*, with measurements for stable isotopes of carbon and oxygen ($\delta^{13}C$ and $\delta^{18}O$) off the Iberian Peninsula (Voelker et al., 2015) but no data for nutrients,

3 Methods

3.1 Data assembly and primary quality control

The data from the 106 new cruises were submitted directly to us or retrieved from data centers: typically the CLIVAR and Carbon Hydrographic Data Office (https://cchdo.ucsd.edu, last access: 03 June 2021~~20 October 2020~~), National Center for Environmental Information (https://www.ncei.noaa.gov, last access 03 June 2021~~20 October 2020~~), and PANGAEA (https://pangaea.de, last access 03 June 2021~~20 October 2020~~). Each cruise is identified by an expedition code (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: 03 June 2021~~20 June 2020~~).

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

7

Each data column (except temperature and pressure, which are assumed "good" if they exist) has an associated column of
280 data flags. For the original data exchange files, these flags conform to the WOCE definitions for water samples and are
listed in Table 2. For the merged and adjusted product files these flags are simplified: questionable (WOCE flag 3) and
bad (WOCE flag 4) data are removed and their flags are set to 9. The same procedure is applied to data flagged 8 (very
few such data exist); WOCE flags 1 (Data not received) and 5 (Data not reported) are also set to 9, while flags of 6 (Mean
of replicate measurements) and 7 (Manual chromatographic peak measurement) are set to 2, if the data appear good. Also,
285 in the merged product files a flag of 0 is used to indicate a value that could be measured but is somehow approximated:
for salinity, oxygen, phosphate, nitrate, and silicate, the approximation is conducted using vertical interpolation; for
seawater CO_2 chemistry variables (TCO_2, TAlk, pH, and fCO_2), the approximation is conducted using calculation from
two measured CO_2 chemistry variables (Sect 3.2.2). Importantly, interpolation of CO_2 chemistry variables is never
performed and thus a flag value of 0 has a unique interpretation.

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

3.2 Secondary quality control

The aim of the secondary QC was to identify and correct any significant biases in the data from the 43~~106~~ new cruises
relative to GLODAPv2.20~~19~~20, 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 202~~0~~1 in order to decide the
300 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 represent are the minimum bias that can be confidently established relative to the
measurement precision for the variables and cruises considered~~are set according to the expected measurement precision~~
~~for each variable~~, and are the same as those used for GLODAPv2.20~~19~~20. In addition to the average magnitude of the
offsets, factors such as the precision of the offsets, persistence towards the various cruises used in the comparison,
305 regional dynamics, and the occurrence of time trends or other variations were considered. Thus, not all offsets larger than
the initial minimum limits have been adjusted. A guiding principle for these considerations was to not apply an
adjustment whenever in doubt. Conversely, in some cases where data and offsets were very precise and the cruise had
been conducted in a region where variability is expected to be small, adjustments lower than the minimum limits were
applied. Any adjustment was applied uniformly to all values for a variable and cruise, i.e., an underlying assumption is
310 that cruises suffer from either no or a single and constant measurement bias. Adjustments for salinity, TCO_2, TAlk and
pH are always additive, while adjustments for oxygen, nutrients and the halogenated transient traces are always
multiplicative. Except where explicitly noted (Sect. 3.3.1), adjustments were not changed for data previously included in
GLODAPv2.20~~19~~20.

Crossover comparisons, multi-linear regressions (MLRs), and comparison of deep-water averages were used to identify
315 offsets for salinity, oxygen, nutrients, TCO_2, TAlk, and pH (Sect. 3.2.2 and 3.2.3). As in GLODAPv2.2020, but 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). As in GLODAPv2.2020 we made extensive use of two

8

predictions from two empirical algorithms~~In contrast to GLODAPv2 and GLODAPv2.2019, evaluation of the internal consistency of the seawater CO₂ chemistry variables was not used for the evaluation of pH (Sect. 3.2.4). New to the present version is more extensive use of two predictions from two empirical algorithms~~ —"CArbonate system And Nutrients concentration from hYdrological properties and Oxygen using a Neural-network version B" (CANYON-B) and "CONsisTency EstimatioN and amounT" (CONTENT), (Bittig et al., 2018)—for the evaluation of offsets in nutrients and seawater CO_2 chemistry data (Section 3.2.5). For the halogenated transient tracers, comparisons of surface saturation levels and the relationships among the tracers were used to assess the data 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 by analysis of water samples (bottle data) and/or directly from the CTD sensor pack. These two measurement types are merged and presented as a single variable in the product. The merging was conducted prior to the consistency checks, ensuring their internal calibration in the product. The merging procedures were only applied to the bottle data files, which commonly include values recorded by the CTD at the pressures where the water samples are collected. Whenever both CTD and bottle data were present in a data file, the merging step considered the deviation between the two and calibrated the CTD values if required and possible. Altogether seven scenarios (Table 4) are possible for each of the CTD-O₂ sensor properties individually, where the fourth ~~(see below)~~ and sixth 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 are available: use CTD values.~~
3. ~~No CTD values are available: use bottle values.~~
4. ~~Too few data of both types are available for comparison and more than 80 % of the records have bottle values: use 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 GLODAPv2.20~~19~~20 data product as the reference data product. The toolbox implements the 'running-cluster' crossover analysis first described by Tanhua et al. (2010). This analysis compares data from two cruises on a station-by-station basis and calculates a weighted mean offset between the two and its weighted standard deviation. The weighting is based on the scatter in the data such that data that have less scatter have a larger influence on the comparison than data with more scatter. Whether the scatter reflects actual variability or data precision is irrelevant in this context as increased scatter nevertheless decreases the confidence in the comparison. Stations are compared when they are within 2° arc distance (~ 200 km) of each other. Only deep data are used, to minimize the effects of natural variability. Either the 1500 or 2000 dbar depth surface was used as upper bound, depending on the number of available data, their variation at

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

As an example of crossover analysis, the crossover for TCO_2 measured on the two cruises 320620170820 (P06E), which is new to this version, and 49NZ20030803, which was included in GLODAPv2, is shown in Fig. 3. For TCO_2 the offset is determined as the difference in accordance with the procedures followed for GLODAPv2. The TCO_2 values from 320620170820 are comparable, with a weighed mean offset of 0.84 ± 3.12 µmol kg^{-1} compared to those measured on 49NZ20030803.

For each of the 43 new cruises, such a crossover comparison was conducted against all possible cruises in GLODAPv2.2020, 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 on 320620170820 is shown in Fig. 4. The TCO_2 data measured on this cruise are 2.15 ± 1.04 µmol kg^{-1} higher when compared to the data measured on nearby cruises included in GLODAPv2.2020. This is well within the initial minimum adjustment limit for TCO_2 of 4 µmol kg^{-1} (Table 3), and as such does not qualify for an adjustment of the data in the merged data product. All other variables show the same high consistency (not shown), thus, no adjustment is given to any variable on cruise 320620170820 in GLODAPv2.2021. This is supported by the CANYON-B and CONTENT results (Sect. 3.2.5). As an example of crossover analysis, the crossover for TCO_2 measured on the two cruises 49UP20160109, which is new to this version, and 49UP20160703, which was included in GLODAPv2.2019, is shown in Fig. 3. For TCO_2 the offset is determined as the difference, as is the case for salinity, TAlk, and pH. For the nutrients, oxygen, and the halogenated transient tracers, ratios are used. This is in accordance with the procedures followed for GLODAPv2. The TCO_2 values from 49UP20160109 are higher, with a weighed mean offset of 3.62 ± 2.67 µmol kg^{-1} compared to those measured on 49UP20160703.

For each of the 106 new cruises, such a crossover comparison was conducted against all possible cruises in GLODAPv2.2019, i.e., all cruises that had stations closer than 2° arc distance to any station for the cruise in question. The summary figure for TCO_2 on 49UP20160109 is shown in Fig. 4. The TCO_2 data measured on this cruise are high by 3.68 ± 0.83 µmol kg^{-1} when compared to the data measured on nearby cruises included in GLODAPv2.2019. This is slightly less than the initial minimum adjustment limit for TCO_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: this is somewhat less than indicated by the crossover analysis, but a smaller adjustment is supported by the CANYON-B and CONTENT results (Sect. 3.2.5).

395 Adjustments are typically round numbers ~~relative to the precision of the variable being considered~~ (e.g., -3 not -3.4 for TCO$_2$ and 0.005 not 0.0047 for pH) to avoid ~~the~~ communicating that the ideal adjustments are known to high precision. ~~One exception to the above described procedure exists, namely in the Sea of Japan where six new cruises were added. In this region, only two other cruises were included in GLODAPv2.2019. Therefore, all eight cruises were compared against each other and strong outliers were adjusted accordingly, instead of adjusting the six new cruises towards the existing~~
400 ~~two.~~

3.2.3 Other consistency analyses

MLR analyses and deep water averages, broadly following Jutterström et al. (2010), were also used for the secondary QC of salinity, oxygen, nutrients, TCO$_2$, and TAlk data. These approaches are particularly valuable when a cruise has either very few or no valid crossovers with GLODAPv2, but are used more generally to provide more insight on the consistency
405 of the data. For the 43 new cruises of the present update, no adjustment decisions were made on the basis of MLR and deep water average analyses alone. ~~The latter was the case for the 106 new cruises; i.e., no adjustment decisions were reached on the basis of MLR and deep water average analyses alone. For the MLRs, the~~The presence of bias in the data was identified by comparing the MLR-generated values with the measured values. Both analyses were conducted on samples collected deeper than the 1500 or 2000 dbar pressure level to minimize the effects of natural variations, and both
410 used available GLODAPv2.20~~19~~20 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
415 were suspect for the cruise in question were avoided (e.g., if oxygen appeared biased it was not included as an independent variable). The MLRs could be based on 10 to 500 samples, and the robustness of the fit (r^2, RMSE) and quantity of fitting data were considered when using the results to guide whether to apply a correction. The same applies for the deep-water averages (i.e., the standard deviation of the mean). MLR and deep-water average results showing offsets above the minimum adjustment limits were carefully scrutinized, along with available crossover values and
420 CANYON-B and CONTENT estimates, to determine whether or not to apply an adjustment.

