



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

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**Abstract.** The Global Ocean Data Analysis Project (GLODAP) is a synthesis effort providing regular compilations of surface-to-bottom ocean biogeochemical data, with an emphasis on seawater inorganic carbon chemistry and related variables determined through chemical analysis of seawater samples. GLODAPv2.2020 is an update of the previous version, GLODAPv2.2019. The major changes are data from 106 new cruises added, extension of time coverage to 2019, and the inclusion of available (also for historical cruises) discrete fugacity of CO<sub>2</sub> ( $f\text{CO}_2$ ) 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<sub>4</sub>) have undergone extensive quality control with a focus on systematic evaluation of bias. The data are available in two formats: (i) as submitted by the data originator but updated to WOCE exchange format and (ii) as a merged data product with adjustments applied to minimize bias. These adjustments were derived by comparing the data from the 106 new cruises with the data from the 840 quality-controlled cruises of the GLODAPv2.2019 data product using crossover analysis. Comparisons to empirical algorithm estimates provided additional context for adjustment decisions; this is new to this version. The adjustments are intended to remove potential biases from errors related to measurement, calibration, and data-handling practices without removing known or likely time trends or variations in the variables evaluated. The compiled and adjusted data product is believed to be consistent to better than 0.005 in salinity, 1 % in oxygen, 2 % in nitrate, 2 % in silicate, 2 % in phosphate, 4  $\mu\text{mol kg}^{-1}$  in dissolved inorganic carbon, 4  $\mu\text{mol kg}^{-1}$  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  $f\text{CO}_2$ , were not subjected to bias comparison or adjustments.

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

## 1 Introduction

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

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

The oceanographic community largely adheres to principles and practices for ensuring open access to research data, such as the FAIR (Findable, Accessible, Interoperable, Reusable) initiative (Wilkinson et al., 2016), but the plethora of file formats and different levels of documentation, combined with the need to retrieve data on a per-cruise basis from different access points, limits the realization of their full scientific potential. For biogeochemical data there is the added complexity of different levels of standardization and calibration, and even different units used for the same variable, such that the comparability between datasets is often poor. Standard operating procedures have been de-

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

Variable	Units	Product file name	WOCE flag name <sup>a</sup>	Second QC flag name <sup>b</sup>	Exchange file name
Assigned sequential cruise number		cruise			
Station		station			STANBR
Cast		cast			CASTNO
Year		year			DATE
Month		month			DATE
Day		day			DATE
Hour		hour			TIME
Minute		minute			TIME
Latitude		latitude			LATITUDE
Longitude		longitude			LONGITUDE
Bottom depth	m	bottomdepth			
Pressure of the deepest sample	dbar	maxsampdepth			DEPTH
Niskin bottle number		bottle			BTLNBR
Sampling pressure	dbar	pressure			CTDPRS
Sampling depth	m	depth			
Temperature	°C	temperature			CTDTMP
Potential temperature	°C	theta			
Salinity		salinity	salinityf	salinityqc	CTDSAL/SALNTY
Potential density anomaly	kg m <sup>-3</sup>	sigma0	(salinityf)		
Potential density anomaly, ref 1000 dbar	kg m <sup>-3</sup>	sigma1	(salinityf)		
Potential density anomaly, ref 2000 dbar	kg m <sup>-3</sup>	sigma2	(salinityf)		
Potential density anomaly, ref 3000 dbar	kg m <sup>-3</sup>	sigma3	(salinityf)		
Potential density anomaly, ref 4000 dbar	kg m <sup>-3</sup>	sigma4	(salinityf)		
Neutral density anomaly	kg m <sup>-3</sup>	gamma	(salinityf)		
Oxygen	μmol kg <sup>-1</sup>	oxygen	oxygenf	oxygenqc	CTDOXY/OXYGEN
Apparent oxygen utilization	μmol kg <sup>-1</sup>	aou	aouf		
Nitrate	μmol kg <sup>-1</sup>	nitrate	nitratef	nitrateqc	NITRAT
Nitrite	μmol kg <sup>-1</sup>	nitrite	nitritef		NITRIT
Silicate	μmol kg <sup>-1</sup>	silicate	silicatef	silicateqc	SILCAT
Phosphate	μmol kg <sup>-1</sup>	phosphate	phosphatef	phosphateqc	PHSPHT
TCO <sub>2</sub>	μmol kg <sup>-1</sup>	tco2	tco2f	tco2qc	TCARBON
TALK	μmol kg <sup>-1</sup>	talk	talkf	talkqc	ALKALI
pH on total scale, 25 °C and 0 dbar of pressure		phts25p0	phts25p0f	phtsqc	PH_TOT
pH on total scale, in situ temperature and pressure		phtsinsitup	phtsinsitupf	phtsqc	
fCO <sub>2</sub> at 20 °C and 0 dbar of pressure	μatm	fco2	fco2f		FCO2/PCO2
fCO <sub>2</sub> temperature <sup>c</sup>	°C	fco2temp	(fco2f)		FCO2_TMP/PCO2_TMP
CFC-11	pmol kg <sup>-1</sup>	cfc11	cfc11f	cfc11qc	CFC-11
pCFC-11	ppt	pcfc11	(cfc11f)		
CFC-12	pmol kg <sup>-1</sup>	cfc12	cfc12f	cfc12qc	CFC-12
pCFC-12	ppt	pcfc12	(cfc12f)		
CFC-113	pmol kg <sup>-1</sup>	cfc113	cfc113f	cfc113qc	CFC-113
pCFC-113	ppt	pcfc113	(cfc113f)		
CCl <sub>4</sub>	pmol kg <sup>-1</sup>	ccl4	ccl4f	ccl4qc	CCL4
pCCl <sub>4</sub>	ppt	pccl4	(ccl4f)		
SF <sub>6</sub>	fmol kg <sup>-1</sup>	sf6	sf6f		SF6
pSF <sub>6</sub>	ppt	psf6	(sf6f)		
δ <sup>13</sup> C	‰	c13	c13f	c13qc	DELC13
Δ <sup>14</sup> C	‰	c14	c14f		DELC14
Δ <sup>14</sup> C counting error	‰	c14err			C14ERR
<sup>3</sup> H	TU	h3	h3f		TRITIUM
<sup>3</sup> H counting error	TU	h3err			TRITER
δ <sup>3</sup> He	‰	he3	he3f		DELHE3
<sup>3</sup> He counting error	‰	he3err			DELHER
He	nmol kg <sup>-1</sup>	he	hef		HELIUM
He counting error	nmol kg <sup>-1</sup>	heerr			HELIER
Ne	nmol kg <sup>-1</sup>	neon	neonf		NEON
Ne counting error	nmol kg <sup>-1</sup>	neonerr			NEONER
δ <sup>18</sup> O	‰	o18	o18f		DELO18
Total organic carbon	μmol L <sup>-1</sup> d	toc	tocf		TOC
Dissolved organic carbon	μmol L <sup>-1</sup> d	doc	docf		DOC
Dissolved organic nitrogen	μmol L <sup>-1</sup> d	don	donf		DON
Dissolved total nitrogen	μmol L <sup>-1</sup> d	tdn	tdnf		TDN
Chlorophyll <i>a</i>	μg kg <sup>-1</sup> d	chl <sub>a</sub>	chl <sub>a</sub> f		CHLORA

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

veloped for some variables (Dickson et al., 2007; Hood et al., 2010; Becker et al., 2020), and certified reference materials (CRMs) exist for seawater TCO<sub>2</sub> and TALK measurements (Dickson et al., 2003) and for nutrients in seawater (CRMNS; Aoyama et al., 2012; Ota et al., 2010). Despite this, biases in data still occur. These can arise from poor sampling and preservation practices, calibration procedures, instrument design, and inaccurate calculations. The use of CRMs does not by itself ensure accurate measurements of seawater CO<sub>2</sub> chemistry (Bockmon and Dickson, 2015), and the CRMNSs have only become available recently and are not universally used. For salinity and oxygen, lack of calibration of the data from conductivity–temperature–depth (CTD) profiler mounted sensors is an additional and widespread problem, particularly for oxygen (Olsen et al., 2016). For halogenated transient tracers, uncertainties in standard gas composition, extracted water volume, and purge efficiency typically provide the largest sources of uncertainty. In addition to bias, occasional outliers occur. In rare cases poor precision – many multiples worse than that expected with current measurement techniques – can render a set of data of limited use. GLODAP deals with these issues by presenting the data in a uniform format, including any metadata either publicly available or submitted by the data originator, and by subjecting the data to primary and secondary quality control assessments, focusing on precision and consistency, respectively. The secondary quality control focuses on deep data, where natural variability is minimal. Adjustments are applied to the data to minimize cases of bias that could be confidently established relative to the measurement precision for the variables and cruises considered.

GLODAPv2.2020 builds on earlier synthesis efforts for biogeochemical data obtained from research cruises, GLODAPv1.1 (Key et al., 2004; Sabine et al., 2005), Carbon dioxide in the Atlantic Ocean (CARINA) (Key et al., 2010), Pacific Ocean Interior Carbon (PACIFICA) (Suzuki et al., 2013), and notably GLODAPv2 (Olsen et al., 2016). GLODAPv1.1 combined data from 115 cruises with biogeochemical measurements from the global ocean. The vast majority of these were the sections covered during the World Ocean Circulation Experiment and the Joint Global Ocean Flux Study (WOCE/JGOFS) in the 1990s, but data from important “historical” cruises were also included, such as from the Geochemical Ocean Sections Study (GEOSECS), Transient Tracers 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.,

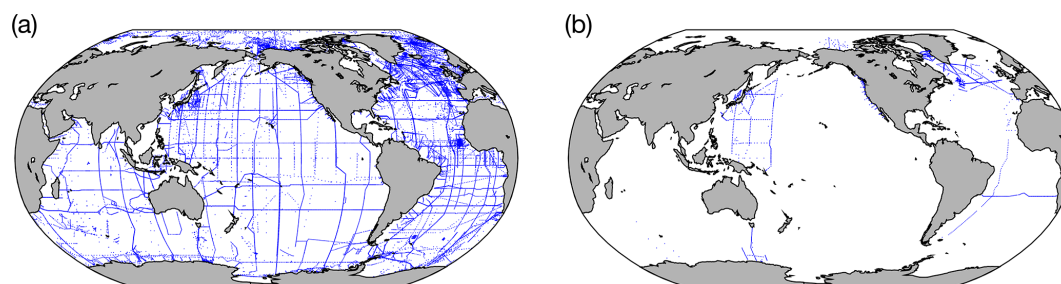
2019). GLODAPv2 is now updated regularly using the “living data format” of *Earth System Science Data* to document significant additions and changes to the dataset.

