The annual update GLODAPv2.2023: the global interior ocean biogeochemical data product

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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 bottle data, with an emphasis on seawater inorganic carbon chemistry and related variables determined through chemical analysis of seawater samples. GLODAPv2.2023 is an update of the previous version, GLODAPv2.2022 (Lauvset et al., 2022). The major changes are as follows: data from 23 new cruises were added. In addition, a number of changes were made to data included in GLODAPv2.2022. GLODAPv2.2023 includes measurements from more than 1.4 million water samples from the global oceans collected on 1108 cruises. The data for the now 13 GLODAP core variables (salinity, oxygen, nitrate, silicate, phosphate, dissolved inorganic carbon, total alkalinity, pH, chlorofluorocarbon-11 (CFC-11), CFC-12, CFC-113, CCl_4, and SF_6) 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 converted to World Ocean Circulation Experiment (WOCE) exchange format and (ii) as a merged data product with adjustments applied to minimize bias. For the present annual update, adjustments for the 23 new cruises were derived by comparing those data with the data from the 1085 quality-controlled cruises in the GLODAPv2.2022 data product using crossover analysis. SF_6 data from all cruises were evaluated by comparison with CFC-12 data measured on the same cruises. For nutrients and ocean carbon dioxide (CO_2) chemistry comparisons to estimates based on empirical algorithms provided additional context for adjustment decisions. The adjustments that we applied are intended to remove potential biases from errors related to measurement, calibration, and data handling practices without removing known or likely time trends or variations in the variables evaluated. The compiled and adjusted data product is believed to be consistent to better than 0.005 in salinity, 1 % in oxygen, 2 % in nitrate, 2 % in silicate, 2 % in phosphate, 4 μmol kg^{-1} in dissolved inorganic carbon, 4 μmol kg^{-1} in total alkalinity, 0.01–0.02 in pH (depending on region), and 5 % in the halogenated transient tracers. The other variables included in the compilation, such as isotopic tracers and discrete CO_2 fugacity (fCO$_2$), were not subjected to bias comparison or adjustments.

The original data, their documentation and DOI codes are available at the Ocean Carbon and Acidification Data System of NOAA NCEI, which also provides access to the merged data product. This 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/zyrq-ht66 (Lauvset et al., 2023). These bias-adjusted product files also include significant ancillary and approximated data, which were obtained by interpolation of, or calculation from, measured data. This living data update documents the GLODAPv2.2023 methods and provides a broad overview of the secondary quality control procedures and results.

1 Introduction

The oceans mitigate climate change by absorbing both atmospheric CO_2 corresponding to a significant fraction of anthropogenic CO_2 emissions (Friedlingstein et al., 2022; Gruber et al., 2019; Müller et al., 2023) and most of the excess heat in the Earth system caused by the enhanced greenhouse effect (Cheng et al., 2017; Cheng et al., 2020). The objective of GLODAP (Global Ocean Data Analysis Project, www.glodap.info, last access: 07 Sep 2023) is to provide high-quality and bias-corrected water column bottle data from the ocean surface to the sea floor. These data should be used to document the state and the evolving changes in physical and chemical ocean properties, e.g., the inventory of anthropogenic CO_2 in the ocean, natural oceanic carbon, ocean acidification, ventilation rates, oxygen levels, and vertical nutrient transports (Tanhua et al., 2021). The core quality-controlled and bias-adjusted variables of GLODAP are salinity, dissolved oxygen, inorganic macronutrients (nitrate, silicate, and phosphate), seawater CO_2 chemistry variables (dissolved inorganic carbon

– TCO$_2$, total alkalinity – TAlk, and pH on the total hydrogen ion, or H$^+$, scale), the halogenated transient tracers chlorofluorocarbon-11 (CFC-11), CFC-12, CFC-113, carbon tetrachloride (CCl$_4$), and sulfur hexafluoride (SF$_6$).

Other chemical tracers are measured on many cruises included in GLODAP, such as dissolved organic carbon and nitrogen, as well as stable and radioactive isotope ratios. In many cases, a subset of these data is distributed as part of the GLODAP

75   data product, however, such data have not been extensively quality controlled or checked for measurement biases in this effort. For some of these variables better sources of data exist, for example the product by Jenkins et al. (2019) for helium isotope and tritium data or the dissolved organic matter product by Hansell et al. (2021). GLODAP also includes some common derived variables to facilitate interpretation, such as potential density anomalies and apparent oxygen utilization (AOU). A full list of variables included in the data product is provided in Table 1.