3.2.4 pH scale conversion and quality control

Altogether 13 of the 43 new cruises included measured pH data, and none required adjustment (Sect. 4.2). All new pH data were reported on the total scale and at 25 °C so no scale and/or temperature conversion was necessary. For details on scale and temperature conversions in previous versions of GLODAPv2 we refer the reader to Olsen et al. (2020). In
425 contrast to past quality control of GLODAP pH data, evaluation of the internal consistency of CO$_2$ system variables was not used for the secondary quality control of the pH data of the 13 new cruises; only crossover analysis was used, supplemented by CONTENT and CANYON-B comparisons (Sect. 3.2.5). Recent literature has demonstrated that internal consistency evaluation procedures are subject to errors owing to incomplete understanding of the thermodynamic constants, major ion concentrations, measurement biases, and potential contribution of organic compounds or other
430 unknown protolytes to alkalinity. These complications lead to pH-dependent offsets in calculated pH compared with cruise spectrophotometric pH measurements (Álvarez et al., 2020; Carter et al., 2018; Fong and Dickson, 2019), but not with those derived in lab conditions using ISFET (Ion Sensitive Field Effect Transistor) sensors (Takeshita et al., 2020).

The pH-dependent offsets may be interpreted as biases and generate false corrections. ~~Altogether 82 of the 106 new cruises included measured pH data. For one of these, the pH data were not supplied on the total scale or at 25 °C and 0 dbar pressure, which is the GLODAP standard, and were thus converted. The conversion was conducted using CO2SYS (Lewis and Wallace, 1998) for MATLAB (van Heuven et al., 2011) with reported pH and TAlk as inputs, and generating pH output values at total scale at 25 °C and 0 dbar of pressure (named phts25p0 in the product). Missing TAlk data were approximated as 67 times salinity. The proportionality (67) is the mean ratio of TAlk to salinity in GLODAPv2 data. The uncertainties introduced with this approximation are negligible (order 10^{-7} pH units) for the scale conversions and order 10^{-3} pH units for the temperature and pressure conversion (evaluated by repeating conversions with 2 times the standard deviation of the ratio, i.e., 67 ± 4.1). This is sufficiently accurate relative to other sources of uncertainty, which are discussed below. Data for phosphate and silicate are also needed, and were, whenever missing, determined using CANYON B (Bittig et al., 2018). The conversion was conducted with the carbonate dissociation constants of Lueker et al. (2000), the bisulfate dissociation constant of Dickson (1990), and the borate to salinity ratio of Uppström (1974). These procedures are the same as used for GLODAPv2.2019 (Olsen et al., 2019).~~

~~In contrast to past GLODAP pH QC, evaluation of the internal consistency of CO_2 system variables was not used for the secondary quality control of the pH data of the 106 new cruises; only crossover analysis was used, supplemented by CONTENT and CANYON B (Sect. 3.2.5). Recent literature has demonstrated that internal consistency evaluation procedures are subject to errors owing to incomplete understanding of the thermodynamic constants, major ion concentrations, measurement biases, and potential contribution of organic compounds or other unknown protolytes to alkalinity (Takeshita et al., 2020), which lead to pH dependent offsets in calculated pH (Álvarez et al., 2020; Carter et al., 2018): these may be interpreted as biases and generate false corrections.~~ The offsets are particularly strong at pH levels below 7.7, when calculated and measured pH are different by on average between 0.01 and 0.02 units. For the North Pacific this is a problem as pH values below 7.7 can occur at the depths interrogated during the QC (>1500 dbar for this region, Olsen et al., 2016). Since any corrections, which may thus be an artifact, are applied to the full profiles, we use a minimum adjustment ~~we assign an uncertainty~~ of 0.02 to the North Pacific pH data in the merged product files. Elsewhere, the ~~uncertainties~~inconsistencies that have arisen are smaller, since deep pH is typically larger than 7.7 (Lauvset et al., 2020), and at such levels the difference between calculated and measured pH is less than 0.01 on average (Álvarez et al., 2020; Carter et al., 2018). Outside the North Pacific, we believe, therefore that the pH data are consistent to 0.01. Avoiding interconsistency considerations for these intermediate products helps to reduce the problem, but since the reference data set (also as used for the generation of the CANYON-B and CONTENT algorithms) has these issues, a full re-evaluation, envisioned for GLODAPv3, is needed to address the problem satisfactorily.

3.2.5 CANYON-B and CONTENT analyses

CANYON-B and CONTENT (Bittig et al., 2018) were used to support decisions regarding application of adjustments (or not). CANYON-B is a neural network for estimating nutrients and seawater CO_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.

Used in the correct way and with caution this tool is a powerful supplement to the traditional crossover analyses. Specifically, we gave no weight to comparisons where the crossover analyses had suggested that the S and/or O_2 data were biased as this would lead to error in the predicted values. We also considered the uncertainties of the CANYON-B and CONTENT estimates. These uncertainties are determined for each predicted value, and for each comparison the ratio of the difference (between measured and predicted values) to the local uncertainty was used to gauge the comparability. As an example, the CANYON-B/CONTENT analyses of the data obtained for 320620170820 are presented in Fig. 5. The CANYON-B and CONTENT results confirmed the crossover comparisons for TCO_2 discussed in Sect. 3.2.2. The magnitude of the inconsistency for both the CONTENT and the CANYON-B estimates was 0.6 µmol kg^{-1}, i.e., less than the weighted mean crossover offset of 2.1 µmol kg^{-1} (Fig. 4). ~~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 inconsistency 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 these procedures provide estimates at the level of individual data points, e.g., pH values are determined for every sampling location and depth where T, S, and O_2 data are available. Cases of strong differences between measured and estimated values are always examined. This has helped to identify primary QC issues for some cruises and variables, for example a case of an inverted pH profile on cruise 32PO20130829, which was identified and amended in GLODAPv2.2020.
~~This has helped to identify primary QC issues for some variables and cruises, for example a case of an inverted pH profile at cruise 32PO20130829, which has been amended.~~

3.2.6 Halogenated transient tracers

For the halogenated transient tracers (CFC-11, CFC-12, CFC-113, and CCl_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 concentrations at depth. As for GLODAPv2, the procedures were the same as those applied for CARINA (Jeansson et al., 2010; Steinfeldt et al., 2010). No QC is performed for SF_6 in GLODAP, but there are plans to include this in future versions.

3.3 Merged product generation

The merged product file for GLODAPv2.2021~~0~~ was created by correcting known issues in the GLODAPv2.202~~0~~2019
510   merged file, and then appending a merged and bias-corrected file containing the 43~~106~~ new cruises to this error-corrected
GLODAPv2.202~~0~~2019 file.

3.3.1 Updates and corrections for GLODAPv2.202~~0~~2019

Several minor omissions and errors have been identified in the GLODAPv2.2020 data product since the release in 2020.
Most of these have been corrected in this release, but some issues, such as those relating to pH in the North Pacific (Sect.
515   3.2.4), will not be remedied before GLODAPv3. In addition, some recently available data have been added for a few
cruises. The changes are:

- Individual suspicious samples, identified and reported by users and data providers, have been deleted from the
product. This affects oxygen on cruises 31DS19940126 and 29HE20130320; nutrients on cruises 316N19950829
and 06BE20001128; salinity on cruises 06BE20001128, 316N19921006, 318M19730822, 35A319950221,
520   49K619940107, and 32PO20130829; and TAlk on cruises 58P320011031, 33RO20071215, and 316N19821201.
- For data with missing (except Gerard bottles, Sect. 3.3.2) or bad temperature all other data have been set to NaN.
For future updates we will attempt to find the missing temperatures and, where possible, restore the now deleted
data.
- Corrected all cases where a secondary QC-flag of 1 had been erroneously assigned. This happened for cases where
525   the secondary QC flag was 1, but the data fields of the entire cruise were only NaN. The only case where this
would be correct is if a -777 is given in the adjustment table; all other cases were changed to a secondary QC-flag
of 0.
- All fCO_2 data are reported at a constant temperature of 20°C as described in Olsen et al. (2020). In some cases
temperature was not reported for calculated fCO_2, so where missing, a temperature of 20 °C has been assigned to
530   calculated fCO_2 data.
- Cruise 18SN19950803 has been given a 8% downward adjustment on phosphate and cruise 49NZ20020822 has
been given a 6% upward adjustment for phosphate. Both were identified as clear outliers when analyzing
crossovers for the seven new cruises in the area (JOIS, Table A1), and the addition of so many new crossovers
allowed for robust assessment of necessary adjustments.
535   - TAlk has been updated for station 106 on cruise 33RO19980123.
- Updated data for dissolved total nitrogen (tdn), pH, and TAlk was submitted and included for cruise
33RR20160208. Missing carbon variables have also been calculated for these updated data, and assigned a flag 0.
- $\Delta^{14}C$ data on 33MW19910711 have been updated.
- On cruise 33RO20161119 $\Delta^{14}C$ and $\delta^{13}C$ data have been added, and BTLNBR updated.
540   CTDPRS for station 5 (cast 2) on cruise 33RO20131223 have been corrected~~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.

- All $\delta^{13}C$ values from the large volume Gerard barrels (identified by bottle number greater than 80) were removed from the product files as these values often have poor precision and accuracy related to gas extraction procedures.

- For 33HQ20150809, temperatures of station 52 cast 1 were found bad (less than -2 °C) and have been removed, hence all other samples were removed for this cast as well (the same depths and variables were sampled at the other casts, however). Temperatures for casts 2 and 8 were replaced with updated values; these changes are very minor, on the order of 0.001 °C.

- For cruises 33RO20110926, 33RO20150525, and 33RO20150410, $\delta^{13}C$ and $\Delta^{14}C$ data have become available and were added to the product.

- Ship code for all RV *Maria S. Merian* cruises have been changed from MM to M2.

- For cruises 49SH20081021 and 49UF20121024, an adjustment of + 6 µmol kg^{-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.

- Neutral density values in GLODAPv2 and GLODAPv2.2019 had been calculated using the polynomial approximation of Sérazin (2011). All of these values were replaced with neutral density calculated following Jackett and McDougall (1997).

- Discrete fCO$_2$ data are now included in the product files whenever available. Discrete fCO$_2$ is one of the variables that describe 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 in combination with TCO_2 to calculate TAlk. 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 seawater CO_2 chemistry variables (Carter et al., 2018; Fong and Dickson, 2019; Takeshita et al., 2020; Álvarez et al., 2020). A total of 33 924 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 *f*CO₂ data have not been subjected to secondary QC. The inclusion of discrete *f*CO₂ data has led to some changes in the calculations of missing seawater CO₂ 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:

590

- Data from the 43~~106~~ new cruises were merged and sorted according to EXPOCODE, station, and pressure. GLODAP cruise numbers were assigned consecutively, starting from 32~~001~~, so they can be distinguished from the GLODAPv2.2019 cruises, which ~~that~~ ended at 2106~~1116~~.