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.

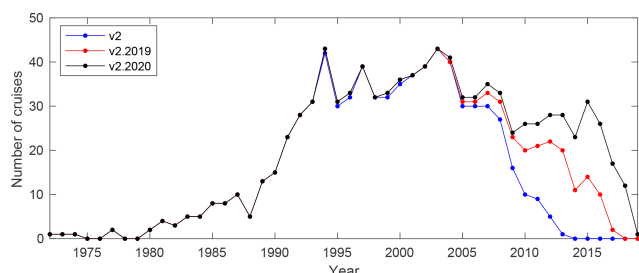
Creating and interpreting inversions and other checks of the full dataset needed for full updates are too demanding in terms of time and resources to be performed every year or 2 years. The aim is to conduct a full analysis (i.e., including an inversion) again after the third GO-SHIP survey has been completed. This completion is currently scheduled for 2023, and we anticipate that GLODAPv3 will become available a few years thereafter. In the interim, presented here is the second intermediate update, which adds data from 106 new cruises to the last update, GLODAPv2.2019 (Olsen et al., 2019).

## 2 Key features of the update

GLODAPv2.2020 (Olsen et al., 2020) contains data from 946 cruises, covering the global ocean from 1972 to 2019, compared to 840 for the period 1972–2017 for GLODAPv2.2019. Information on the 106 cruises added to this version is 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 abovementioned 12 core variables; for example, cruises with only seawater CO<sub>2</sub> chemistry or transient tracer data are still included even without accompanying nutrient data due to their value towards computation of, for example, carbon inventories. In some other cases, cruises without any of these properties measured were included – this was because they did contain data for other carbon-related tracers such as carbon isotopes, with the main intention of ensuring their wider availability. The added cruises are from the years 2004–2019, with most being more recent than 2010. The majority of the new data were



**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.

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, 2017). Another important addition are 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  $\text{CO}_2$  chemistry data; the 2016 occupation of the OVIDE line (Pérez et al., 2018); the 2019 occupation of A17 on board *RV Hesperides*; the 2018 occupation of A9.5 on board *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 sub-polar NA sampling (35TH20080825) and a 2007 *RV Pelagia* cruise (64PE20071026) covering the northeast Atlantic. The final Atlantic cruise is 29GD20120910 on board *RV García del Cid*, with measurements for stable isotopes of carbon and oxygen ( $\delta^{13}\text{C}$  and  $\delta^{18}\text{O}$ ) off the Iberian Peninsula (Voelker et al., 2015) but no data for nutrients, seawater  $\text{CO}_2$  chemistry, or transient tracers. Two new Indian Ocean cruises are included, and both took place in the far south, in the Indian sector of the Southern Ocean: an Argo deployment cruise south and west of Kerguelen Island on board the *RV S. A. Agulhas I* and the 2018 occupation of GO-SHIP

line SR03 on board the *RV Investigator*. The JOIS cruise in 2015 is the sole addition for the Arctic. Finally, new data along the US West Coast are from two cruises conducted on board the *RVs Wecoma* (WCOA2011, 32WC20110812) and *Ronald H. Brown* (WCOA2016, 33RO20160505) as part of NOAA’s ocean acidification program.

All new cruises were subjected to primary (Sect. 3.1) and secondary (Sect. 3.2) quality control (QC). These procedures are essentially the same as for GLODAPv2.2019, aiming to ensure the consistency of the data from the 106 new cruises with the previous release of this data product (in this case, the GLODAPv2.2019 adjusted data product).

### 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: 20 October 2020), National Centers for Environmental Information (<https://www.ncei.noaa.gov>, last access: 20 October 2020), and PANGAEA (<https://pangaea.de>, last access: 20 October 2020). Each cruise is identified by an expedition code (EXPCODE). The EXPCODE is guaranteed to be unique and constructed by combining the country code and platform code with the date of departure in the format YYYYMMDD. The country and platform codes were taken from the ICES (International Council for the Exploration of the Sea) library (<https://vocab.ices.dk/>, last access: 20 June 2020).

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 ( $\text{mL L}^{-1}$ ; oxygen) or micromoles per liter ( $\mu\text{mol L}^{-1}$ ; nutrients) to micromoles per kilogram of seawater ( $\mu\text{mol kg}^{-1}$ ). The default conversion procedure for nutrients was to use seawater density at reported salinity, an assumed measurement temperature of 22 °C, and pressure of 1 atm. For oxygen, the factor 44.66 was used for the conversion of milliliters of oxygen to micromoles of oxygen, while the density required for the conversion of per liter to per kilogram 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.

Each data column (except temperature and pressure, which are assumed “good” if they exist) has an associated column of data flags. For the original data exchange files, these flags conform to the WOCE definitions for water samples and are listed in Table 2. For the merged and adjusted product files these flags are simplified: questionable (WOCE flag 3) and bad (WOCE flag 4) data are removed and their flags are set to 9. The same procedure is applied to data flagged 8 (very few such data exist); WOCE flags 1 (data not received) and 5 (data not reported) are also set to 9, while flags of 6 (mean of replicate measurements) and 7 (manual chromatographic peak measurement) are set to 2, if the data appear good. Also, in the merged product files a flag of 0 is used to indicate a value that could be measured but is somehow approximated: for salinity, oxygen, phosphate, nitrate, and silicate, the approximation is conducted using vertical interpolation; for seawater  $\text{CO}_2$  chemistry variables ( $\text{TCO}_2$ ,  $\text{TALK}$ ,  $\text{pH}$ , and  $f\text{CO}_2$ ), the approximation is conducted using calculation from two measured  $\text{CO}_2$  chemistry variables (Sect. 3.2.2). Importantly, interpolation of  $\text{CO}_2$  chemistry variables is never performed, and thus a flag value of 0 has a unique interpretation.

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 106 new cruises relative to GLODAPv2.2019, while retaining any signal due to temporal changes. To this end, secondary QC in the form of consistency analyses was conducted to identify offsets in the data. All identified offsets were scrutinized by the GLODAP reference group through a series of teleconferences during March and April 2020 in order to decide the adjustments to be applied to correct for the offset (if any). To guide this process, a set of initial minimum adjustment limits was used (Table 3). These are set according to the expected measurement precision for each variable and are the same as those used for GLODAPv2.2019. In addition to the average magnitude of the offsets, factors such as the precision of the offsets, persistence towards the various cruises used in the comparison, regional dynamics, and the occurrence of time trends or other variations were considered. Thus, not all offsets larger than the initial minimum limits have been adjusted. A guiding principle for these considerations was to not apply an adjustment whenever in doubt. Conversely, in some cases where data and offsets were very precise and the cruise had been conducted in a region where variability is expected to be small, adjustments lower than the minimum limits were applied. Any adjustment was applied uniformly to all values for a variable and cruise, i.e., an underlying assumption is that cruises suffer from either no or a single and constant measurement bias. Adjustments for salinity,  $\text{TCO}_2$ ,  $\text{TALK}$ , and  $\text{pH}$  are always additive, while adjustments for oxygen, nutrients, and the halogenated transient tracers are always multiplicative. Except where explicitly noted (Sect. 3.3.1), adjustments were not changed for data previously included in GLODAPv2.2019.

Crossover comparisons, multi-linear regressions (MLRs), and comparison of deep-water averages were used to identify offsets for salinity, oxygen, nutrients,  $\text{TCO}_2$ ,  $\text{TALK}$ , and  $\text{pH}$  (Sect. 3.2.2 and 3.2.3). In contrast to GLODAPv2 and GLODAPv2.2019, evaluation of the internal consistency of the seawater  $\text{CO}_2$  chemistry variables was not used for the evaluation of  $\text{pH}$  (Sect. 3.2.4). New to the present version is more extensive use of 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  $\text{CO}_2$  chemistry data (Sect. 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

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

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

<sup>a</sup> Flag set to 9 in product files. <sup>b</sup> Data are not included in the GLODAPv2.2020 product files and their flags set to 9. <sup>c</sup> Data are included, but flag set to 2.

**Table 3.** Initial minimum adjustment limits.

Variable	Minimum adjustment
Salinity	0.005
Oxygen	1 %
Nutrients	2 %
TCO <sub>2</sub>	4 μmol kg <sup>-1</sup>
TAlk	4 μmol kg <sup>-1</sup>
pH	0.01
CFCs	5 %

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 are possible for each of the CTD-O<sub>2</sub> sensor properties individually, where the fourth (see below) never occurred during our analyses but is included to maintain consistency with GLODAPv2.

1. No data are available: no action needed.
2. No bottle values 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 GLODAPv2.2019 data product as the reference data product. The toolbox implements the “running-cluster” crossover analysis first described by Tanhua et al. (2010). This analysis compares data from two cruises on a station-by-station basis and calculates a weighted mean offset between the two and its weighted standard deviation. The weighting is based on the scatter in the data such that data that have less scatter have a larger influence on the comparison than data with more scatter. Whether the scatter reflects actual variability or data precision is irrelevant in this context as increased scatter nevertheless decreases the confidence in the comparison. Stations are compared when they are within 2 arcdeg 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 the 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, 2017). 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-water 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  $\text{TCO}_2$  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  $\text{TCO}_2$  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  $\text{TCO}_2$  values from 49UP20160109 are higher, with a weighed mean offset of  $3.62 \pm 2.67 \mu\text{mol kg}^{-1}$  compared to those measured on 49UP20160703.