80   **Table 1.** Variables in the GLODAPv2.2023 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 (e.g., G2cruise).

Variable	Units	Product file name	WOCE flag name[a]	2nd QC flag name[b]	WHP-exchange name
Expocode		expocode			
Digital Object Identifier		doi			
Assigned sequential cruise number		cruise			
Basin identifier[c]		region			
Station		station			STNNBR
Cast		cast			CASTNO
Year		year			DATE
Month		month			DATE
Day		day			DATE
Hour		hour			TIME
Minute		minute			TIME
Latitude		latitude			LATITUDE
Longitude		longitude			LONGITUDE
Bottom depth	m	bottomdepth			
Pressure of the deepest sample	dbar	maxsampdepth			DEPTH
Niskin botttle number		bottle			BTLNBR
Sampling pressure	dbar	pressure			CTDPRS
Sampling depth	m	depth			
Temperature	°C	temperature			CTDTMP
Potential temperature	°C	theta			
Salinity		salinity	salinityf	salinityqc	CTDSAL/SALNTY
Potential density anomaly	kg m^{-3}	sigma0	(salinityf)		
Potential density anomaly, ref 1000 dbar	kg m^{-3}	sigma1	(salinityf)		
Potential density anomaly, ref 2000 dbar	kg m^{-3}	sigma2	(salinityf)		
Potential density anomaly, ref 3000 dbar	kg m^{-3}	sigma3	(salinityf)		

Variable	Units	Product file name	WOCE flag name[a]	2nd QC flag name[b]	WHP-exchange name
Potential density anomaly, ref 4000 dbar	kg m^{-3}	sigma4	(salinityf)		
Neutral density anomaly	kg m^{-3}	gamma	(salinityf)		
Oxygen	µmol kg^{-1}	oxygen	oxygenf	oxygenqc	CTDOXY/OXYGEN
Apparent oxygen utilization	µmol kg^{-1}	aou	aouf		
Nitrate	µmol kg^{-1}	nitrate	nitratef	nitrateqc	NITRAT
Nitrite	µmol kg^{-1}	nitrite	nitritef		NITRIT
Silicate	µmol kg^{-1}	silicate	silicatef	silicateqc	SILCAT
Phosphate	µmol kg^{-1}	phosphate	phosphatef	phosphateqc	PHSPHT
TCO$_2$	µmol kg^{-1}	tco2	tco2f	tco2qc	TCARBON
TAlk	µmol kg^{-1}	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		phtsinsitutp	phtsinsitutpf	phtsqc	
fCO$_2$ at 20° C and 0 dbar of pressure	µatm	fco2	fco2f		FCO2/PCO2
fCO$_2$ temperature [d]	°C	$f$co2temp	(fco2f)		FCO2_TMP/PCO2_TMP
CFC-11	pmol kg^{-1}	cfc11	cfc11f	cfc11qc	CFC-11
pCFC-11	ppt	pcfc11	(cfc11f)		
CFC-12	pmol kg^{-1}	cfc12	cfc12f	cfc12qc	CFC-12
pCFC-12	ppt	pcfc12	(cfc12f)		
CFC-113	pmol kg^{-1}	cfc113	cfc113f	cfc113qc	CFC-113
pCFC-113	ppt	pcfc113	(cfc113f)		
CCl$_4$	pmol kg^{-1}	ccl4	ccl4f	ccl4qc	CCL4
pCCl$_4$	ppt	pccl4	(ccl4f)		
SF$_6$	fmol kg^{-1}	sf6	sf6f	sf6qc	SF6
pSF6	ppt	psf6	(sf6f)		
δ^{13}C	‰	c13	c13f	c13qc	DELC13
Δ^{14}C	‰	c14	c14f		DELC14
Δ^{14}C counting error	‰	c14err			C14ERR
^{3}H	TU	h3	h3f		TRITIUM
^{3}H counting error	TU	h3err			TRITER
δ^{3}He	%	he3	he3f		DELHE3
^{3}He counting error	%	he3err			DELHER
He	nmol kg^{-1}	he	hef		HELIUM
He counting error	nmol kg^{-1}	heerr			HELIER
Ne	nmol kg^{-1}	neon	neonf		NEON
Ne counting error	nmol kg^{-1}	neonerr			NEONER
δ^{18}O	‰	o18	o18f		DELO18