- For some cruises the combined concentration of nitrate and nitrite was reported instead of nitrate. If explicit nitrite concentrations were also given, these were subtracted to get the nitrate values. If not, the combined concentration was renamed to nitrate. As nitrite concentrations are very low in the open ocean, this has no practical implications.

595

- 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.

600

- Whenever temperature was missing in the original data file, all data for that record were removed and their flags set to 9. The same was done when both pressure and depth were missing. For all surface samples collected using buckets or similar, the bottle number was set to zero. There are some exceptions to this, in particular for cruises that also used Gerard barrels for sampling. These may have valuable tracer data that are not accompanied by a temperature, so such data have been retained.

605

- All data with WOCE quality flags 3, 4, 5, or 8 were excluded from the product files and their flags set to 9. Hence, in the product files a flag 9 can indicate not measured (as is also the case for the original exchange formatted data files) or excluded from the product; in any case, no data value appears. All flags 6 (replicate measurement) and 7 (manual chromatographic peak measurement) were set to 2, provided the data appeared good.

610

- Missing sampling pressures (depths) were calculated from depths (pressures) following UNESCO (1981).

- For both oxygen and salinity, CTD and bottle values were merged following procedures summarized in Sect. 3.2.1.

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

615

- The data for the 12 core variables were corrected for bias using the adjustments determined during the secondary QC.

- Values for potential temperature and potential density anomalies (referenced to 0, 1000, 2000, 3000, and 4000 dbar) were calculated using Fofonoff (1977) and Bryden (1973). Neutral density for all 989 cruises was calculated using Jackett and McDougall (1997). ~~, thus neutral density for all 946 cruises are calculated using this procedure~~

620

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

16

- Partial pressures for CFC-11, CFC-12, CFC-113, CCl4, 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).

625
- 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

630
regard to which pair to use for the calculation of fCO$_2$. We followed two simple principles. First, TCO_2 and TAlk was the preferred pair to calculate pH and fCO$_2$, because we have higher confidence in the TCO_2 and TAlk data than pH (given the issues summarized in Sect. 3.2.4) and fCO$_2$ (because it was not subjected to secondary QC). Second, if either TCO_2 or TAlk was missing and both pH and fCO$_2$ data existed, pH was preferred (because fCO$_2$ has not been subjected to secondary QC). All other combinations involve only two measured variables. The

635
calculations were conducted using CO2SYS (Lewis and Wallace, 1998) for MATLAB (van Heuven et al., 2011), 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) as in GLODAPv2.2020 and earlier versions (Olsen et al., 2020). We are aware that the borate-to-salinity ratio of Lee et al. (2010) is becoming community standard, but here maintain Uppström (1974) in order to maintain consistency between versions. with the constants set as for the

640
pH conversions (Sect. 3.2.4). For calculations involving TCO_2, TAlk, and pH, if less than a third of the total number of values, measured and calculated combined, for a specific cruise were measured, then all these were replaced by calculated values. The reason for this is that secondary QC of the few measured values was often not possible in such cases, for example due to a limited number of deep data available. Such replacements were not done for calculations involving fCO$_2$, as this would either overwrite all measured fCO$_2$ values or would entail

645
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., fCO$_2$). Calculated seawater CO_2 chemistry values have been assigned WOCE flag 0. Seawater CO_2 chemistry values have not been interpolated, so the interpretation of the 0 flag is unique.

- The resulting merged file for the 43106 new cruises was appended to the merged product file for

650
GLODAPv2.201209.

4 Secondary quality control results and adjustments

All material produced during the secondary QC is available via the online GLODAP Adjustment Table hosted by GEOMAR, Kiel, Germany at https://glodapv2-2021.geomar.de/ (last access: 29 June 2021), https://glodapv2-2020.geomar.de/ (last access: 18 June 2020), and which can also be accessed through www.glodap.info. This is similar in

655
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 75 % of the 43 new cruises both CTD and bottle data of salinity were included in the original cruise data files and for all these cruises

660 the two data types were found to be consistent. This is similar to the GLODAPv2.2020 results. For oxygen, 63 % of the new cruises included both CTD O_2 and bottle values, which is much more than for GLODAPv2.2020 (25%), but comparable to GLODAPv2.2019. 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_2 665 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 670 calibration of the CTD values (23 out of 27 cruises), while for four cruises no good fit could be obtained and their CTD O_2 data are not included in the product. 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

675 The secondary QC has 5 different outcomes, provided there are data. These are summarized in Table 5, along with the corresponding codes that appear in the online Adjustment Table and that are also occasionally used as shorthand for decisions in the coming text. The level of secondary QC varies among the cruises. Specifically, in some cases data were too shallow or geographically too isolated for full and conclusive consistency analyses. A secondary QC flag has been included in the merged product files to enable their identification, with "0" used for variables and cruises not subjected to 680 full secondary QC (corresponding to code -888 in Table 5) and "1" for variables and cruises that were subjected to full secondary QC. The secondary QC flags are assigned per cruise and variable, not for individual data points and are independent of—and included in addition to—the primary (WOCE) QC flag. For example, interpolated (salinity, oxygen, nutrients) or calculated (TCO_2, TAlk, pH) values, which have a primary QC flag 0, may have a secondary QC flag of 1 if the measured data these values are based on have been subjected to full secondary QC. Conversely, individual data points 685 may have a secondary QC flag of 0, even if their primary QC flag is 2 (good data). A 0 flag means that data were too shallow or geographically too isolated for consistency analyses or that these analyses were inconclusive, but that we have no reasons to believe that the data in question are of poor quality. Prominent examples for this version are the two new cruises in the Salish Sea: no data were available in this region in GLODAPv2.2020, which, combined with quite shallow sampling depths, rendered conclusive secondary QC impossible. Prominent examples for this version are the 10 new 690 Davis Strait cruises: no data were available in this region in GLODAPv2.2019, which, combined with complex hydrography and differences in sampling locations, rendered conclusive secondary QC impossible. As a consequence, most, but not all, of these data (some being excluded because of poor precision after consultation with the PI) are included with a secondary QC flag of 0.

The secondary QC actions for the 12 core variables and the distribution of applied adjustments are summarized in Table 6 695 and Fig. 6, respectively. For most variables, only a very small fraction of the data are adjusted: no salinity or pH data, 4.5 % of TCO_2 and TAlk data, 7 % of oxygen data, 14 % of nitrate and phosphate data, and 21 % of silicate data. For the CFCs, no data required adjustment. Overall, the magnitudes of the various adjustments applied are also small. There is a larger fraction of data requiring adjustments to nutrients in GLODAPv2.2021 compared to

GLODAPv2.2020. However, the tendency observed during the production of GLODAPv2.2019 and GLODAPv2.2020 remains, namely that the large majority of recent cruises are consistent with earlier releases of the GLODAP data product. Only 13 out of the 43 new cruises included measured pH data and none received an adjustment. However, we have not performed a new crossover and inversion analysis of all pH data in the northwestern Pacific (though such analysis is planned for the next full update of GLODAP, i.e., GLODAPv3). Therefore, for now the conclusion from GLODAPv2.2020 remains and some caution should be exercised if looking at trends in ocean pH in the northwestern Pacific using GLODAPv2.2020 or GLODAPv2.2021.

no salinity data, 1 % of oxygen and nitrate data, 2 % of TCO$_2$ data, 5 % of TAlk data, 7 % of phosphate data, and 9 % of silicate data are adjusted. For the CFCs, data from one of 16 cruises with CFC-11 are adjusted, while for CFC-12 and CFC-113 the fractions are two of 21 cruises and one of three cruises respectively. The magnitudes of the various adjustments applied are also small, overall. Thus, the tendency observed during the production of GLODAPv2.2019 remains, namely that the large majority of recent cruises are consistent with earlier releases of this product.

For the Sea of Japan cruises, (where two existed in GLODAPv2.2019 and six were added in this version – Sect. 3.2.2), the crossover results showed biased TCO$_2$ data for one of the older cruises (49HS20081021, which is now adjusted up by 6 µmol kg^{-1}), and biased TAlk data for two of the presently added cruises (49UF20111004 and 49UF20121024, adjusted up by 5 and 6 µmol kg^{-1}, respectively)

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

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

The improvement in data consistency due to the secondary QC process is evaluated by comparing the weighted mean of the absolute offsets for all crossovers before and after the adjustments have been applied. This "consistency improvement" for core variables is presented in Table 7. The data for CFCs were omitted from these analyses for previously discussed reasons (Sect. 3.2.6). Globally, the improvement is modest. Considering the initial data quality, this result was expected. However, this does not imply that the data initially were consistent everywhere. Rather, for some regions and variables there are substantial improvements when the adjustments are applied.

For example, silicate in the Atlantic Ocean shows a considerable improvement and nutrients in general show improvements in almost all regions, including globally.

For example, Arctic Ocean phosphate, Indian Ocean silicate and TAlk, and Pacific Ocean pH data all show considerable improvements. For the latter, the improvement is a result of exclusion of data and not application of adjustments, as discussed above.

The various iterations of GLODAP provide insight into initial data quality covering more than 4 decades. Figure 78 summarizes the applied absolute adjustment magnitude per decade. These distributions are broadly unchanged compared to GLODAPv2.202019 (Fig. 86 in Olsen et al., 202019). Most TCO_2 and TAlk data from the 1970s needed an adjustment, but this fraction steadily declines until only a small percentage is adjusted in recent years. This is encouraging and demonstrates the value of standardizing sampling and measurement practices (Dickson et al., 2007), the widespread use of CRMs (Dickson et al., 2003), and instrument automation. The pH adjustment frequency also has a downward trend; however, there remain issues with the pH adjustments and this is a topic for future development in GLODAP, with the support from the OCB Ocean Carbonate System Intercomparison Forum (OCSIF, https://www.us-ocb.org/ocean-carbonate-system-intercomparison-forum/, last accessed: 20 June 202003 June 2021) working group (Álvarez et al., 2020). For the nutrients and oxygen, only the phosphate adjustment frequency decreases from decade to decade. However, we do note that the more recent data from the 2010s receive the fewest adjustments. This may reflect recent increased attention that seawater nutrient measurements have received through an operation manual (Becker et al., 2019; Hydes et al., 2012) availability of CRMNS (Aoyama et al., 2012; Ota et al., 2010), and the SCOR working group #147, Towards comparability of global oceanic nutrient data (COMPONUT). For silicate, the fraction of cruises receiving adjustments peaks in the 1990s and 2000s. This is related to the 2 % offset between US and Japanese cruises in the Pacific Ocean that was revealed during production of GLODAPv2 and discussed in Olsen et al. (2016). For salinity and the halogenated transient tracers, the number of adjusted cruises is small in every decade.