For each of the 106 new cruises, such a crossover comparison was conducted against all possible cruises in GLODAPv2.2019, i.e., all cruises that had stations closer than 2 arcdeg distance to any station for the cruise in question. The summary figure for  $\text{TCO}_2$  on 49UP20160109 is shown in Fig. 4. The  $\text{TCO}_2$  data measured on this cruise are high by  $3.68 \pm 0.83 \mu\text{mol kg}^{-1}$  when compared to the data measured on nearby cruises included in GLODAPv2.2019. This is slightly less than the initial minimum adjustment limit for  $\text{TCO}_2$  of  $4 \mu\text{mol kg}^{-1}$  (Table 3), but the offset is present against all cruises and there is no obvious time trend (particularly important for  $\text{TCO}_2$ ) and as such qualifies for an adjustment of the data in the merged data product. In this case  $-3 \mu\text{mol kg}^{-1}$  was applied: this is somewhat less than indicated by the crossover analysis, but a smaller adjustment is supported by the CANYON-B and CONTENT results (Sect. 3.2.5). Adjustments are typically round numbers

relative to the precision of the variable being considered (e.g.,  $-3$  not  $-3.4$  for  $\text{TCO}_2$  and  $0.005$  not  $0.0047$  for pH) to avoid communicating that the ideal adjustments are known to high precision.

One exception to the above-described procedure exists, namely in the Sea of Japan where six new cruises were added. In this region, only two other cruises were included in GLODAPv2.2019. Therefore, all eight cruises were compared against each other and strong outliers were adjusted accordingly, instead of adjusting the six new cruises towards the existing two.

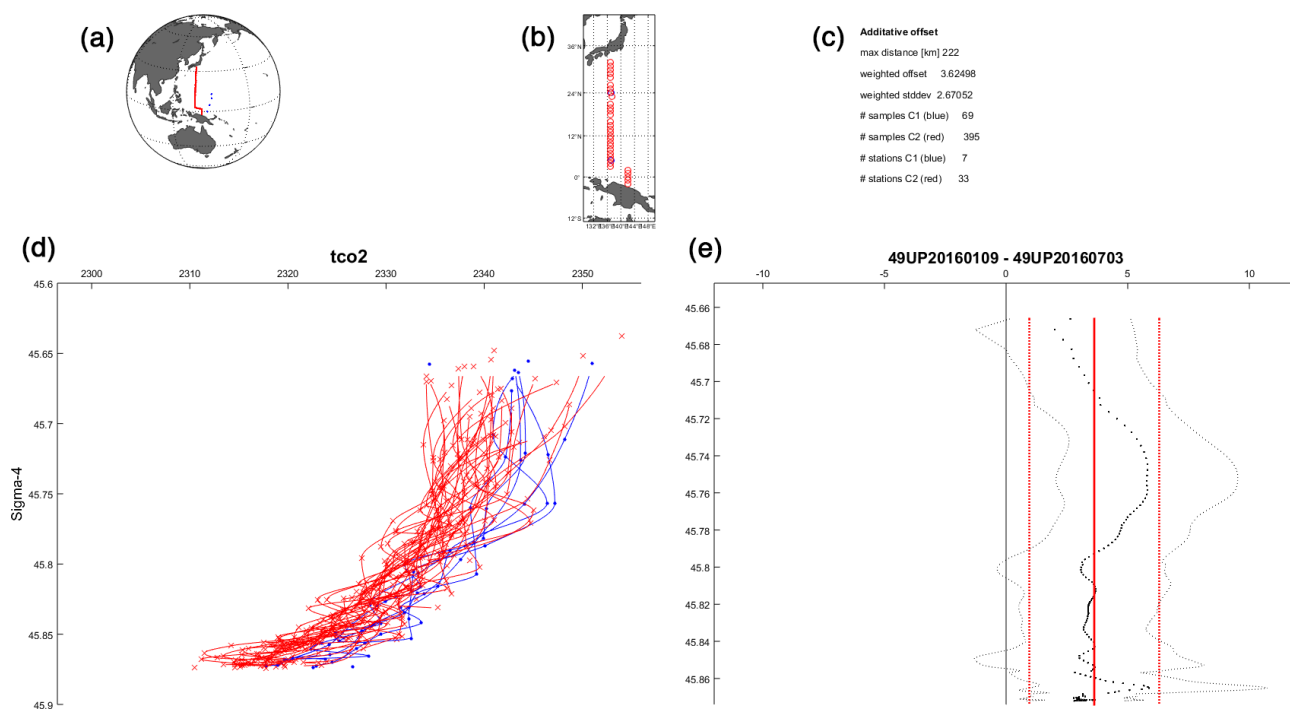
### 3.2.3 Other consistency analyses

MLR analyses and deep-water averages, broadly following Jutterström et al. (2010), were also used for the secondary QC of salinity, oxygen, nutrients,  $\text{TCO}_2$ , and TALK data. These approaches are particularly valuable when a cruise has either very few or no valid crossovers but are also used more generally to provide more insight into the consistency of the data. The latter was the case for the 106 new cruises; i.e., no adjustment decisions were reached on the basis of MLR and deep-water average analyses alone. For the MLRs, the presence of bias in the data was identified by comparing the MLR-generated values with the measured values. Both analyses were conducted on samples collected deeper than the 1500 or 2000 dbar pressure level to minimize the effects of natural variations, and both used available GLODAPv2.2019 data from within  $2^\circ$  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 abovementioned variables could be included among the independent variables (e.g., for a TALK MLR, salinity, oxygen, nutrients, and  $\text{TCO}_2$  were allowed), with the exact selection determined based on the statistical robustness of the fit, as evaluated using the coefficient of determination ( $r^2$ ) and root-mean-square error (RMSE). MLRs based on variables that were suspect for the cruise in question were avoided (e.g., if oxygen appeared biased it was not included as an independent variable). The MLRs could be based on 10 to 500 samples, and the robustness of the fit ( $r^2$ , RMSE) and quantity of fitting data were considered when using the results to guide whether to apply a correction. The same applies for the deep-water averages (i.e., the standard deviation of the mean). MLR and deep-water average results showing offsets above the minimum adjustment limits were carefully scrutinized, along with available crossover values and CANYON-B and CONTENT estimates, to determine whether or not to apply an adjustment.

### 3.2.4 pH scale conversion and quality control

Altogether 82 of the 106 new cruises included measured pH data. For one of these, the pH data were not supplied on the total scale or at  $25^\circ\text{C}$  and 0 dbar pressure, which is the



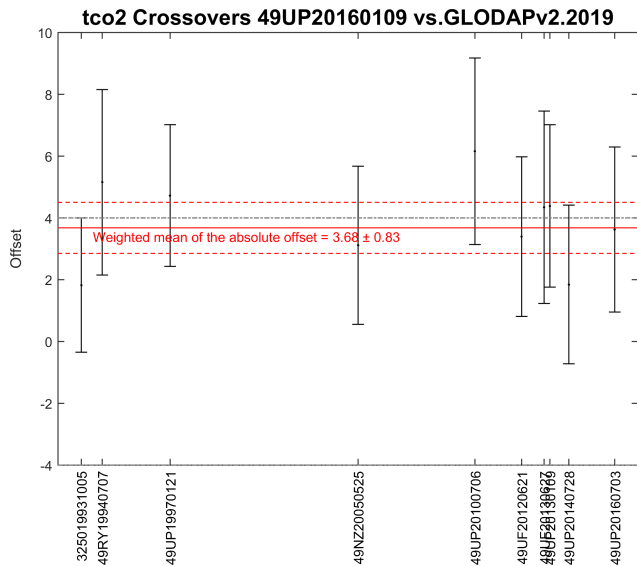


**Figure 3.** Example crossover figure, for  $\text{TCO}_2$  for cruises 49UP20160109 (blue) and 49UP20160703 (red), as it was generated during the crossover analysis. Panel (a) shows all station positions for the two cruises and (b) shows the specific stations used for the crossover analysis. Panel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

GLODAP standard, and were thus converted. The conversion was conducted using CO2SYS (Lewis and Wallace, 1998) for MATLAB (van Heuven et al., 2011) with reported pH and TALK as inputs and generating pH output values at total scale at 25 °C and 0 dbar of pressure (named phts25p0 in the product). Missing TALK data were approximated as 67 times salinity. The proportionality (67) is the mean ratio of TALK to salinity in GLODAPv2 data. The uncertainties introduced with this approximation are negligible (order  $10^{-7}$  pH units) for the scale conversions and order  $10^{-3}$  pH units for the temperature and pressure conversion (evaluated by repeating conversions with 2 times the standard deviation of the ratio, i.e.,  $67 \pm 4.1$ ). This is sufficiently accurate relative to other sources of uncertainty, which are discussed below. Data for phosphate and silicate are also needed and were, whenever missing, determined using CANYON-B (Bittig et al., 2018). The conversion was conducted with the carbonate dissociation constants of Lueker et al. (2000), the bisulfate dissociation constant of Dickson (1990), and the borate-to-salinity ratio of 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  $\text{CO}_2$  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 assign an uncertainty of 0.02 to the North Pacific pH data in the merged product files. Elsewhere, the uncertainties that have arisen are smaller, since deep pH is typically larger than 7.7 (Lauvset et al., 2020), and at such levels the difference between calculated and measured pH is less than 0.01 on av-



**Figure 4.** Example summary figure, for TCO<sub>2</sub> crossovers for 49UP20160109 versus the cruises in GLODAPv2.2019 (with cruise EXPCODE listed on the 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 ( $\mu\text{mol kg}^{-1}$ ). The weighted mean and standard deviation of all these offsets are shown in the red lines and are  $3.68 \pm 0.83 \mu\text{mol kg}^{-1}$ . The black dashed line is the reference line for a  $+4 \mu\text{mol kg}^{-1}$  offset (the corresponding line for  $-4 \mu\text{mol kg}^{-1}$  offset is right on top of the x axis and not visible).