Variable	Units	Product file name	WOCE flag name[a]	2nd QC flag name[b]	WHP-exchange name
Total organic carbon	µmol L^{-1} [e]	toc	tocf		TOC
Dissolved organic carbon	µmol L^{-1} [e]	doc	docf		DOC
Dissolved organic nitrogen	µmol L^{-1} [e]	don	donf		DON
Dissolved total nitrogen	µmol L^{-1} [e]	tdn	tdnf		TDN
Chlorophyll *a*	µg kg^{-1} [e]	chla	chlaf		CHLORA

[a]The only derived variable assigned a separate WOCE flag is AOU as it depends strongly on both temperature and oxygen (and less strongly on salinity). For the other derived variables, the applicable WOCE flag is given in parentheses. [b] Secondary QC flags indicate whether data have been subjected to full secondary QC (1) or not (0), as described in Sect. 3. [c] 1 is the Atlantic Ocean, 4 is the Arctic Mediterranean Sea (i.e., the Arctic Ocean plus the Nordic Seas), 8 is the Pacific Ocean, and 16 is the Indian Ocean. [d] Included for clarity, is 20 °C for all occurences. [e]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.

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, limit the realization of their full scientific potential. In addition, the manual data retrieval is time consuming and prone to data handling errors (Tanhua et al., 2021). For biogeochemical data there is the added complexity of different levels of standardization and calibration, and even different units and scales used for the same variable such that the comparability between datasets is often poor. Standard operating procedures have been developed for some variables (Dickson et al., 2007; Hood et al., 2010; Becker et al., 2020), certified reference materials (CRMs) exist for seawater TCO$_2$ and TAlk measurements (Dickson et al., 2003), and reference materials for nutrients in seawater (RMNS, certified based on International Organization for Standardization Guide 34; Aoyama et al., 2012; Ota et al., 2010) are also available. Despite all this, biases in data still exist. These can arise from poor sampling and preservation practices, calibration procedures, instrument design and calibration, and inaccurate calculations. The use of CRMs does not by itself ensure accurate measurements of seawater CO$_2$ chemistry (Bockmon and Dickson, 2015), and the RMNS have only become available recently and are not universally used. For salinity and oxygen, the 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 rigorous primary and secondary quality control assessments, focusing on precision and consistency, respectively. The secondary quality control focuses on deep data, in which natural variability is minimal. Adjustments are applied to the data to minimize cases of bias that could be confidently established relative to the measurement precision for the variables and cruises considered. Key metadata are provided in the header of each data file, and original unadjusted data along with full cruise reports submitted by the data providers (where available) are accessible through the GLODAPv2 cruise summary table hosted by the Ocean Carbon and Acidification Data System (OCADS) at the National Oceanographic and Atmospheric Administration (NOAA) National Centers for Environmental Information (NCEI) (https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2023/cruise_table_v2023.html, last access: 12 October 2023).

This most recent GLODAPv2.2023 data product builds on earlier synthesis efforts for biogeochemical data obtained from research cruises, namely, GLODAPv1.1 (Key et al., 2004; Sabine et al., 2005), Carbon dioxide in the Atlantic Ocean (CARINA) (Key et al., 2010), Pacific Ocean Interior Carbon (PACIFICA) (Suzuki et al., 2013), and notably GLODAPv2 (Olsen et al., 2016). GLODAPv1.1 combined data from 115 cruises with biogeochemical measurements from the global ocean. The vast majority of these were the sections covered during the World Ocean Circulation Experiment and the Joint Global Ocean Flux Study (WOCE/JGOFS) in the 1990s, but data from important "historical" cruises were also included, such as from the Geochemical Ocean Sections Study (GEOSECS), Transient Traces in the Ocean (TTO), and South Atlantic Ventilation Experiment (SAVE). GLODAPv2, which forms the basis for the update presented here, was released in 2016 with data from 724 scientific cruises, including those from GLODAPv1.1, CARINA, and PACIFICA, as well as data from 168 additional cruises. GLODAPv2 not only combined all previous efforts, but it also created ocean-wide consistency across all cruise data through an inversion analysis. A particularly important source of additional data was 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 updated regularly using the "living data process" of *Earth System Science Data* to document significant additions and modifications to the data product.