5 Data availability

The GLODAPv2.2021 merged and adjusted data product is archived at NOAA NCEI under https://doi.org/10.25921/ttgq-n825 (Lauvset et al., 2021). 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.ncei.noaa.gov/access/ocean-carbon-data-system/oceans/GLODAPv2_2021/https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2_2020/ (last access: 22 07 Junely 20210). The data are available as comma-separated ascii files (*.csv) and as binary MATLAB files (*.mat) that use the open-source Hierarchical Data Format version 5 (HDF5) data format. The data product is also made available as an Ocean Data View (ODV) file which can be easily explored using the "webODV Explore" online data service (https://explore.webodv.awi.de/, last access: 07 July 2021). 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. 89. 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, and a similar table is provided for matching the GLODAP cruise number with the data DOI. In the MATLAB files this information (EXPOCODE and DOI) is available as a cell array. A "known issues document" accompanies the data files and provides an overview of known errors and omissions in the data product files. It is regularly updated, and users are encouraged to inform us whenever any new issues are identified. It is critical that users consult this document whenever the data products are used.

The original cruise files, with updated flags determined during additional primary GLODAP QC, are available through the GLODAPv2.2021 cruise summary table (CST) hosted by NOAA NCEI: https://www.ncei.noaa.gov/access/ocean-carbon-data-system/oceans/GLODAPv2_2021/cruise_table_v2021.html (last access: 07 July 2021). Each of these files has been assigned a doi, which is included in the data product files, but not listed here. The original cruise files are available through the GLODAPv2.2020 cruise summary table (CST) hosted by NOAA NCEI: https://www.node.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 GLODAPv2.2021 is made available without any restrictions, users of the data should adhere to the fair data use principles:

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

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

6 Summary

GLODAPv2.2021 is an update of GLODAPv2.2020. Data from 43 new cruises have been added to supplement the earlier release and extend temporal coverage by 1 year. GLODAP now includes 47 years, 1972–2020, of global interior ocean biogeochemical data from 989 cruises.

The total number of data records is 1 334 269. Records with measurements for all 12 core variables (salinity, oxygen, nitrate, silicate, phosphate, TCO_2, TAlk, pH, CFC-11, CFC-12, CFC-113, and CCl_4) are very rare; only 2029 records have measured data for all 12 in the merged product file (interpolated and calculated data excluded). Requiring only two out of the four measured seawater CO_2 chemistry variables, in addition to all the other core variables, brings the number of available records up to 9231, so this is also very rare. A major limiting factor to having all core variables is the simultaneous availability of data for all four transient tracer species: only 26 137 records have measurements of CFC-11, CFC-12, CFC-113, and CCl_4 while 422 029 have data for at least one of these (not considering availability of other core variables). A total of 423 544 records have measured data for two out of the three CO_2 chemistry core variables. The number of measured fCO$_2$ data is 33 844; note again that these data were not subjected to quality control. The number of records with measured data for salinity, oxygen, and nutrients is 832 566, while the number of records with salinity and

oxygen data is 1 127 477. All of the above numbers concern measured data, not interpolated or calculated values. 2% (27 538) of the total data records do not have salinity. There are several reasons for this, the main one being the inability to vertically interpolate due to too large separation (Section 3.3.2) between measured samples. Other reasons for missing salinity include salinity not being reported and missing depth or pressure. Note that there are slightly fewer records with fCO$_2$ and all CFC data in GLODAPv2.2021 compared to GLODAPv2.2020. This is due to the removal of data with missing temperatures (Section 3.3.1).

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.

The total number of data records are 1 275 558. Records with measurements for all 12 core variables, salinity, oxygen, nitrate, silicate, phosphate, TCO$_2$, TAlk, pH, CFC-11, CFC-12, CFC-113, and CCl$_4$ are very rare; only 2026 records have measured data for all 12 in the merged product file (interpolated and calculated data excluded). Requiring only two measured seawater CO$_2$ chemistry variables in addition to all the other core variables brings the number of available records up to 9 230, so this is also very rare. A major limiting factor is simultaneous availability of data for all four freon species, only 26 277 records have measurements of CFC-11, CFC-12, CFC-113, and CCl$_4$ while 400 587 have data for at least one of these (not considering availability of other core variables). A total of 398 757 records have measured data for two out of the three CO$_2$ chemistry core variables. The number of measured fCO$_2$ data are 33 924; note that these data were not subjected to quality control. The number of records with measured data for salinity, oxygen, and nutrients are 798 703, while the number of records with salinity and oxygen data are 1 077 859. All of these numbers are for measured data, not interpolated or calculated values.

Figure 910 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 101 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. 101a) and density (Fig. 101b) 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 the 12 core variables were subjected to primary quality control to identify questionable or bad data points (outliers) and secondary quality control to identify systematic measurement biases. The data are provided in two ways: as a set of individual exchange-formatted original cruise data files with assigned WOCE flags, and as globally and regionally merged data product files with adjustments applied to the data according to the outcome of the consistency analyses. Importantly, no adjustments were applied to data in the individual cruise files while primary-QC changes were applied.

The consistency analyses were conducted by comparing the data from the 43106 new cruises to GLODAPv2.202019. Adjustments were only applied when the offsets were believed to reflect biases relative to the earlier data product release related to measurement calibration and/or data handling practices, and not to natural variability or anthropogenic trends.

The Adjustment Table at https://glodapv2-2021.geomar.de/ (last access: 29 June 2021) ~~https://glodapv2-2020.geomar.de/ (last access: 18 June 2020)~~ lists all applied adjustments and provides a brief justification for each. The consistency analyses rely on deep ocean data (>1500 or 2000 dbar depending on region), but supplementary CANYON-B and CONTENT analyses consider data below 500 dbar. Data consistency for cruises with exclusively shallow sampling was not examined. All new pH data for this version were comprehensively reviewed using crossover analysis, and none required adjustment. Regardless, full reanalysis of all available pH data, particularly in the North Pacific, will be conducted for GLODAPv3. ~~No pH data were adjusted for this version, but we note that this is largely a consequence of problems in establishing a reasonable pH baseline level in the deep northwest Pacific (Sect. 4.2). A comprehensive analysis of all available pH data in that region should be conducted for the next update~~.

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 flags of 0 indicate that the values were calculated from two other 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 resulting from the adjustments (Table 7), the data subjected to consistency analyses are believed to be consistent to better than 0.005 in salinity, 1 % in oxygen, 2 % in nitrate, 2 % in silicate, 2 % in phosphate, 4 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. As mentioned above, the included fCO_2 data have not been subjected to quality control, therefore no ~~uncertainty~~ consistency estimate is given for this variable. This should be conducted in future efforts.

7 Author contributions.

SKL~~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~~PYTHON~~ scripts for the merging of the data, and works on converting all code used for the GLODAP effort to Python. All authors contributed to the interpretation of the secondary QC results and decisions on whether to apply actual adjustments. Many conducted ancillary QC analyses. SKL and AO wrote the manuscript with input from all authors.

8 Competing interests

The authors declare that they have no competing interests.

9 Acknowledgements

References

Álvarez, M., Fajar, N. M., Carter, B. R., Guallart, E. F., Pérez, F. F., Woosley, R. J., and Murata, A.: Global ocean spectrophotometric pH assessment: consistent inconsistencies, Environ. Sci. Technol., doi: 10.1021/acs.est.9b06932, 2020. 2020.

Amante, C. and Eakins, B. W.: ETOPO1 1 Arc-minute global relief model: procedures, data sources and analysis, NOAA Technical Memorandum NESDIS NGDC-24, National Geophysial Data Center, Marine Geology and Geophysics Division, Boulder, CO, U.S.A., 2009.

Aoyama, M.: Global certified-reference-material- or reference-material-scaled nutrient gridded dataset GND13, Earth Syst. Sci. Data, 12, 487-499, 2020.

Aoyama, M., Ota, H., Kimura, M., Kitao, T., Mitsuda, H., Murata, A., and Sato, K.: Current status of homogeneity and stability of the reference materials for nutrients in Seawater, Anal. Sci., 28, 911-916, 2012.

Azetsu-Scott, K., Petrie, B., Yeats, P., and Lee, C.: Composition and fluxes of freshwater through Davis Strait using multiple chemical tracers, J. Geophys. Res. Oceans, 117, 2012.

935 Becker, M., Andersen, N., Erlenkeuser, H., Humphreys, M. P., Tanhua, T., and Körtzinger, A.: An internally consistent dataset of δ^{13}C-DIC in the North Atlantic Ocean - NAC13v1, Earth Syst. Sci. Data, 8, 559-570, 2016.

Becker, S., Aoyama, M., Woodward, E. M. S., Bakker, K., Coverly, S., Mahaffey, C., and Tanhua, T.: GO-SHIP repeat hydrography nutrient manual: The precise and accurate determination of dissolved inorganic nutrients in seawater, using Continuous Flow Analysis methods. In: The GO-SHIP Repeat Hydrography Manual: A Collection of Expert

940 Reports and Guidelines, Hood, E. M., Sabine, C., and Sloyan, B. M. (Eds.), IOCCP Report Number 14, ICPO Publication Series Number 134, 2019.

Bittig, H. C., Steinhoff, T., Claustre, H., Fiedler, B., Williams, N. L., Sauzède, R., Körtzinger, A., and Gattuso, J.-P.: An alternative to static climatologies: Robust estimation of open ocean CO_2 variables and nutrient concentrations from T, S, and O_2 data using Bayesian Neural Networks, Frontiers in Marine Science, 5, 2018.

945 Bockmon, E. E. and Dickson, A. G.: An inter-laboratory comparison assessing the quality of seawater carbon dioxide measurements, Mar. Chem., 171, 36-43, 2015.

Brakstad, A., Våge, K., Håvik, L., and Moore, G. W. K.: Water Mass Transformation in the Greenland Sea during the Period 1986-2016, J. Phys. Oceanogr., 49, 121-140, 2019.

Bryden, H. L.: New polynomials for thermal-expansion, adiabatic temperature gradient and potential temperature of sea-

950 water, Deep-Sea Res., 20, 401-408, 1973.