erage (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 dataset (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<sub>2</sub> chemistry variables from temperature, salinity, and oxygen. CONTENT additionally considers the consistency among the estimated CO<sub>2</sub> chemistry variables to further refine them. These approaches were developed using the data included in the GLODAPv2 data product. Their advantage compared to crossover analyses for evaluating consistency among cruise data is that effects of water mass changes on ocean properties are represented in the non-linear relationships in the underlying neural network. For example, if elevated nutrient values are measured on a cruise but are not due to a measurement bias but actual aging of the

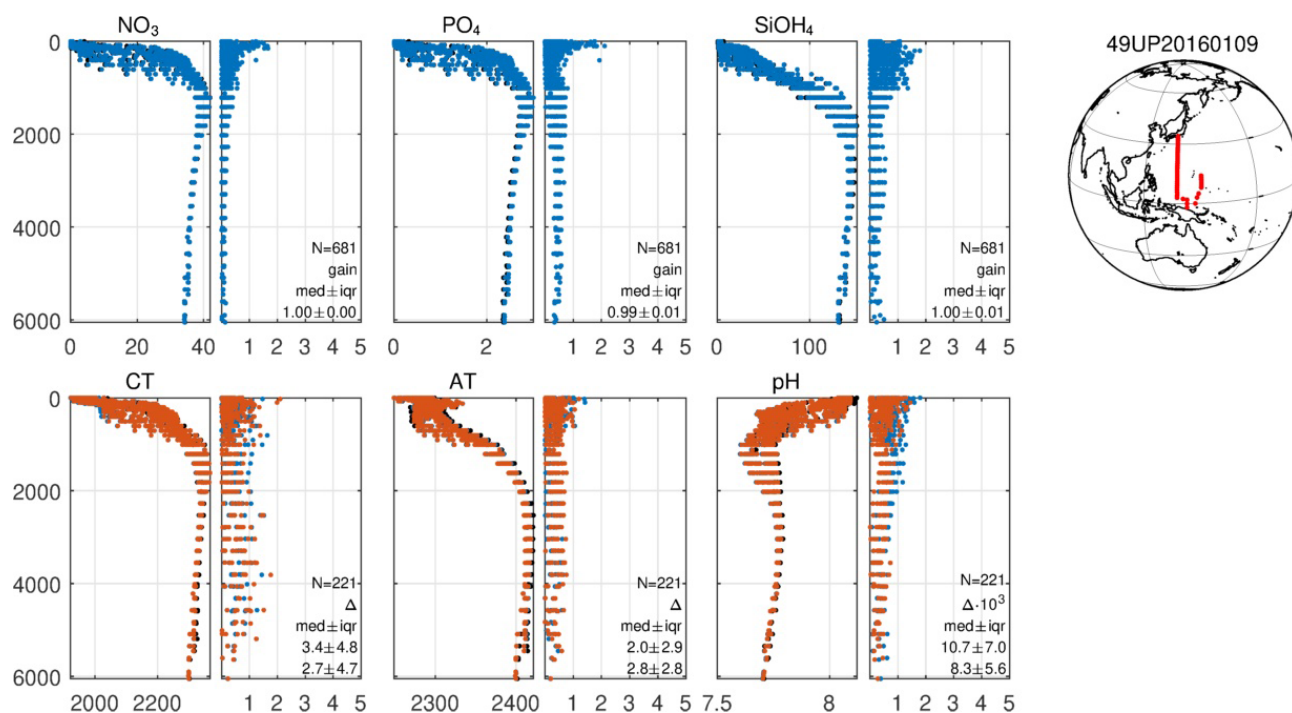
water mass(es) that have been sampled and as such accompanied by a decrease in oxygen concentrations, the measured values and the CANYON-B estimates will be similar. Vice versa, if the nutrient values are biased, the measured values and CANYON-B predictions will be dissimilar.

Used in the correct way and with caution this tool is a powerful supplement to the traditional crossover analyses. Specifically, we gave no weight to comparisons where the crossover analyses had suggested that the S and/or O<sub>2</sub> data were biased as this would lead to error in the predicted values. We also considered the uncertainties of the CANYON-B and CONTENT estimates. These uncertainties are determined for each predicted value, and for each comparison the ratio of the difference (between measured and predicted values) to the local uncertainty was used to gauge the comparability. As an example, the CANYON-B/CONTENT analyses of the data obtained at 49UP20160109 are presented in Fig. 5. The CANYON-B and CONTENT results confirmed the positive offset in the TCO<sub>2</sub> values revealed in the crossover comparisons discussed in Sect. 3.2.2. The magnitude of the inconsistency for the CANYON-B estimate was  $3.4 \mu\text{mol kg}^{-1}$ , i.e., slightly less than that the weighted mean crossover offset of  $3.7 \mu\text{mol kg}^{-1}$ , while the CONTENT estimate gave an inconsistency of  $2.7 \mu\text{mol kg}^{-1}$ . The differences between these consistency estimates owe to differences in the actual approach, the weighting across stations, stations considered (i.e., crossover comparisons use only stations within  $\sim 200$  km of each other, while CANYON-B and CONTENT consider all stations where necessary variables are sampled), and depth range considered ( $> 500$  dbar for CANYON-B and CONTENT vs.  $> 1500/2000$  dbar for crossovers). The specific difference between the CANYON-B and CONTENT estimates is a result of the seawater CO<sub>2</sub> chemistry considerations by the latter. For the other variables, the inconsistencies are low and agree with the crossover results (not shown here but results can be accessed through the adjustment table) with the exception of pH. The pH results are further discussed in Sect. 4.2.

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

### 3.2.6 Halogenated transient tracers

For the halogenated transient tracers (CFC-11, CFC-12, CFC-113, and CCl<sub>4</sub>; CFCs for short) inspection of surface saturation levels and evaluation of relationships between the tracers for each cruise were used to identify biases, rather than crossover analyses. Crossover analysis is of limited



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

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).

### 3.3 Merged product generation

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

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

Several minor omissions and errors have been identified in the GLODAPv2 and v2.2019 data products since their release in 2016 and 2019, respectively. Most of these have been corrected in this release. In addition, some recently available

data have been added for a few cruises. The changes are as follows.

- 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,  $\text{SF}_6$ , and  $\text{CCl}_4$  were replaced with new ones received from the principal investigator, and recently published data for  $\delta^{13}\text{C}$  and  $\Delta^{14}\text{C}$  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 a 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  $\delta^{13}\text{C}$  values of station 7 bottle 32 and station 16 bottle 22 were found to be bad (values were less than  $-6\%$ ) and have been removed from the product file.
- For 35MF19850224, the  $\delta^{13}\text{C}$  value of station 21 cast 3 bottle 4 was found to be bad and has been removed.
- For 74JC20100319 the  $\delta^{13}\text{C}$  value at station 37 bottle 7 was found to be bad and has been removed.
- All  $\delta^{13}\text{C}$  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 to be bad (less than  $-2^\circ\text{C}$ ) 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  $0.001^\circ\text{C}$ .
- For cruises 33RO20110926, 33RO20150525, and 33RO20150410,  $\delta^{13}\text{C}$  and  $\Delta^{14}\text{C}$  data have become available and were added to the product.
- Ship codes for all RV *Maria S. Merian* cruises have been changed from MM to M2.
- For cruises 49SH20081021 and 49UF20121024, an adjustment of  $+6\ \mu\text{mol kg}^{-1}$  is now applied to the  $\text{TCO}_2$  values.
- Additional primary QC has been applied to the cruises with *Keifu Maru II* and *Ryofu Maru III* that were included in GLODAPv2.2019.
- Neutral density values in GLODAPv2 and GLODAPv2.2019 had been calculated using the polynomial approximation of Sérazin (2011). All of these values were replaced with neutral density calculated following Jackett and McDougall (1997).
- Discrete  $f\text{CO}_2$  data are now included in the product files whenever available. Discrete  $f\text{CO}_2$  is one of the variables that describe seawater  $\text{CO}_2$  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  $f\text{CO}_2$  data were included indirectly in both GLODAPv1.1 and GLODAPv2 as they had been used in combination with  $\text{TCO}_2$  to calculate TALK. We have now chosen to include the discrete  $f\text{CO}_2$  values in the product files. This increases transparency and traceability of the product; the  $f\text{CO}_2$  data

are also highly relevant for ongoing efforts toward resolving recently identified inconsistencies in our understanding of the relationships among the seawater  $\text{CO}_2$  chemistry variables (Carter et al., 2018; Fong and Dickson, 2019; Takeshita et al., 2020; Álvarez et al., 2020). A total of 33 924 discrete  $f\text{CO}_2$  measurements from 34 cruises conducted between 1983–2014 are now included. All values were converted to  $20^\circ\text{C}$  and 0 dbar pressure using CO2SYS for MATLAB (van Heuven et al., 2011). This was also used for the conversion of partial pressure of  $\text{CO}_2$  ( $p\text{CO}_2$ ) to  $f\text{CO}_2$  for the 20 cruises where  $p\text{CO}_2$  was reported. The procedures for these conversions, in terms of dissociation constants and approximation of missing variables, were the same as for the pH conversions (Sect. 3.2.4). These  $f\text{CO}_2$  data have not been subjected to secondary QC. The inclusion of discrete  $f\text{CO}_2$  data has led to some changes in the calculations of missing seawater  $\text{CO}_2$  chemistry variables; these are described towards the end of the next section.