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) in which all data points are subject to potential adjustment. This was carried out for the creation of 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 from previous releases are not changed or adjusted during intermediate updates. Note that 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, as well as other checks of the entire dataset needed for full updates, are too demanding in terms of time and resources to be performed every year or every 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 2024. Work on GLODAPv3 commences in fall 2023, and we anticipate that GLODAPv3 will become available at the end of 2025. In the interim, the fifth intermediate update is presented here, which adds data from 23 cruises to the last update, GLODAPv2.2022 (Lauvset et al., 2022). Given the anticipated schedule towards GLODAPv3, this will be the final intermediate update of GLODAPv2.

2 Key features of the update

GLODAPv2.2023 contains data from 1108 cruises covering the global ocean from 1972 to 2021, compared to 1085 for the period 1972-2021 for the previous GLODAPv2.2022 (Lauvset et al., 2022). Information about the 23 cruises added to this version is provided in Table A1 in the Appendix. Cruise sampling locations are shown alongside those of GLODAPv2.2023 in Fig. 1, while the coverage in time is shown in Fig. 2. Not all cruises have data for all the above-mentioned 13 core variables. For example, cruises with only seawater CO_2 chemistry or transient tracer data are still included even without

accompanying nutrient data due to their value towards the computation of carbon inventories. In a few cases, cruises without any of these properties are included because they do contain data for other carbon-related tracers such as carbon isotopes, with the intention of ensuring their wider availability. The added cruises are from 2002 to 2021, with the majority being more recent than 2018. This update consists of:

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- 5 cruises in the northeast North Atlantic from Marine Institute Ireland
- 3 time series datasets in the Arctic Ocean
- A dataset from the Greenland-Scotland ridge including multiple stations in the Irminger and Iceland Seas over the years 2002-2006, and the Iceland standard section at 64°20'N
- 4 Japanese cruises in the Northwest Pacific Ocean
165
- 1 Chinese National Arctic Research Expedition (CHINARE) cruise from the Arctic (Chukchi Sea) in 2008
- An update of the Irminger and Iceland Sea time series with new data from 2014 – 2019
- 1 Line-P cruise (2015)
- 3 coastal cruises out of Iquique from the Coastal Ecosystem and Environmental Change lab (ECCO-Lab) in Chile
- 1 Discovery cruise in the Southern Ocean
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- A20 and A22 occupations from 2021
- The 2018 Observatoire de la variabilité interannuelle et décennale en Atlantique Nord (OVIDE) cruise

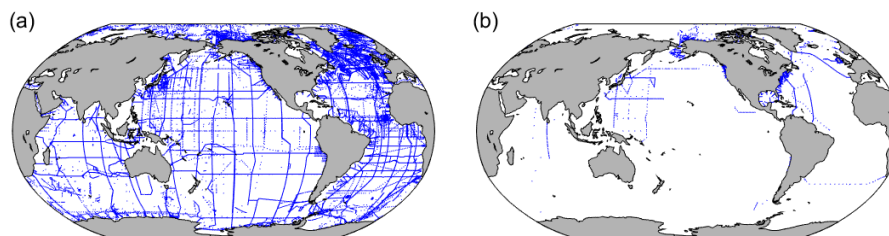
All new cruises in GLODAPv2.2023 include seawater CO_2 chemistry data, and 8 of these also include data on halogenated transient tracers.

175

Figure 1. Location of stations in (a) GLODAPv2.2022 and for (b) the new data added in this update.