Bu, X. and Warner, M. J.: Solubility of chlorofluorocarbon-113 in water and seawater, Deep-Sea Res Pt I, 42, 1151-1161, 1995.

Bullister, J. L. and Wisegarver, D. P.: The solubility of carbon tetrachloride in water and seawater, Deep-Sea Res. Pt I, 45, 1285-1302, 1998.

955 Bullister, J. L., Wisegarver, D. P., and Menzia, F. A.: The solubility of sulfur hexafluoride in water and seawater, Deep-Sea Res. Pt I, 49, 175-187, 2002.

Carter, B. R., Feely, R. A., Williams, N. L., Dickson, A. G., Fong, M. B., and Takeshita, Y.: Updated methods for global locally interpolated estimation of alkalinity, pH, and nitrate, Limnol. Oceanogr.-Meth., 16, 119-131, 2018.

Cheng, L. J., Abraham, J., Zhu, J., Trenberth, K. E., Fasullo, J., Boyer, T., Locarnini, R., Zhang, B., Yu, F. J., Wan, L. Y.,

960 Chen, X. R., Song, X. Z., Liu, Y. L., and Mann, M. E.: Record-setting ocean warmth continued in 2019, Adv. Atmos. Sci, 37, 137-142, 2020.

Cheng, L. J., Trenberth, K. E., Fasullo, J., Boyer, T., Abraham, J., and Zhu, J.: Improved estimates of ocean heat content from 1960 to 2015, Sci. Adv., 3, 2017.

Dickson, A. G.: Standard potential of the reaction: AgCl(s) + ½H_2(g) = Ag(s) + HCl(aq) and the standard acidity constant

965 of the ion HSO_4^- in synthetic sea water from 273.15 to 318.15 K, J. Chem. Thermodyn., 22, 113-127, 1990.

Dickson, A. G., Afghan, J. D., and Anderson, G. C.: Reference materials for oceanic CO_2 analysis: a method for the certification of total alkalinity, Mar. Chem., 80, 185-197, 2003.

Dickson, A. G., Sabine, C. L., and Christian, J. R.: Guide to Best Practices for Ocean CO_2 measurements, PICES Special Publication 3, 191 pp., 2007.

970 Falck E. and Olsen, A.: Nordic Seas dissolved oxygen data in CARINA, Earth Syst. Sci. Data, 2, 123-131, 2010.

Fofonoff, N. P.: Computation of potential temperature of seawater for an arbitrary reference pressure, Deep-Sea Res., 24, 489-491, 1977.

Fong, M. B. and Dickson, A. G.: Insights from GO-SHIP hydrography data into the thermodynamic consistency of CO_2 system measurements in seawater, Mar. Chem., 211, 52-63, 2019.

975 Friedlingstein, P., Jones, M. W., O'Sullivan, M., Andrew, R. M., Hauck, J., Peters, G. P., Peters, W., Pongratz, J., Sitch, S., Le Quere, C., Bakker, D. C. E., Canadell, J. G., Ciais, P., Jackson, R. B., Anthoni, P., Barbero, L., Bastos, A., Bastrikov, V., Becker, M., Bopp, L., Buitenhuis, E., Chandra, N., Chevallier, F., Chini, L. P., Currie, K. I., Feely, R. A., Gehlen, M., Gilfillan, D., Gkritzalis, T., Goll, D. S., Gruber, N., Gutekunst, S., Harris, I., Haverd, V., Houghton, R. A., Hurtt, G., Ilyina, T., Jain, A. K., Joetzjer, E., Kaplan, J. O., Kato, E., Goldewijk, K. K., Korsbakken, J. I.,

980 Landschutzer, P., Lauvset, S. K., Lefevre, N., Lenton, A., Lienert, S., Lombardozzi, D., Marland, G., McGuire, P. C., Melton, J. R., Metzl, N., Munro, D. R., Nabel, J. E. M. S., Nakaoka, S. I., Neill, C., Omar, A. M., Ono, T., Peregon, A., Pierrot, D., Poulter, B., Rehder, G., Resplandy, L., Robertson, E., Rodenbeck, C., Seferian, R., Schwinger, J., Smith, N., Tans, P. P., Tian, H. Q., Tilbrook, B., Tubiello, F. N., van der Werf, G. R., Wiltshire, A. J., and Zaehle, S.: Global Carbon Budget 2019, Earth Syst. Sci. Data, 11, 1783-1838, 2019.

985 Friis, K., Körtzinger, A., and Wallace, D. W. R.: The salinity normalization of marine inorganic carbon chemistry data, Geophys. Res. Lett., 30, 2003.

Fröb, F., Olsen, A., Våge, K., Moore, G. W. K., Yashayaev, I., Jeansson, E., and Rajasakaren, B.: Irminger Sea deep convection injects oxygen and anthropogenic carbon to the ocean interior, Nat. Commun., 7, 2016.

Garcia, H. E. and Gordon, L. I.: Oxygen solubility in seawater - Better fitting equations, Limnol. Oceanogr., 37, 1307-

990 1312, 1992.

Gordon, A. L.: Deep Antarctic covection west of Maud Rise, J. Phys. Oceanogr., 8, 600-612, 1978.

Gruber, N., Clement, D., Carter, B. R., Feely, R. A., van Heuven, S., Hoppema, M., Ishii, M., Key, R. M., Kozyr, A., Lauvset, S. K., Lo Monaco, C., Mathis, J. T., Murata, A., Olsen, A., Perez, F. F., Sabine, C. L., Tanhua, T., and Wanninkhof, R.: The oceanic sink for anthropogenic CO_2 from 1994 to 2007, Science, 363, 1193-1199, 2019.

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

Hydes, D. J., Aoyama, A., Aminot, A., Bakker, K., Becker, S., Coverly, S., Daniel, A., Dickson, A. G., Grosso, O., Kerouel, R., van Ooijen, J., Sato, K., Tanhua, T., Woodward, E. M. S., and Zhang, J.-Z.: Determination of dissolved
1000   nutrients in seawater with high precision and intercomparability using gas-segmented continuous flow analysers. In: The GO SHIP Repeat Hydrography Manual: A Collection of Expert Reports and Guidelines, Hood, E. M., Sabine, C., and Sloyan, B. M. (Eds.), IOCCP Report Number 14, ICPO Publication Series Number 134, 2012.

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

1005   Jeansson, E., Olsson, K. A., Tanhua, T., and Bullister, J. L.: Nordic Seas and Arctic Ocean CFC data in CARINA, Earth Syst. Sci. Data, 2, 79-97, 2010.

Jenkins, W. J., Doney, S. C., Fendrock, M., Fine, R., Gamo, T., Jean-Baptiste, P., Key, R., Klein, B., Lupton, J. E., Newton, R., Rhein, M., Roether, W., Sano, Y. J., Schlitzer, R., Schlosser, P., and Swift, J.: A comprehensive global oceanic dataset of helium isotope and tritium measurements, Earth Syst. Sci. Data, 11, 441-454, 2019.

1010   Jutterström, S., Anderson, L. G., Bates, N. R., Bellerby, R., Johannessen, T., Jones, E. P., Key, R. M., Lin, X., Olsen, A., and Omar, A. M.: Arctic Ocean data in CARINA, Earth Syst. Sci. Data, 2, 71-78, 2010.

Key, R. M., Kozyr, A., Sabine, C. L., Lee, K., Wanninkhof, R., Bullister, J. L., Feely, R. A., Millero, F. J., Mordy, C., and Peng, T. H.: A global ocean carbon climatology: Results from Global Data Analysis Project (GLODAP), Global Biogeochem. Cy., 18, 2004.

1015   Key, R. M., Tanhua, T., Olsen, A., Hoppema, M., Jutterström, S., Schirnick, C., van Heuven, S., Kozyr, A., Lin, X., Velo, A., Wallace, D. W. R., and Mintrop, L.: The CARINA data synthesis project: introduction and overview, Earth Syst. Sci. Data, 2, 105-121, 2010.

King, B., Sanchez-Franks, A., Firing, Y. et al.: RRS James Cook Cruise JC159 28 February – 11 April 2018. Hydrographic sections from the Brazil to the Benguela Current across 24S in the Atlantic (National Oceanography
1020   Centre Cruise Report, 60), National Oceanography Centre, Southampton, 193 pp., 2019.

Lauvset, S. K. and Tanhua, T.: A toolbox for secondary quality control on ocean chemistry and hydrographic data, Limnol. Oceanogr.-Meth., 13, 601-608, 2015.

Lauvset, S. K., Key, R. M., Olsen, A., van Heuven, S., Velo, A., Lin, X., Schirnick, C., Kozyr, A., Tanhua, T., Hoppema, M., Jutterström, S., Steinfeldt, R., Jeansson, E., Ishii, M., Perez, F. F., Suzuki, T., and Watelet, S.: A new global
1025   interior ocean mapped climatology: the 1° × 1° GLODAP version 2, Earth Syst. Sci. Data, 8, 325-340, 10.5194/essd-8-325-2016, 2016.

Lauvset, S. K., Carter, B. R., Perez, F. F., Jiang, L.-Q., Feely, R. A., Velo, A., and Olsen, A.: Processes Driving Global Interior Ocean pH Distribution, Global Biogeochemical Cycles, 34, e2019GB006229, 10.1029/2019gb006229, 2020.

Lauvset, S. K., Lange, N., Tanhua, T., Bittig, H. C., Olsen, A., Kozyr, A., Álvarez, M., Becker, S., Brown, P. J., Carter,
1030   B. R., Cotrim da Cunha, L., Feely, R. A., van Heuven, S., Hoppema, M., Ishii, M., Jeansson, E., Jutterström, S., Jones, S. D., Karlsen, M. K., Lo Monaco, C., Michaelis, P., Murata, A., Pérez, F. F., Pfeil, B., Schirnick, C., Steinfeldt, R., Suzuki, T., Tilbrook, B., Velo, A., Wanninkhof, R., Woosley, R. J., Key, R. M. Global Ocean Data Analysis Project version 2.2021 (GLODAPv2.2021) (NCEI Accession 0237935). NOAA National Centers for Environmental Information. Dataset. https://doi.org/10.25921/ttgq-n825, 2021.

1035   Lee, K., Kim, T. W., Byrne, R. H., Millero, F. J., Feely, R. A., and Liu, Y. M.: The universal ratio of boron to chlorinity for the North Pacific and North Atlantic oceans, Geochimica Et Cosmochimica Acta, 74, 1801-1811, 10.1016/j.gca.2009.12.027, 2010.