### 3.3.2 Merging

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

- Data from the 106 new cruises were merged and sorted according to EXPCODE, station, and pressure. GLODAP cruise numbers were assigned consecutively, starting from 2001, so they can be distinguished from the GLODAPv2.2019 cruises that ended at 1116.
- For some cruises the combined concentration of nitrate and nitrite was reported instead of nitrate. If explicit nitrite concentrations were also given, these were subtracted to get the nitrate values. If not, the combined concentration was renamed to nitrate. As nitrite concentrations are very low in the open ocean, this has no practical implications.
- When bottom depths were not given, they were approximated as the deepest sample pressure +10 dbar or extracted from ETOPO1 (Amante and Eakins, 2009), whichever was greater. For GLODAPv2, bottom depths were extracted from the Terrain Base (National Geophysical Data Center/NESDIS/NOAA/U.S. Department of Commerce, 1995). The intended use of this variable is only drawing approximate bottom topography for sections.
- Whenever temperature was missing in the original data file, all data for that record were removed and their flags set to 9. The same was done when both pressure and

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

depth were missing. For all surface samples collected using buckets or similar, the bottle number was set to zero. There are some exceptions to this, in particular for cruises that also used Gerard barrels for sampling. These may have valuable tracer data that are not accompanied by a temperature, so such data have been retained.

- All data with WOCE quality flags 3, 4, 5, or 8 were excluded from the product files and their flags set to 9. Hence, in the product files a flag 9 can indicate not measured (as is also the case for the original exchange formatted data files) or excluded from the product; in any case, no data value appears. All flags 6 (replicate measurement) and 7 (manual chromatographic peak measurement) were set to 2, provided the data appeared good.
- Missing sampling pressures (depths) were calculated from depths (pressures) following UNESCO (1981).
- For both oxygen and salinity, CTD and bottle values were merged following procedures summarized in Sect. 3.2.1.
- Missing salinity, oxygen, nitrate, silicate, and phosphate values were vertically interpolated whenever practical, using a quasi-Hermetian piecewise polynomial. “Whenever practical” means that interpolation was limited to the vertical data separation distances given in Table 4 in Key et al. (2010). Interpolated salinity, oxygen, and nutrient values have been assigned a WOCE quality flag 0.
- The data for the 12 core variables were corrected for bias using the adjustments determined during the secondary QC.
- Values for potential temperature and potential density anomalies (referenced to 0, 1000, 2000, 3000, and 4000 dbar) were calculated using Fofonoff (1977) and Bryden (1973). Neutral density was calculated using Jackett and McDougall (1997); thus neutral density for all 946 cruises is calculated using this procedure.
- Apparent oxygen utilization was determined using the combined fit in Garcia and Gordon (1992).
- Partial pressures for CFC-11, CFC-12, CFC-113, CCl<sub>4</sub>, and SF<sub>6</sub> were calculated using the solubilities by Warner and Weiss (1985), Bu and Warner (1995), Bullister and Wisegarver (1998), and Bullister et al. (2002).
- Missing seawater CO<sub>2</sub> chemistry variables were calculated whenever possible. The procedures for these calculations have been slightly altered as the product now contains four such variables; earlier versions of GLODAPv2 (Olsen et al., 2016; Olsen et al., 2019) included only three, so whenever two were included the one to calculate was unequivocal. Four CO<sub>2</sub> chemistry variables give more degrees of freedom in this respect, e.g., a particular record may have measured data for TCO<sub>2</sub>, TAlk, and pH, and then a choice needs to be made with regard to which pair to use for the calculation of *f*CO<sub>2</sub>. We followed two simple principles. First, TCO<sub>2</sub> and TAlk was the preferred pair to calculate pH and *f*CO<sub>2</sub>, because we have higher confidence in the TCO<sub>2</sub> and TAlk data than pH (given the issues summarized in Sect. 3.2.4) and *f*CO<sub>2</sub> (because it was not subjected to secondary QC). Second, if either TCO<sub>2</sub> or TAlk was missing and both pH and *f*CO<sub>2</sub> data existed, pH was preferred (because *f*CO<sub>2</sub> has not been subjected to sec-

ondary QC). All other combinations involve only two measured variables. The calculations were conducted using CO2SYS (Lewis and Wallace, 1998) for MATLAB (van Heuven et al., 2011), with the constants set as for the pH conversions (Sect. 3.2.4). For calculations involving TCO<sub>2</sub>, TAlk, and pH, if less than a third of the total number of values, measured and calculated combined, for a specific cruise were measured, then all these were replaced by calculated values. The reason for this is that secondary QC of the few measured values was often not possible in such cases, for example due to a limited number of deep data available. Such replacements were not done for calculations involving *f*CO<sub>2</sub>, as this would either overwrite all measured *f*CO<sub>2</sub> values or would entail replacing a measured variable that has been subjected to secondary QC (i.e., TCO<sub>2</sub>, TAlk, or pH) with one calculated from a variable that has not been subjected to secondary QC (i.e., *f*CO<sub>2</sub>). Calculated seawater CO<sub>2</sub> chemistry values have been assigned WOCE flag 0. Seawater CO<sub>2</sub> chemistry values have not been interpolated, so the interpretation of the 0 flag is unique.

- The resulting merged file for the 106 new cruises was appended to the merged product file for GLODAPv2.2019.

#### 4 Secondary quality control results and adjustments

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

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

Table 4 summarizes the actions taken for the merging of the CTD and bottle data for salinity and oxygen. For 81 % of the 106 cruises added with this update, both CTD and bottle data were included for salinity in the original cruise data files and for all these cruises the two data types were found to be consistent. This is similar to the GLODAPv2.2019 results. For oxygen, only 25 % of the cruises included both CTD O<sub>2</sub> and bottle values; this is much less than for GLODAPv2.2019 where 50 % of the cruises included both. Having both CTD and bottle values in the data files is highly preferred as the information is valuable for quality control (bottle mistrips, leaking Niskin bottles, and oxygen sensor drift are among the issues that can be revealed). The extent to which the bottle data (i.e., OXYGEN in the individual cruise exchange files)

**Table 5.** Possible outcomes of the secondary QC and their codes in the online adjustment table.

Secondary QC result	Code
The data are of good quality, consistent with the rest of the dataset and should not be adjusted.	0/1 <sup>a</sup>
The data are of good quality but are biased: adjust by adding (for salinity, TCO <sub>2</sub> , TAlk, pH) or by multiplying (for oxygen, nutrients, CFCs) the adjustment value.	Adjustment value
The data have not been quality controlled, are of uncertain quality, and are 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 and coastal regions, without crossovers or similar, prohibits full secondary QC.	–888
No data exist for this variable for the cruise in question.	–999

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

in reality are mislabeled CTD data (i.e., should be CTDOXY) is uncertain. Regardless, the large majority of the CTD and bottle oxygen were consistent and did not need any further calibration of the CTD values (23 out of 25 cruises), while for two cruises no good fit could be obtained and their CTD O<sub>2</sub> data are not included in the product.

##### 4.2 Adjustment summary

The secondary QC has five different outcomes, provided there are data. These are summarized in Table 5, along with the corresponding codes that appear in the online adjustment table and that are also occasionally used as shorthand for decisions in the coming text. The level of secondary QC varies among the cruises. Specifically, in some cases data were too shallow or geographically too isolated for full and conclusive consistency analyses. A secondary QC flag has been included in the merged product files to enable their identification, with “0” used for variables and cruises not subjected to full secondary QC (corresponding to code –888 in Table 5) and “1” for variables and cruises that were subjected to full secondary QC. The secondary QC flags are assigned per cruise and variable, not for individual data points, and are independent of – and included in addition to – the primary (WOCE) QC flag. For example, interpolated (salinity, oxygen, nutrients) or calculated (TCO<sub>2</sub>, TAlk, pH) values, which have a primary QC

flag 0, may have a secondary QC flag of 1 if the measured data these values are based on have been subjected to full secondary QC. Conversely, individual data points may have a secondary QC flag of 0, even if their primary QC flag is 2 (good data). A 0 flag means that data were too shallow or geographically too isolated for consistency analyses or that these analyses were inconclusive but that we have no reasons to believe that the data in question are of poor quality. Prominent examples for this version are the 10 new Davis Strait cruises: no data were available in this region in GLODAPv2.2019, which, combined with complex hydrography and differences in sampling locations, rendered conclusive secondary QC impossible. As a consequence, most, but not all, of these data (some being excluded because of poor precision after consultation with the PI) are included with a secondary QC flag of 0.

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

For the Sea of Japan cruises, (where two existed in GLODAPv2.2019 and six were added in this version – Sect. 3.2.2), the crossover results showed biased TCO<sub>2</sub> data for one of the older cruises (49HS20081021, which is now adjusted up by 6 μmol kg<sup>-1</sup>) and biased TALK data for two of the presently added cruises (49UF20111004 and 49UF20121024, adjusted up by 5 and 6 μmol kg<sup>-1</sup>, respectively).