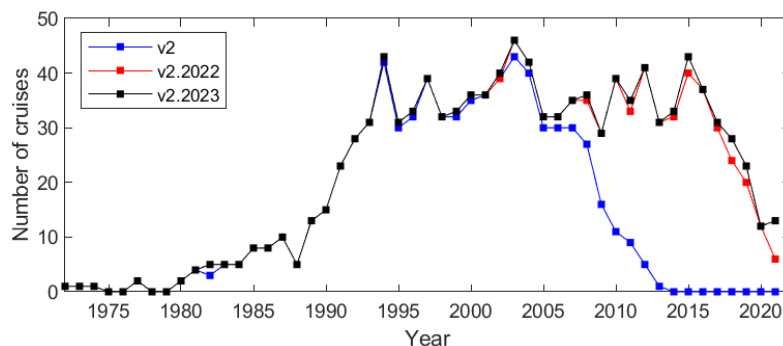



Figure 2. Number of cruises per year in GLODAPv2, GLODAPv2.2022, and GLODAPv2.2023.

180   All new cruises were subjected to primary (Sect. 3.1) and secondary (Sect. 3.2) quality control (QC). These procedures are very similar to those used for GLODAPv2.2022 and previous versions, aiming to ensure the consistency of the data from the 23 new cruises with the previous release of the GLODAP data product (in this case, the GLODAPv2.2022 adjusted data product). As for GLODAPv2.2022 we also apply secondary QC routines to SF_6 data.

For GLODAPv2.2021 we added a basin identifier to the product files, where 1 is the Atlantic Ocean, 4 the Arctic

185   Mediterranean Sea (i.e., the Arctic Ocean plus the Nordic Seas), 8 the Pacific Ocean, and 16 the Indian Ocean. These regions are abbreviated AO, AMS, PO, and IO, respectively, in the adjustment table. Data in the Mediterranean Sea, Caribbean Sea, and Gulf of Mexico are classified as belonging to the Atlantic Ocean (1). These basin identifiers were added to the product files, first in GLODAPv2.2022, to make it easier for users to identify which ocean basin an individual cruise belongs to without having to use one of the four regional files. This remains in GLODAPv2.2023. Note that there is no

190   overlap between the regional files or for our basin identifiers, and cruises in the Southern Ocean are placed in the basin where most of the data were collected. As in the previous version, GLODAPv2.2022, we include the DOI for each cruise in all product files with the aim of easing access to the original data and metadata, as well as improving the visibility of data providers.

3 Methods

3.1 Data assembly and primary quality control

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Data from the 23 new cruises were submitted directly to us or retrieved from data centers – typically OCADS (https://www.ncei.noaa.gov/products/ocean-carbon-acidification-data-system, last access : 7 Sep 2023), the CLIVAR and Carbon Hydrographic Data Office (https://cchdo.ucsd.edu, last access: 7 Sep 2023), and PANGAEA (https://pangaea.de, last access: 7 Sep 2023). Each cruise is identified by an expedition code (EXPOCODE). The EXPOCODE is guaranteed to

200   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 7 Sep 2023).

The individual cruise data files were converted to the WHP-exchange format: a comma-delimited ascii format for data from hydrographic cruises, with different and specific versions for CTD and bottle data. GLODAP only includes WHP-exchange

205   in bottle format, with data and CTD data at bottle trip depths. An overview of the significant points is given below, with full details provided at https://exchange-format.readthedocs.io/ (v1.2.0 as of 2022-03-22, last access: 7 Sep 2023), derived from 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 creation date time stamp in ISO8601 (YYYYMMDD) format, as well as the identification of the group and person who prepared the file. The latter follows a convention of including the division/group, the institution,

210   and the initials of the person. The omnipresent "PRINUNIVRMK" thus acknowledges the enormous effort by Robert M. Key at Princeton University. Next follows the README section, which 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 is 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

215   as file update notes are included. The only rule for the README section is that it must be concise and informative, and each line must start with the comment character (#). The README is followed by variable names and units on separate lines, and then the data. The names and units are standardized and provided in Table 1 for the variables included in

GLODAP, with full specifications provided at https://exchange-format.readthedocs.io/en/latest/parameters.html (v1.2.0 as of 2022-03-22, last access: 7 Sep 2023). For consistency with previous updates, and to ease the use of existing methods and code, GLODAP still uses the WHP-exchange format instead of adopting the new naming structure as outlined in Jiang et al. (2022).