Lewis, E. and Wallace, D. W. R.: Program developed for CO_2 system calculations, ORNL/CDIAC-105, Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, TN, U.S.A., 1998.

1040   Lueker, T. J., Dickson, A. G., and Keeling, C. D.: Ocean pCO_2 calculated from dissolved inorganic carbon, alkalinity, and equations for K-1 and K-2: validation based on laboratory measurements of CO_2 in gas and seawater at equilibrium, Mar. Chem., 70, 105-119, 2000.

McGrath, T., Cronin, M., Kerrigan, E., Wallace, D., Gregory, C., Normandeau, C., and McGovern, E.: A rare intercomparison of nutrient analysis at sea: lessons learned and recommendations to enhance comparability of open-
1045   ocean nutrient data, Earth Syst. Sci. Data, 11, 355-374, 2019.

Oka, E., Ishii, M., Nakano, T., Suga, T., Kouketsu, S., Miyamoto, M., Nakano, H., Qiu, B., Sugimoto, S., and Takatani, Y.: Fifty years of the 137A degrees E repeat hydrographic section in the western North Pacific Ocean, J. Oceanogr., 74, 115-145, 2018.

Oka, E., Katsura, S., Inoue, H., Kojima, A., Kitamoto, M., Nakano, T., and Suga, T.: Long-term change and variation of salinity in the western North Pacific subtropical gyre revealed by 50-year-long observations along 137 degrees E, J. Oceanogr., 73, 479-490, 2017.

Olsen, A., Key, R. M., van Heuven, S., Lauvset, S. K., Velo, A., Lin, X. H., Schirnick, C., Kozyr, A., Tanhua, T., Hoppema, M., Jutterstrom, S., Steinfeldt, R., Jeansson, E., Ishii, M., Perez, F. F., and Suzuki, T.: The Global Ocean Data Analysis Project version 2 (GLODAPv2) - an internally consistent data product for the world ocean, Earth Syst. Sci. Data, 8, 297-323, 2016.

Olsen, A., Lange, N., Key, R. M., Tanhua, T., Bittig, H. C., Kozyr, A., Àlvarez, M., Azetsu-Scott, K., Becker, S., Brown, P. J., Carter, B. R., Cotrim da Cunha, L., Feely, R. A., van Heuven, S., Hoppema, M., Ishii, M., Jeansson, E., Jutterström, S., Landa, C. S., Lauvset, S., Michaelis, P., Murata, A., Pérez, F. F., Pfeil, B., Schirnick, C., Steinfedt, R., Suzuki, T., Tilbrook, B., Velo, A., Wanninkhof, R., and Woosley, R. J.: Global ocean data analysis project version 2.2020 (GLODAPv2.2020), NOAA, National Centers for Environmental Information, https://doi.org/10.25921/2c8h-sa89, 2020.

Olsen, A., Lange, N., Key, R. M., Tanhua, T., Alvarez, M., Becker, S., Bittig, H. C., Carter, B. R., da Cunha, L. C., Feely, R. A., van Heuven, S., Hoppema, M., Ishii, M., Jeansson, E., Jones, S. D., Jutterstrom, S., Karlsen, M. K., Kozyr, A., Lauvset, S. K., Lo Monaco, C., Murata, A., Perez, F. F., Pfeil, B., Schirnick, C., Steinfeldt, R., Suzuki, T., Telszewski, M., Tilbrook, B., Velo, A., and Wanninkhof, R.: GLODAPv2.2019-an update of GLODAPv2, Earth Syst. Sci. Data, 11, 1437-1461, 2019.

Olsen, A., Lange, N., Key, R. M., Tanhua, T., Bittig, H. C., Kozyr, A., Álvarez, M., Azetsu-Scott, K., Becker, S., Brown, P. J., Carter, B. R., Cotrim da Cunha, L., Feely, R. A., van Heuven, S., Hoppema, M., Ishii, M., Jeansson, E., Jutterström, S., Landa, C. S., Lauvset, S. K., Michaelis, P., Murata, A., Pérez, F. F., Pfeil, B., Schirnick, C., Steinfeldt, R., Suzuki, T., Tilbrook, B., Velo, A., Wanninkhof, R., and Woosley, R. J.: An updated version of the global interior ocean biogeochemical data product, GLODAPv2.2020, Earth Syst. Sci. Data, 12, 3653-3678, 10.5194/essd-12-3653-2020, 2020.

Ota, H., Mitsuda, H., Kimura, M., and Kitao, T.: Reference materials for nutrients in seawater: Their development and present homogenity and stability. In: Comparability of nutrients in the world's oceans, Aoyama, A., Dickson, A. G., Hydes, D. J., Murata, A., Oh, J. R., Roose, P., and Woodward, E. M. S. (Eds.), Mother Tank, Tsukuba, Japan, 2010.

Panassa, E., Santana Casiano, J. M., Gonzalez Davila, M., Hoppema, M., van Heuven, S., Völker, C., Wolf Gladrow, D., and Hauck, J.: Variability of nutrients and carbon dioxide in the Antarctic Intermediate Water between 1990 and 2014, Ocean Dyn., 68, 295-308, 2018.

Pérez, F. F., Fontela, M., García Ibáñez, M. I., Mercier, H., Velo, A., Lherminier, P., Zunino, P., de la Paz, M., Alonso Pérez, F., Guallart, E. F., and Padin, X. A.: Meridional overturning circulation conveys fast acidification to the deep Atlantic Ocean, Nature, 554, 515-518, 2018.

Sabine, C., Key, R. M., Kozyr, A., Feely, R. A., Wanninkhof, R., Millero, F. J., Peng, T.-H., Bullister, J. L., and Lee, K.: Global Ocean Data Analysis Project (GLODAP): Results and Data, ORNL/CDIAC-145, NDP-083, Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, TN, U.S.A., 2005.

Sérazin, G.: An approximate neutral density variable for the World's oceans, Master's Thesis, Ecole Centrale, Lyon, Ècully, France, 2011.

Sloyan, B. M., Wanninkhof, R., Kramp, M., Johnson, G. C., Talley, L. D., Tanhua, T., McDonagh, E., Cusack, C., O'Rourke, E., McGovern, E., Katsumata, K., Diggs, S., Hummon, J., Ishii, M., Azetsu-Scott, K., Boss, E., Ansorge, I., Perez, F. F., Mercier, H., Williams, M. J. M., Anderson, L., Lee, J. H., Murata, A., Kouketsu, S., Jeansson, E., Hoppema, M., and Campos, E.: The Global Ocean Ship-Based Hydrographic Investigations Program (GO-SHIP): A Platform for Integrated Multidisciplinary Ocean Science, Frontiers in Marine Science, 6, 2019.

Steinfeldt, R., Tanhua, T., Bullister, J. L., Key, R. M., Rhein, M., and Köhler, J.: Atlantic CFC data in CARINA, Earth Syst. Sci. Data, 2, 1-15, 2010.

Suzuki, T., Ishii, M., Aoyama, A., Christian, J. R., Enyo, K., Kawano, T., Key, R. M., Kosugi, N., Kozyr, A., Miller, L. A., Murata, A., Nakano, T., Ono, T., Saino, T., Sasaki, K., Sasano, D., Takatani, Y., Wakita, M., and Sabine, C.: PACIFICA Data Synthesis Project, ORNL/CDIAC-159, NDP-092, Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U. S. Department of Energy, Oak Ridge, TN, U.S.A., 2013.

Swift, J.: Reference-quality water sample data: Notes on aquisition, record keeping, and evaluation. In: The GO-SHIP Repeat Hydrography Manual: A Collection of Expert Reports and Guidelines, Hood, E. M., Sabine, C., and Sloyan, B. M. (Eds.), IOCCP Report Number 14, ICPO Publication Series Number 134, 2019.

Swift, J. and Diggs, S. C.: Description of WHP exchange format for CTD/Hydrographic data, CLIVAR and Carbon Hydrographic Data Office, UCSD Scripps Institution of Oceanography, San Diego, Ca, US, 2008.

Takeshita, Y., Johnson, K. S., Coletti, L. J., Jannasch, H. W., Walz, P. M., and Warren, J. K.: Assessment of pH dependent errors in spectrophotometric pH measurements of seawater, Mar. Chem., 223, 103801, 2020.

Talley, L. D., Feely, R. A., Sloyan, B. M., Wanninkhof, R., Baringer, M. O., Bullister, J. L., Carlson, C. A., Doney, S. C., Fine, R. A., Firing, E., Gruber, N., Hansell, D. A., Ishii, M., Johnson, G. C., Katsumata, K., Key, R. M., Kramp, M., Langdon, C., Macdonald, A. M., Mathis, J. T., McDonagh, E. L., Mecking, S., Millero, F. J., Mordy, C. W., Nakano,

T., Sabine, C. L., Smethie, W. M., Swift, J. H., Tanhua, T., Thurnherr, A. M., Warner, M. J., and Zhang, J. Z.: Changes in ocean heat, carbon content, and ventilation: A review of the first decade of GO-SHIP global repeat hydrography, Annu. Rev. Mar. Sci., 8, 185-215, 2016.

Tanhua, T., van Heuven, S., Key, R. M., Velo, A., Olsen, A., and Schirnick, C.: Quality control procedures and methods of the CARINA database, Earth Syst. Sci. Data, 2, 35-49, 2010.

Tanhua, T., Lauvset, S. K., Lange, N., Olsen, A., Álvarez, M., Diggs, S., Bittig, H. C., Brown, P. J., Carter, B. R., da Cunha, L. C., Feely, R. A., Hoppema, M., Ishii, M., Jeansson, E., Kozyr, A., Murata, A., Pérez, F. F., Pfeil, B., Schirnick, C., Steinfeldt, R., Telszewski, M., Tilbrook, B., Velo, A., Wanninkhof, R., Burger, E., O'Brien, K., and Key, R. M.: A vision for FAIR ocean data products, Communications Earth & Environment, 2, 136, 10.1038/s43247-021-00209-4, 2021.

UNESCO: Tenth report of the joint panel on oceanographic tables and standards, UNESCO Technical Paper in Marine Science, 36, 13-21, 1981.

Uppström, L. R.: Boron/Chlorinity ratio of deep-sea water from Pacific Ocean, Deep-Sea Res,, 21, 161-162, 1974.

van Heuven, S., Pierrot, D., Rae, J. W. B., Lewis, E., and Wallace, D. W. R.: MATLAB program developed for CO_2 system calculations, ORNL/CDIAC-105b, Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, TN, U.S.A., 2011.