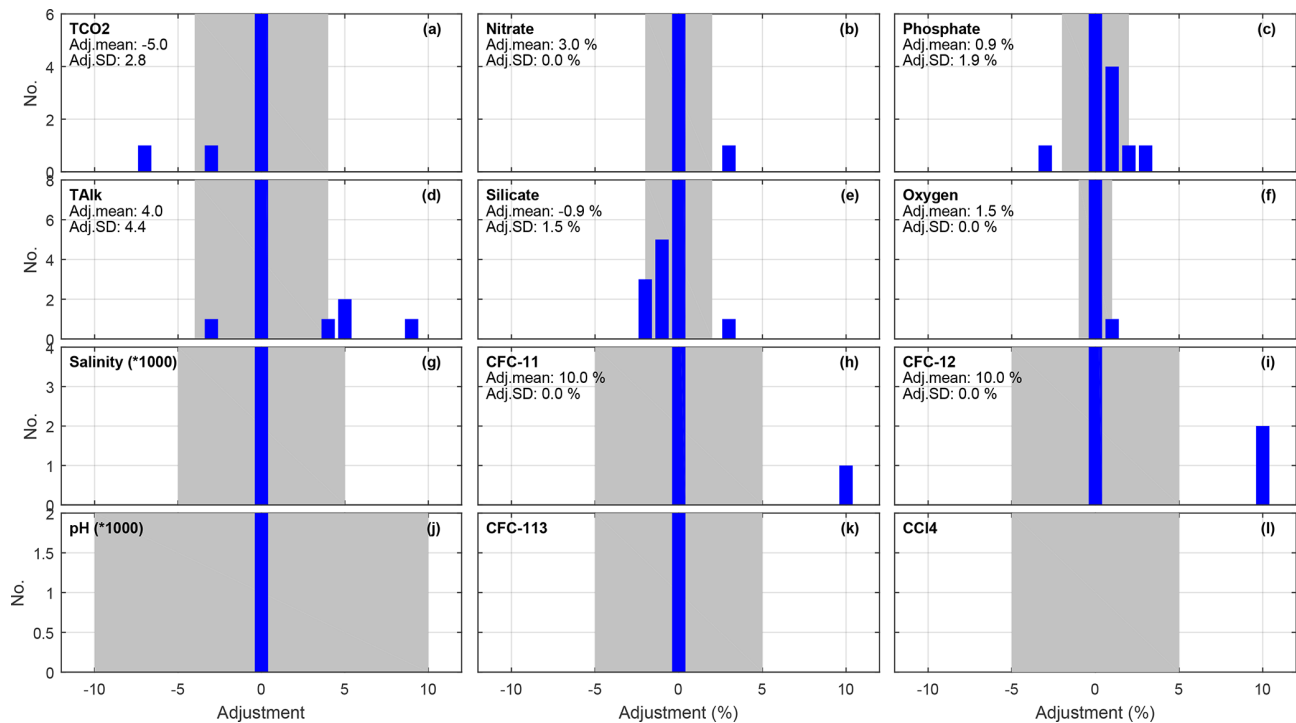
The quality control of pH data proved challenging for this version. The large majority of new pH data had been collected in the northwestern Pacific on cruises conducted by the Japan Meteorological Agency. Figure 7 shows the distribution of pH crossover offsets vs. GLODAPv2.2019. Most of the pH values are higher, some by up to 0.02 pH units; this is considerable, particularly as the data that are compared are from deeper than 2000 dbar where no changes due to ocean acidification are expected. The challenging aspect lies in the fact that the data added are comparatively many (~ 70 cruises vs. ~ 130 already included in this region in v2.2019) and also are more recent (2010–2018 vs. 1993–2016). As such they might be of higher quality given advances in pH measurement techniques over the years. Adjusting a large fraction of the new cruises down (following the adjustment limit of 0.01) is not advisable. We therefore chose to not adjust any pH data but to exclude the most serious outliers from

the product file (using a limit of |0.015|, which led to exclusion of pH data from five cruises) and include the rest of the data without adjustments. We expect that a crossover and inversion analysis of all pH data in the northwestern Pacific will provide more information on the consistency among the cruises, and such an analysis will be conducted for the next update. For now, some caution should be exercised if looking at trends in ocean pH in the northwestern Pacific using GLODAPv2.2020. The crossover and inversion might also result in re-inclusion of the excluded data. The formal decision for the excluded outliers is therefore to “suspend” them (Table 6).

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

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

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



**Figure 6.** Distribution of applied adjustments for each core variable that received secondary QC, in micromoles per kilogram for  $\text{TCO}_2$  and TALK and 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)  $\times$  100). 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).

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

	Sal.	Oxy.	$\text{NO}_3$	Si	$\text{PO}_4$	$\text{TCO}_2$	TALK	pH	CFC-11	CFC-12	CFC-113	$\text{CCl}_4$
With data	106	101	97	97	97	92	96	82	16	21	3	0
No data	0	5	9	9	9	14	10	24	90	85	103	106
Unadjusted <sup>a</sup>	89	85	82	73	75	68	67	65	12	17	2	0
Adjusted <sup>b</sup>	0	1	1	9	7	2	6	0	1	2	0	0
–888 <sup>c</sup>	17	14	14	14	14	22	23	12	2	2	1	0
–666 <sup>d</sup>	0	0	0	0	0	0	0	5	0	0	0	0
–777 <sup>e</sup>	0	1	0	1	1	0	0	0	1	0	0	0

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

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

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

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

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

surement 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 2020) working group (Álvarez et al., 2020).

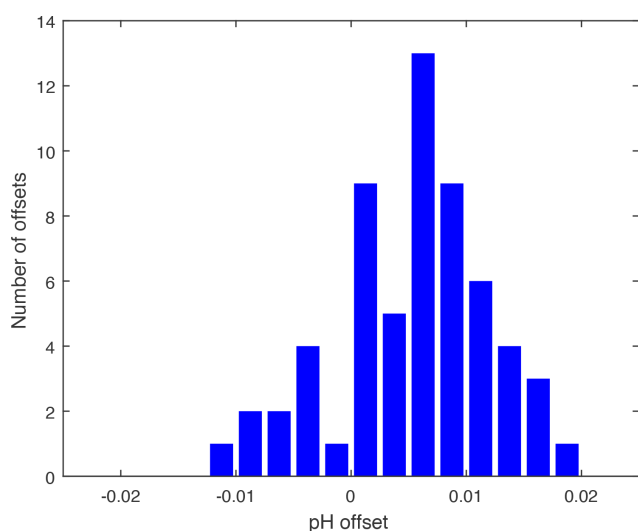
For the nutrients and oxygen, only the phosphate adjustment frequency decreases from decade to decade. However, we do note that the more recent data from the 2010s receive the fewest adjustments. This may reflect recent increased attention that seawater nutrient measurements have received through an operation manual (Becker et al., 2020; Hydes et al., 2012), availability of CRMNS (Aoyama et al., 2012; Ota et al., 2010), and the Scientific Committee on Oceanic Research (SCOR) working group no. 147, “Towards compara-



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

	ARCTIC		ATLANTIC		INDIAN		PACIFIC		GLOBAL		$n$ (global)
	Unadj	Adj	Unadj	Adj	Unadj	Adj	Unadj	Adj	Unadj	Adj	
Sal ( $\times 1000$ )	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
NO <sub>3</sub> (%)	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
PO <sub>4</sub> (%)	5.0	⇒ 2.6	2.2	⇒ 2.0	0.8	⇒ 0.8	0.8	⇒ 0.7	0.8	⇒ 0.8	2047
TCO <sub>2</sub> ( $\mu\text{mol kg}^{-1}$ )	3.4	⇒ 3.4	2.6	⇒ 2.6	1.9	⇒ 1.9	2.1	⇒ 1.8	2.2	⇒ 1.9	512
TAlk ( $\mu\text{mol kg}^{-1}$ )	2.9	⇒ 2.9	1.7	⇒ 1.7	2.4	⇒ 1.6	2.5	⇒ 2.1	2.4	⇒ 2.1	521
pH ( $\times 1000$ )	NA	⇒ NA	8.5	⇒ 8.5	NA	⇒ NA	8.3	⇒ 7.4	8.3	⇒ 7.5	458

NA: not available.

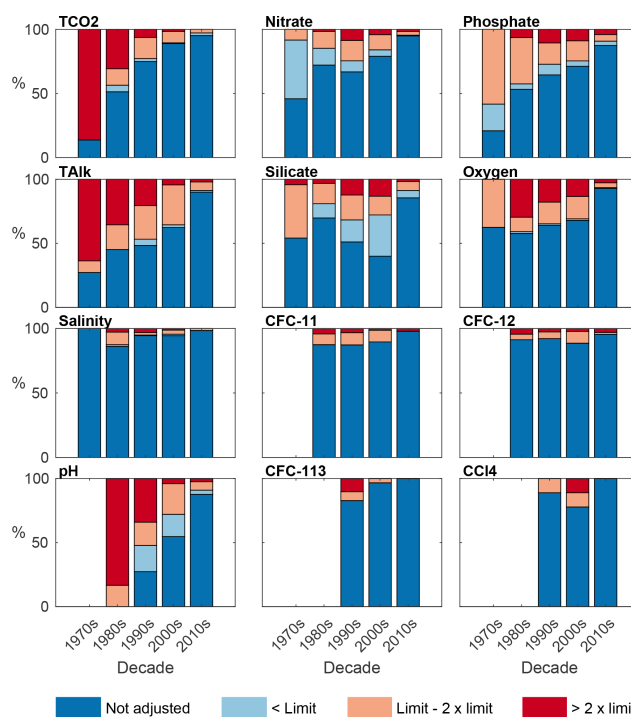


**Figure 7.** Distribution of pH offsets versus GLODAPv2.2019 for the cruises from the Japan Meteorological Agency added in GLODAPv2.2020.

bility of global oceanic nutrient data” (COMONUT). For silicate, the fraction of cruises receiving adjustments peaks in the 1990s and 2000s. This is related to the 2% offset between US and Japanese cruises in the Pacific Ocean that was revealed during production of GLODAPv2 and discussed in Olsen et al. (2016). For salinity and the halogenated transient tracers, the number of adjusted cruises is small in every decade.