Voelker, A. H. L., Colman, A., Olack, G., Waniek, J. J., and Hodell, D.: Oxygen and hydrogen isotope signatures of Northeast Atlantic water masses, Deep-Sea Res, Pt II, 116, 89-106, 2015.

Warner, M. J. and Weiss, R. F.: Solubilities of chlorofluorocarbon-11 and chlorofluorocarbon-12 in water and seawater, Deep-Sea Res., 32, 1485-1497, 1985.

Weatherall, P., Marks, K. M., Jakobsson, M., Schmitt, T., Tani, S., Arndt, J. E., Rovere, M., Chayes, D., Ferrini, V., and Wigley, R.: A new digital bathymetric model of the world's oceans, Earth Space Sci., 2, 331-345, 2015.

Wilkinson, M. D., Dumontier, M., Aalbersberg, I. J., Appleton, G., Axton, M., Baak, A., Blomberg, N., Boiten, J.-W., da Silva Santos, L. B., Bourne, P. E., Bouwman, J., Brookes, A. J., Clark, T., Crosas, M., Dillo, I., Dumon, O., Edmunds, S., Evelo, C. T., Finkers, R., Gonzalez-Beltran, A., Gray, A. J. G., Groth, P., Goble, C., Grethe, J. S., Heringa, J., 't Hoen, P. A. C., Hooft, R., Kuhn, T., Kok, R., Kok, J., Lusher, S. J., Martone, M. E., Mons, A., Packer, A. L., Persson, B., Rocca-Serra, P., Roos, M., van Schaik, R., Sansone, S.-A., Schultes, E., Sengstag, T., Slater, T., Strawn, G., Swertz, M. A., Thompson, M., van der Lei, J., van Mulligen, E., Velterop, J., Waagmeester, A., Wittenburg, P., Wolstencroft, K., Zhao, J., and Mons, B.: The FAIR Guiding Principles for scientific data management and stewardship, Scientific Data, 3, 160018, 2016.

Yashayaev, I. and Loder, J. W.: Further intensification of deep convection in the Labrador Sea in 2016, Geophys. Res. Lett., 44, 1429-1438, 2017.

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			
Basin identifier		region			
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

Variable	Units	Product file name	WOCE flag name[a]	2nd QC flag name[b]	Exchange file name
pH on total scale, 25° C and 0 dbar of pressure		phts25p0	phts25p0f	phtsqc	PH_TOT
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	$f$co2temp	(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^3He	%	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 parentheses. [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.

1150

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

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

[a]Flag set to 9 in product files

1155   [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

Table 3. Initial minimum adjustment limits. These limits represent ~~are~~ the minimum bias that can be confidently established relative to the measurement precision for the variables and cruises considered. Note that these limits are not uncertainties, but rather a priori estimates of global inter-cruise consistency in the data product.

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 %

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 are available: use CTD values.	20	5
3	No CTD values are available: use bottle values.	0	67
4	Too few data of both types are available for comparison and >80% of the 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 CTD values 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

Case	Description	Salinity	Oxygen
1	No data are available: no action needed.	0	1
2	No bottle values are available: use CTD values.	8	1
3	No CTD values are available: use bottle values.	2	14
4	Too few data of both types are available for comparison and >80% of the 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.	33	23
6	The CTD values deviate significantly from bottle values: calibrate CTD values using linear fit and replace missing bottle values with calibrated CTD values.	0	0
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	4

1165

33

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

Secondary QC result	Code
The data are of good quality, consistent with the rest of the dataset and should not be adjusted.	0/1[a]
The data are of good quality but are biased: adjust by adding (for salinity, TCO_2, TAlk, pH) or by multiplying (for oxygen, nutrients, CFCs) the adjustment value	Adjustment value
The data have not been QC'd, are of uncertain quality, and suspended until full secondary QC has been carried out	-666
The data are of poor quality and excluded from the data product.	-777
The data appear of good quality but their nature, being from shallow depths, coastal regions, without crossovers or similar, prohibits full secondary QC	-888
No data exist for this variable for the cruise in question	-999

[a]The value of 0 is used for variables with additive adjustments (salinity, TCO_2, TAlk, pH) and 1 for variables with multiplicative adjustments (for oxygen, nutrients, CFCs). This is mathematically equivalent to 'no adjustment' in each case

1170

Table 6. Summary of secondary QC results for the 43~~106~~ new cruises, in number of cruises per result and per variable.

	Sal.	Oxy.	NO₃	Si	PO₄	TCO₂	TAlk	pH	CFC-11	CFC-12	CFC-113	CCl₄
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

	Sal.	Oxy.	NO₃	Si	PO₄	TCO₂	TAlk	pH	CFC-11	CFC-12	CFC-113	CCl₄
With data	43	42	41	41	40	36	35	13	8	13	1	0
No data	0	1	2	2	3	7	8	30	35	30	42	43
Unadjusted[a]	36	32	27	23	27	28	28	13	8	13	1	0
Adjusted[b]	0	3	6	9	6	2	2	0	0	0	0	0
-888[c]	7	7	7	8	7	6	4	0	0	0	0	0
-666[d]	0	0	0	0	0	0	0	0	0	0	0	0
-777[e]	0	0	1	1	0	0	0	0	0	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.

Table 7. Improvements resulting from quality control of the 106 new cruises, per basin and for the global data set. The ~~values~~numbers in the table are the weighted mean of the absolute offset of unadjusted and adjusted data versus GLODAPv2.20~~1~~209. *n* is the total number of valid crossovers in the global ocean for the variable in question. The values in this table represent the inter-cruise consistency in the GLODAPv2.2021 product.

-	ARCTIC				ATLANTIC				INDIAN				PACIFIC				GLOBAL			*n* (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	2841
Oxy (%)	0.8	⇒	0.8		0.7	⇒	0.7		0.5	⇒	0.5		0.5	⇒	0.5		0.5	⇒	0.5	2462
NO₃ (%)	0.9	⇒	0.9		1.6	⇒	1.5		0.6	⇒	0.6		0.5	⇒	0.5		0.5	⇒	0.5	2158
Si (%)	3.6	⇒	3.6		2.5	⇒	2.4		1.9	⇒	1.1		1.0	⇒	0.8		1.0	⇒	0.8	1956
PO₄ (%)	5.0	⇒	2.6		2.2	⇒	2.0		0.8	⇒	0.8		0.8	⇒	0.7		0.8	⇒	0.8	2047
TCO₂ (µmol/kg)	3.4	⇒	3.4		2.6	⇒	2.6		1.9	⇒	1.9		2.1	⇒	1.8		2.2	⇒	1.9	512
TAlk (µmol/kg)	2.9	⇒	2.9		1.7	⇒	1.7		2.4	⇒	1.6		2.5	⇒	2.1		2.4	⇒	2.1	521
pH (x1000)	NA	⇒	NA		8.5	⇒	8.5		NA	⇒	NA		8.3	⇒	7.4		8.3	⇒	7.5	458

1185

-	ARCTIC				ATLANTIC				INDIAN				PACIFIC				GLOBAL			*n* (global)
-	Unadj	-	Adj	-	Unadj	-	Adj	-	Unadj	-	Adj	-	Unadj	-	Adj	-	Unadj	-	Adj	
Sal (x1000)	3.0	⇒	3.0	-	4.2	⇒	4.2	-	2.4	⇒	2.4	-	2.5	⇒	2.5	-	2.9	⇒	2.9	917
Oxy (%)	0.9	⇒	0.9		0.9	⇒	0.8		0.8	⇒	0.8		1.3	⇒	1.2		1.0	⇒	1.0	842
NO₃ (%)	1.5	⇒	1.3		3.3	⇒	1.4		1.0	⇒	1.0		1.4	⇒	1.0		1.5	⇒	1.1	670
Si (%)	4.0	⇒	3.6		9.2	⇒	1.8		1.5	⇒	1.2		1.1	⇒	0.8		1.7	⇒	1.2	665
PO₄ (%)	3.4	⇒	2.8		2.6	⇒	1.7		0.7	⇒	0.7		2.0	⇒	1.8		2.2	⇒	1.8	643
TCO₂ (µmol/kg)	3.2	⇒	3.2		1.9	⇒	1.9		1.9	⇒	1.9		2.6	⇒	2.3		2.6	⇒	2.4	328
TAlk (µmol/kg)	3.0	⇒	3.0		5.5	⇒	5.5		2.2	⇒	2.2		2.9	⇒	2.4		3.2	⇒	3.0	262
pH (x1000)	NA	⇒	NA		4.9	⇒	4.9		14.8	⇒	14.8		11.0	⇒	11.0		9.0	⇒	9.0	99

36

1190 **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.ncei.noaa.gov/access/ocean-carbon-data-system/oceans/GLODAPv2_2021/cruise_table_v2021.html ~~at https://www.node.noaa.gov/ocads/oceans/GLODAPv2_2020/cruise_table_v2020.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	Pacifie	ks201009	20101203	20101222	*Keifu Maru II*
2031	49UF20111004	Pacifie	ks201109	20111004	20111127	*Keifu Maru II*
2032	49UF20111205	Pacifie	ks201110	20111205	20111221	*Keifu Maru II*
2033	49UF20120410	Pacifie	ks201203	20120410	20120424	*Keifu Maru II*
2034	49UF20120602	Pacifie	ks201205	20120602	20120614	*Keifu Maru II*
2035	49UF20131006	Pacifie	ks201307	20131006	20131022	*Keifu Maru II*
2036	49UF20131029	Pacifie	ks201308	20131029	20131210	*Keifu Maru II*
2037	49UF20140107	Pacifie	ks201401	20140107	20140125	*Keifu Maru II*
2038	49UF20140206	Pacifie	ks201402	20140206	20140326	*Keifu Maru II*
2039	49UF20140410	Pacifie	ks201403	20140410	20140505	*Keifu Maru II*
2040	49UF20140512	Pacifie	ks201404	20140512	20140617	*Keifu Maru II*
2041	49UF20140623	Pacifie	ks201405, P09, P13	20140623	20140826	*Keifu Maru II*
2042	49UF20140904	Pacifie	ks201406	20140904	20141019	*Keifu Maru II*
2043	49UF20150107	Pacifie	ks201501	20150107	20150126	*Keifu Maru II*
2044	49UF20150202	Pacifie	ks201502	20150202	20150306	*Keifu Maru II*
2045	49UF20150415	Pacifie	ks201504	20150415	20150504	*Keifu Maru II*
2046	49UF20150511	Pacifie	ks201505	20150511	20150611	*Keifu Maru II*
2047	49UF20150620	Pacifie	ks201506, P09, P13	20150620	20150823	*Keifu Maru II*
2048	49UF20151021	Pacifie	ks201508	20151021	20151202	*Keifu Maru II*
2049	49UF20160107	Pacifie	ks201601	20160107	20160126	*Keifu Maru II*
2050	49UF20160201	Pacifie	ks201602	20160201	20160310	*Keifu Maru II*
2051	49UF20160407	Pacifie	ks201604	20160407	20160507	*Keifu Maru II*
2052	49UF20160512	Pacifie	ks201605	20160512	20160610	*Keifu Maru II*
2053	49UF20160618	Pacifie	ks201606	20160618	20160723	*Keifu Maru II*
2054	49UF20160730	Pacifie	ks201607	20160730	20160912	*Keifu Maru II*
2055	49UF20160917	Pacifie	ks201608	20160917	20161007	*Keifu Maru II*
2056	49UF20161116	Pacifie	ks201609	20161116	20161219	*Keifu Maru II*
2057	49UF20170110	Pacifie	ks201701, P09, P10	20170110	20170223	*Keifu Maru II*
2058	49UF20170228	Pacifie	ks201702	20170228	20170326	*Keifu Maru II*
2059	49UF20170408	Pacifie	ks201703	20170408	20170426	*Keifu Maru II*
2060	49UF20170502	Pacifie	ks201704	20170502	20170606	*Keifu Maru II*
2061	49UF20170612	Pacifie	ks201705	20170612	20170713	*Keifu Maru II*
2062	49UF20170719	Pacifie	ks201706, P09, P10	20170719	20170907	*Keifu Maru II*
2063	49UF20171107	Pacifie	ks201708	20171107	20171208	*Keifu Maru II*
2064	49UF20180129	Pacifie	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
2083	49UP20150426	Pacific	rf201504	20150426	20150528	Ryofu Maru III
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
2093	49UP20170107	Pacific	rf201701	20170107	20170126	Ryofu Maru III
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

No	EXPOCODE	Region	Alias	Start	End	Ship
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*

1195

No	EXPOCODE	Region	Alias	Start	End	Ship
3001	06M220140607	Atlantic	MSM39	20140607	20140625	*Maria S. Merian*
3002	06M220160331	Atlantic	MSM53	20160331	20160509	*Maria S. Merian*
3003	06MT20160828	Atlantic	M130, SFB754	20160828	20161003	*Meteor*
3004	06MT20170302	Pacific	M135, SFB754	20170302	20170407	*Meteor*
3005	06MT20180213	Atlantic	M145	20180213	20180314	*Meteor*
3006	09AR20141205	Pacific	AU1402	20141205	20150125	*Aurora Australis*
3007	18DD20100202	Pacific	LineP-2010-01	20100202	20100216	*John P. Tully*
3008	18DD20100605	Pacific	LineP-2010-13	20100605	20100621	*John P. Tully*
3009	18DD20140210	Pacific	LineP-2014-01	20140210	20140224	*John P. Tully*
3010	18DD20150818	Pacific	LineP-2015-010	20150818	20150903	*John P. Tully*
3011	18DD20160208	Pacific	LineP-2016-001	20160208	20160222	*John P. Tully*
3012	18DD20160816	Pacific	LineP-2016-008	20160816	20160831	*John P. Tully*
3013	18DD20160605	Pacific	LineP-2016-006	20160605	20160625	*John P. Tully*
3014	18DD20170205	Pacific	LineP-2017-001	20170205	20170221	*John P. Tully*
3015	18DD20170604	Pacific	LineP-2017-006	20170604	20170620	*John P. Tully*
3016	18DD20190205	Pacific	LineP-2019-001	20190205	20190223	*John P. Tully*
3017	18DD20190602	Pacific	LineP-2019-006	20190602	20190618	*John P. Tully*
3018	18LU20180218	Pacific	LineP-2018-001	20180218	20180308	*Sir Wilfrid Laurier*
3019	18SN20040725	Arctic	JOIS-2004-16	20040725	20040802	*Louis S. St-Laurent*
3020	18SN20100915	Arctic	JOIS-2010-07	20100915	20101015	*Louis S. St-Laurent*
3021	18SN20110721	Arctic	JOIS-2011-20	20110721	20110818	*Louis S. St-Laurent*
3022	18SN20120802	Arctic	JOIS-2012-11	20120802	20120830	*Louis S. St-Laurent*
3023	18SN20130724	Arctic	JOIS2013-04	20130724	20130902	*Louis S. St-Laurent*
3024	18SN20140921	Arctic	JOIS-2014-11	20140921	20141017	*Louis S. St-Laurent*
3025	18SN20160922	Arctic	JOIS-2016-16	20160922	20161018	*Louis S. St-Laurent*
3026	18VT20141027	Pacific	Salish Sea 2014-50	20141027	20141030	*Vector*
3027	18VT20150401	Pacific	Salish Sea 2015-17	20150401	20150405	*Vector*
3028	29AH20090725	Atlantic	CAIBOX	20090725	20090813	*Sarmiento de Gamboa*
3029	320620170703	Pacific	GO-SHIP P06W, SOCCOM	20170703	20170817	*Nathaniel B. Palmer*
3030	320620170820	Pacific	GO-SHIP P06E, SOCCOM	20170820	20170930	*Nathaniel B. Palmer*
3031	320620180309	Pacific	NBP18_02, SOCCOM	20180309	20180514	*Nathaniel B. Palmer*
3032	325020100509	Pacific	TN249-10, BEST Spring 2010	20100509	20100614	*Thomas G. Thompson*
3033	325020190403	Indian	TN366, GO-SHIP I06S, SOCCOM	20190403	20190514	*Thomas G. Thompson*

3034	33RO20180423	Indian	GO-SHIP I07N	20180423	20180606	*Ronald H. Brown*
3035	33RR20160321	Indian	GO-SHIP I09N	20160321	20160428	*Roger Revelle*
3036	35A320031214	Atlantic	BIOZAIRE III	20031214	20040107	*L'Atalante*
3037	35A320120628	Pacific	Pandora	20120628	20210806	*L'Atalante*
3038	35A320150218	Pacific	OUTPACE	20150218	20150304	*L'Atalante*
3039	35MF19820626	Indian	MEROU-1982-A	19820626	19820703	*Marion Dufresne*
3040	35MF19821003	Indian	MEROU-1982-B	19821003	19821007	*Marion Dufresne*
3041	49NZ20191229	Indian	MR19-04, GO-SHIP I07S, SOCCOM	20191229	20200210	*Mirai*
3042	58JH20190515	Arctic	JH2019205	20190515	20190604	*Johan Hjort*
3043	74JC20181103	Atlantic	GO-SHIP SR01b	20181103	20181123	*James Clark Ross*

1200 **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.

1205 **Figure 3.** Example crossover figure, for TCO₂ for cruises 320620170820 (blue) and 49NZ20030803 (red),~~49UP20160109 (blue) and 49UP20160703 (red)~~, as it was generated during the crossover analysis. Panel **(a)** shows all station positions for the two cruises and **(b)** shows the specific stations used for the crossover analysis. Panel **(d)** shows the data of TCO₂ (μmol kg⁻¹) below the upper depth limit (in this case 2000 dbar) versus potential density anomaly referenced to 4000 dbar, as points and the interpolated profiles as lines. Non-interpolated data either did not meet minimum depth separation requirements (Table 4 in Key et al., 2010) or are the deepest sampling depth. The interpolation does not extrapolate. Panel **(e)** shows the mean TCO₂ (μmol kg⁻¹) difference profile (black, dots) with its standard deviation, and also the weighted mean offset (straight, red) and weighted standard deviation. Summary statistics are provided in **(c)**.

Figure 4. Example summary figure, for TCO₂ crossovers for 3206201708204~~9UP20160109~~ versus the cruises in GLODAPv2.20~~19~~20 (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 (in μmol kg⁻¹). The weighted mean and standard deviation of all these offsets are shown in the red lines and are 2.15 ± 1.04 ~~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 CANYON-B and CONTENT analyses for 3206201708204~~9UP20160109~~. 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 CO₂ chemistry variables (Note, different abbreviations for TCO₂ (CT) and TAlk (AT)). All are shown versus sampling pressure (dbar) and the unit is μmol kg⁻¹ for all except pH, which is on the total scale at *in situ* temperature and pressure.~~which is unitless.~~ Black dots (which to a large extent are hidden by the predicted estimates) are the measured data, blue dots are CANYON-B estimates and red dots are the CONTENT estimates. Each variable has two figure panels. The left shows the depth profile while the right shows the absolute difference between measured and estimated values divided by the CANYON-B/CONTENT uncertainty estimate, which is determined for each estimated value. These values are used to gauge the comparability; a value below 1 indicates a good match as it means that the difference between measured and estimated values is less than the uncertainty of the latter. The statistics in each panel are for all data deeper than 500 dbar and N is the number of samples; considered. A gain ratio and its interquartile range are given for the nutrients. For the seawater CO₂ 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.

1230 **Figure 6.** Distribution of applied adjustments for each core variable that received secondary QC, in μmol kg⁻¹ for TCO₂ and TAlk, unitless for salinity and pH (but multiplied with 1000 in both cases so a common x-axis can be used), while for the other properties adjustments are given in percent ((adjustment ratio-1)x100)). Grey areas depict the initial minimum adjustment limits. The figure includes numbers for data subjected to secondary quality control only. Note also that the y-axis scale is set to render the number of adjustments to be visible, so the bar showing zero offset (the 0 bar) for each variable is cut off (see Table 6 for these numbers).

1235 ~~Figure 7. Distribution of pH offsets for the cruises from Japan Meteorological Agency added in GLODAPv2.2020.~~

Figure 7~~8~~. Magnitude of applied adjustments relative to minimum adjustment limits (Table 3) per decade for the 9~~46~~89 cruises included in GLODAPv2.2021~~0~~.

Figure 8~~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.

1240 **Figure 9~~10~~.** Distribution of data in GLODAPv2.2021~~0~~ in (a) December–February, (b) March–May, (c) June–August, (d) September–November, and (e) number of observations for each month in four latitude bands.

Figure 10~~1~~. 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 1245 point and has data for several variables.

1250