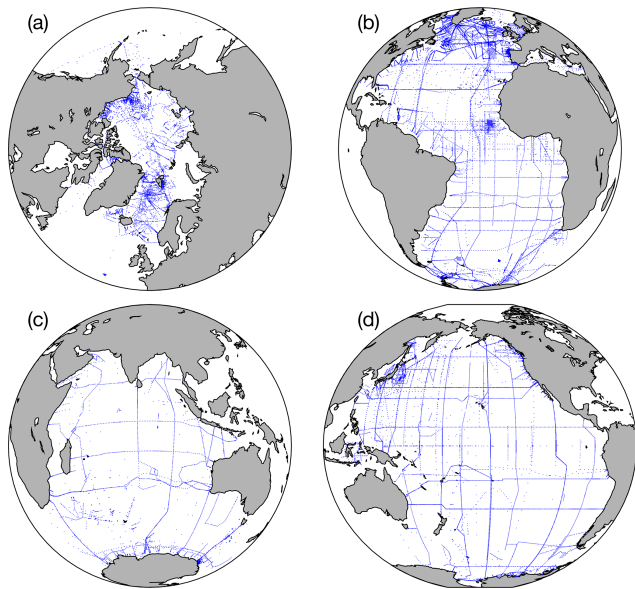
## 5 Data availability

The GLODAPv2.2020 merged and adjusted data product is archived at NOAA NCEI under <https://doi.org/10.25921/2c8h-sa89> (Olsen et al., 2020). These data and ancillary information are also available via our web pages <https://www.glodap.info> and <https://www.glodap.info>



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

[https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2\\_2020/](https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2_2020/) (last access: 22 June 2020). The data are available as comma-separated ascii files (\*.csv) and as binary MATLAB files (\*.mat) that use the open-source Hierarchical Data Format version 5 (HDF5) data format. Regional subsets are available for the Arctic, Atlantic, Pacific, and Indian oceans. There are no data overlaps between regional subsets, and each cruise exists in only one basin file even if data from that cruise cross basin boundaries. The station locations in each basin file are shown in Fig. 9. The product file



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

variables are listed in Table 1. A lookup table for matching the EXPCODE of a cruise with GLODAP cruise number is provided with the data files. In the MATLAB files this information is available as a cell array. A “known issues document” accompanies the data files and provides an overview of known errors and omissions in the data product files. It is regularly updated, and users are encouraged to inform us whenever any new issues are identified. It is critical that users consult this document whenever the data products are used.

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

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

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

data and/or particular region under investigation. This can improve scientific quality and promote data sharing.

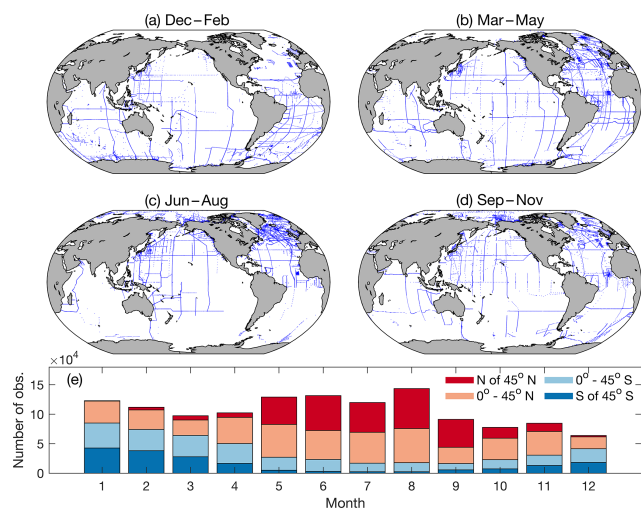
This paper should be cited in any scientific publications that result from usage of the product. Citations provide the most efficient means to track use, which is important for attracting funding to enable the preparation of future updates.

## 6 Summary

GLODAPv2.2020 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 is 1 275 558. Records with measurements for all 12 core variables, salinity, oxygen, nitrate, silicate, phosphate,  $\text{TCO}_2$ , TA, pH, CFC-11, CFC-12, CFC-113, and  $\text{CCl}_4$  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  $\text{CO}_2$  chemistry variables in addition to all the other core variables brings the number of available records up to 9230, 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  $\text{CCl}_4$  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  $\text{CO}_2$  chemistry core variables. The number of measured  $f\text{CO}_2$  data is 33 924; note that these data were not subjected to quality control. The number of records with measured data for salinity, oxygen, and nutrients is 798 703, while the number of records with salinity and oxygen data is 1 077 859. All of these numbers are for measured data, not interpolated or calculated values.

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

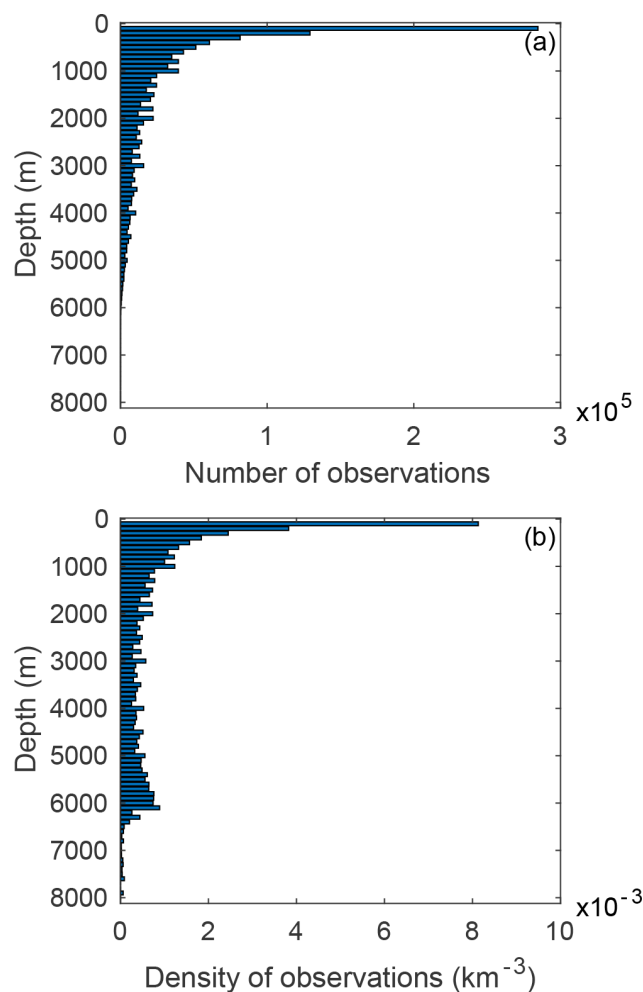


**Figure 10.** Distribution of data in GLODAPv2.2020 in (a) December–February, (b) March–May, (c) June–August, (d) September–November, and (e) number of observations for each month in four latitude bands.

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 106 new cruises to GLODAPv2.2019. Adjustments were only applied when the offsets were believed to reflect biases relative to the earlier data product release related to measurement calibration and/or data-handling practices and not to natural variability or anthropogenic trends. The adjustment table at <https://glodapv2-2020.geomar.de/> (last access: 18 June 2020) lists all applied adjustments and provides a brief justification for each. The consistency analyses rely on deep ocean data ( $> 1500$  or  $2000$  dbar depending on region), but supplementary CANYON-B and CONTENT analyses consider data below 500 dbar. Data consistency for cruises with exclusively shallow sampling was not examined. No pH data were adjusted for this version, but we note that 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)



**Figure 11.** Number (a) and density (b) of observations in 100 m depth layers. The latter was calculated by dividing the number of observations in each layer by its global volume calculated from ETOPO2 (National Geophysical Data Center, 2006). For example, in the layer between 0 and 100 m there are on average approximately 0.008 observations per cubic kilometer. One observation is one water sampling point and has data for several variables.

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

The primary WOCE QC flags in the product files are simplified (e.g., all questionable and bad data were removed). For salinity, oxygen, and the nutrients, any data flagged 0 are interpolated rather than measured. For  $\text{TCO}_2$ , TA, pH, and  $f\text{CO}_2$  any data flags of 0 indicate that the values were calculated from two other measured seawater  $\text{CO}_2$  variables. Finally, while questionable (WOCE flag = 3) and bad (WOCE flag = 4) data have been excluded from the product files,

some may have gone unnoticed through our analyses. Users are encouraged to report on any data that appear suspicious.

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

## Appendix A: Supplementary tables

**Table A1.** Cruises included in GLODAPv2.2020 that did not appear in GLODAPv2.2019. Complete information on each cruise, such as variables included and chief scientist and principal investigator names, is provided in the cruise summary table at [https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2\\_2020/cruise\\_table\\_v2020.html](https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2_2020/cruise_table_v2020.html) (last access: 18 December 2020).

No.	EXPOCODE	Region	Alias	Start (yyyymmdd)	End (yyyymmdd)	Ship
2001	06M220120625	Atlantic	MSM21/2	20120625	20120724	<i>Maria S. Merian</i>
2002	06M220130419	Atlantic	MSM27	20130419	20130506	<i>Maria S. Merian</i>
2003	06M220130509	Atlantic	MSM28	20130509	20130620	<i>Maria S. Merian</i>
2004	06M220140507	Atlantic	MSM38	20140507	20140605	<i>Maria S. Merian</i>
2005	06M220150502	Atlantic	MSM42	20150502	20150522	<i>Maria S. Merian</i>
2006	06M220150525	Atlantic	MSM43	20150525	20150627	<i>Maria S. Merian</i>
2007	06M320100804	Atlantic	M82/2	20100804	20100901	<i>Meteor</i>
2008	096U20180111	Indian	SR03.2018	20180111	20180222	<i>Investigator</i>
2009	18HU20050904	Atlantic	Davis Strait 2005	20050904	20050922	<i>Hudson</i>
2010	18SN20150920	Arctic	JOIS2015	20150920	20151016	<i>Louis S. St-Laurent</i>
2011	29AH20160617	Atlantic	OVIDE-16, A25, A01W	20160617	20160731	<i>Sarmiento de Gamboa</i>
2012	29GD20120910	Atlantic	EUROFLEETS	20120910	20120915	<i>Garcia del Cid</i>
2013	29HE20190406	Atlantic	FICARAM_XIX, A17	20190406	20190518	<i>Hesperides</i>
2014	316N20040922	Atlantic	Davis Strait 2004, KN179-05	20040922	20041004	<i>Knorr</i>
2015	316N20061001	Atlantic	Davis Strait 2006, KN187-02	20061001	20061004	<i>Knorr</i>
2016	316N20071003	Atlantic	Davis Strait 2007, DKN192-02	20071003	20071021	<i>Knorr</i>
2017	316N20080901	Atlantic	Davis Strait 2008, KN194-02	20080901	20080922	<i>Knorr</i>
2018	316N20091006	Atlantic	Davis Strait 2009, KN196-02	20091006	20091028	<i>Knorr</i>
2019	316N20100804	Atlantic	Davis Strait 2010	20100804	20100929	<i>Knorr</i>
2020	316N20101015	Atlantic	KN199-04, GEOTRACES-2010	20101015	20101105	<i>Knorr</i>
2021	316N20111002	Atlantic	Davis Strait 2011, KN203-04	20111002	20111021	<i>Knorr</i>
2022	316N20130914	Atlantic	Davis Strait 2013, KN213-02	20130914	20131003	<i>Knorr</i>
2023	316N20150906	Atlantic	Davis Strait 2015	20150906	20150924	<i>Knorr</i>
2024	32WC20110812	Pacific	WCOA2011	20110812	20110830	<i>Wecoma</i>
2025	33RO20160505	Pacific	WCOA2016	20160505	20160606	<i>Ronald H. Brown</i>
2026	35TH20080825	Atlantic	SUBPOLAR08	20080825	20080915	<i>Thalassa</i>
2027	45CE20170427	Atlantic	CE17007, A02	20170427	20170522	<i>Celtic Explorer</i>
2028	49UF20101002	Pacific	ks201007	20101002	20101104	<i>Keifu Maru II</i>
2029	49UF20101109	Pacific	ks201008	20101109	20101126	<i>Keifu Maru II</i>
2030	49UF20101203	Pacific	ks201009	20101203	20101222	<i>Keifu Maru II</i>
2031	49UF20111004	Pacific	ks201109	20111004	20111127	<i>Keifu Maru II</i>
2032	49UF20111205	Pacific	ks201110	20111205	20111221	<i>Keifu Maru II</i>
2033	49UF20120410	Pacific	ks201203	20120410	20120424	<i>Keifu Maru II</i>
2034	49UF20120602	Pacific	ks201205	20120602	20120614	<i>Keifu Maru II</i>
2035	49UF20131006	Pacific	ks201307	20131006	20131022	<i>Keifu Maru II</i>
2036	49UF20131029	Pacific	ks201308	20131029	20131210	<i>Keifu Maru II</i>
2037	49UF20140107	Pacific	ks201401	20140107	20140125	<i>Keifu Maru II</i>
2038	49UF20140206	Pacific	ks201402	20140206	20140326	<i>Keifu Maru II</i>
2039	49UF20140410	Pacific	ks201403	20140410	20140505	<i>Keifu Maru II</i>
2040	49UF20140512	Pacific	ks201404	20140512	20140617	<i>Keifu Maru II</i>
2041	49UF20140623	Pacific	ks201405, P09, P13	20140623	20140826	<i>Keifu Maru II</i>
2042	49UF20140904	Pacific	ks201406	20140904	20141019	<i>Keifu Maru II</i>
2043	49UF20150107	Pacific	ks201501	20150107	20150126	<i>Keifu Maru II</i>
2044	49UF20150202	Pacific	ks201502	20150202	20150306	<i>Keifu Maru II</i>
2045	49UF20150415	Pacific	ks201504	20150415	20150504	<i>Keifu Maru II</i>
2046	49UF20150511	Pacific	ks201505	20150511	20150611	<i>Keifu Maru II</i>
2047	49UF20150620	Pacific	ks201506, P09, P13	20150620	20150823	<i>Keifu Maru II</i>
2048	49UF20151021	Pacific	ks201508	20151021	20151202	<i>Keifu Maru II</i>
2049	49UF20160107	Pacific	ks201601	20160107	20160126	<i>Keifu Maru II</i>

Table A1. Continued.

No.	EXPCODE	Region	Alias	Start (yyyymmdd)	End (yyyymmdd)	Ship
2050	49UF20160201	Pacific	ks201602	20160201	20160310	<i>Keifu Maru II</i>
2051	49UF20160407	Pacific	ks201604	20160407	20160507	<i>Keifu Maru II</i>
2052	49UF20160512	Pacific	ks201605	20160512	20160610	<i>Keifu Maru II</i>
2053	49UF20160618	Pacific	ks201606	20160618	20160723	<i>Keifu Maru II</i>
2054	49UF20160730	Pacific	ks201607	20160730	20160912	<i>Keifu Maru II</i>
2055	49UF20160917	Pacific	ks201608	20160917	20161007	<i>Keifu Maru II</i>
2056	49UF20161116	Pacific	ks201609	20161116	20161219	<i>Keifu Maru II</i>
2057	49UF20170110	Pacific	ks201701, P09, P10	20170110	20170223	<i>Keifu Maru II</i>
2058	49UF20170228	Pacific	ks201702	20170228	20170326	<i>Keifu Maru II</i>
2059	49UF20170408	Pacific	ks201703	20170408	20170426	<i>Keifu Maru II</i>
2060	49UF20170502	Pacific	ks201704	20170502	20170606	<i>Keifu Maru II</i>
2061	49UF20170612	Pacific	ks201705	20170612	20170713	<i>Keifu Maru II</i>
2062	49UF20170719	Pacific	ks201706, P09, P10	20170719	20170907	<i>Keifu Maru II</i>
2063	49UF20171107	Pacific	ks201708	20171107	20171208	<i>Keifu Maru II</i>
2064	49UF20180129	Pacific	ks201802	20180129	20180309	<i>Keifu Maru II</i>
2065	49UF20180406	Pacific	ks201804	20180406	20180512	<i>Keifu Maru II</i>
2066	49UF20180518	Pacific	ks201805	20180518	20180703	<i>Keifu Maru II</i>
2067	49UF20180709	Pacific	ks201806	20180709	20180829	<i>Keifu Maru II</i>
2068	49UF20180927	Pacific	ks201808	20180927	20181021	<i>Keifu Maru II</i>
2069	49UP20110912	Pacific	rf201109	20110912	20110929	<i>Ryofu Maru III</i>
2070	49UP20120306	Pacific	rf201202	20120306	20120325	<i>Ryofu Maru III</i>
2071	49UP20121116	Pacific	rf201208	20121116	20121218	<i>Ryofu Maru III</i>
2072	49UP20130307	Pacific	rf201302	20130307	20130327	<i>Ryofu Maru III</i>
2073	49UP20130426	Pacific	rf201304	20130426	20130527	<i>Ryofu Maru III</i>
2074	49UP20131128	Pacific	rf201310	20131128	20131223	<i>Ryofu Maru III</i>
2075	49UP20140108	Pacific	rf201401, P09, P10	20140108	20140301	<i>Ryofu Maru III</i>
2076	49UP20140307	Pacific	rf201402	20140307	20140326	<i>Ryofu Maru III</i>
2077	49UP20140429	Pacific	rf201404	20140429	20140530	<i>Ryofu Maru III</i>
2078	49UP20140609	Pacific	rf201405	20140609	20140629	<i>Ryofu Maru III</i>
2079	49UP20141112	Pacific	rf201409	20141112	20141202	<i>Ryofu Maru III</i>
2080	49UP20150110	Pacific	rf201501	20150110	20150223	<i>Ryofu Maru III</i>
2081	49UP20150228	Pacific	rf201502	20150228	20150326	<i>Ryofu Maru III</i>
2082	49UP20150408	Pacific	rf201503	20150408	20150419	<i>Ryofu Maru III</i>
2083	49UP20150426	Pacific	rf201504	20150426	20150528	<i>Ryofu Maru III</i>
2084	49UP20150604	Pacific	rf201505	20150604	20150623	<i>Ryofu Maru III</i>
2085	49UP20150627	Pacific	rf201506	20150627	20150716	<i>Ryofu Maru III</i>
2086	49UP20151115	Pacific	rf201509	20151115	20151216	<i>Ryofu Maru III</i>
2087	49UP20160109	Pacific	rf201601, P09, P10	20160109	20160222	<i>Ryofu Maru III</i>
2088	49UP20160227	Pacific	rf201602	20160227	20160324	<i>Ryofu Maru III</i>
2089	49UP20160408	Pacific	rf201603	20160408	20160421	<i>Ryofu Maru III</i>
2090	49UP20160427	Pacific	rf201604	20160427	20160601	<i>Ryofu Maru III</i>
2091	49UP20160608	Pacific	rf201605	20160608	20160628	<i>Ryofu Maru III</i>
2092	49UP20161021	Pacific	rf201608	20161021	20161206	<i>Ryofu Maru III</i>
2093	49UP20170107	Pacific	rf201701	20170107	20170126	<i>Ryofu Maru III</i>
2094	49UP20170201	Pacific	rf201702	20170201	20170310	<i>Ryofu Maru III</i>
2095	49UP20170425	Pacific	rf201705	20170425	20170508	<i>Ryofu Maru III</i>
2096	49UP20170623	Pacific	rf201707	20170623	20170827	<i>Ryofu Maru III</i>
2097	49UP20170815	Pacific	rf201708	20170815	20171006	<i>Ryofu Maru III</i>
2098	49UP20171125	Pacific	rf201710	20171125	20171224	<i>Ryofu Maru III</i>
2099	49UP20180110	Pacific	rf201801	20180110	20180222	<i>Ryofu Maru III</i>
2100	49UP20180228	Pacific	rf201802	20180228	20180326	<i>Ryofu Maru III</i>
2101	49UP20180501	Pacific	rf201804	20180501	20180605	<i>Ryofu Maru III</i>
2102	49UP20180614	Pacific	rf201805	20180614	20180722	<i>Ryofu Maru III</i>
2103	49UP20180806	Pacific	rf201806, P13	20180806	20180927	<i>Ryofu Maru III</i>
2104	64PE20071026	Atlantic	PE278	20071026	20071117	<i>Pelagia</i>
2105	740H20180228	Atlantic	JC159	20180228	20180410	<i>James Cook</i>
2106	91AA20171209	Indian	NCAOR, SOE2017-18	20171209	20180204	<i>S.A. Agulhas I</i>

### Note on former version

Former versions of this article were published on 15 August 2016 and 25 September 2019 and are available at <https://doi.org/10.5194/essd-8-297-2016> and <https://doi.org/10.5194/essd-11-1437-2019>.

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

**Competing interests.** The authors declare that they have no conflict of interest.

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