Exchange file preparation required unit conversion in some cases, most frequently from concentrations expressed as milliliters per liter (mL L^{-1}; oxygen) or micromoles per liter (μmol L^{-1}; nutrients) to substance contents expressed as micromoles per kilogram of seawater (μmol kg^{-1}). Procedures as described in Jiang et al. (2022) were used for these conversions. The default conversion procedure for nutrients was to use seawater density at reported salinity, an assumed measurement temperature of 22 ºC, and pressure of 1 atm. For oxygen, the factor 44.66 was used for the "milliliters of oxygen" to "micromoles of oxygen" conversion, while the density required for the "per liter" to "per kilogram" conversion was calculated from the reported salinity and draw temperatures whenever possible. However, potential density was used instead when draw temperature was not reported. The potential errors introduced by any of these procedures are insignificant. Missing numbers are indicated by -999.

Table 2. WOCE flags in GLODAPv2.2023 exchange-format original data files (briefly; for full details see Swift, 2010) and the simplified scheme used in the merged product files.

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

[a]Flag set to 9 in product files
[b]Data are not included in the GLODAPv2.2023 product files and their flags set to 9.
[c]Data are included, but flag set to 2

Each data column (except temperature and pressure, which are assumed "good" if they exist) has an associated column of data flags (Joyce and Corry, 1994). 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); 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 approximated: for salinity, oxygen, phosphate, nitrate, and silicate, the approximation is conducted using vertical interpolation; for seawater CO_2 chemistry variables (TCO_2, TAlk, pH, and fCO_2), the approximation is conducted using the calculation from two measured CO_2 chemistry variables (Sect. 3.2.2). Importantly, the interpolation of 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 the GLODAP reference group (https://glodap.info/index.php/group/, last access: 16 October 2023). Regardless, all incoming files were subjected to

250 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. For this task, the GLODAP primary quality control software (Velo et al., 2021) was used as it presents a custom pre-defined schema of property–property plots designed by the consortium to ease the detection of outliers. 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

255 been applied in the GLODAP versions of the original cruise data files in agreement with the data submitter.

3.2 Secondary quality control

The aim of the secondary QC was to identify and correct any significant biases in the data from the 23 new cruises relative to GLODAPv2.2022 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

260 reference group through a series of teleconferences during May 2023 to decide the adjustments to be applied to reduce the apparent offset (if any). To guide this process, a set of initial minimum adjustment limits was prescribed (Table 3). These represent the minimum bias that can be confidently established relative to the measurement precision for the variables and cruises considered and are the same as those used for GLODAPv2.2022. 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

265 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 when 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

270 or a single and constant measurement bias. Adjustments for salinity, TCO_2, TAlk, and pH are always additive, while adjustments for oxygen, nutrients, and the halogenated transient tracers are always multiplicative. Except where explicitly noted (Sect. 3.3.1 and Table A2 in the Appendix) adjustments were not modified for data previously included in GLODAPv2.2022.

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

Variable	Minimum adjustment
Salinity	0.005
Oxygen	1 %
Nutrients	2 %
TCO_2	4 μmol kg^{-1}
TAlk	4 μmol kg^{-1}
pH	0.01
CFCs	5 %

Crossover comparisons were the primary source of information used to identify offsets for salinity, oxygen, nutrients, TCO_2, TAlk, and pH (Sect. 3.2.2). As in GLODAPv2.2022, GLODAPv2.2021 and GLODAPv2.2020 but in contrast to

280 GLODAPv2 and GLODAPv2.2019, the evaluation of the internal consistency of the seawater CO_2 chemistry variables was not used for the evaluation of pH (Sect. 3.2.3). As in the three previous updates (2020, 2021 and 2022) we made extensive use of two predictions from two empirical algorithms – CArbonate system And Nutrients concentration from hYdrological

properties and Oxygen using a Neural-network version B (CANYON-B) and CONsisTency EstimatioN and amounT (CONTENT) (Bittig et al., 2018) – for the evaluation of offsets in nutrients and seawater CO_2 chemistry data (Sect. 3.2.4).

285 For previous versions we have also used multiple linear regression analyses and deep water averages, broadly following Jutterström et al. (2010), for additional information for the secondary QC of salinity, oxygen, nutrients, TCO_2, and TAlk data. As in GLODAPv2.2022 we did not have to rely on the results of the MLR analyses to make decisions about adjustments, and, in general, we are increasingly moving towards only using CANYON-B and CONTENT estimates (Sect. 3.2.4) as additional information when the crossover analysis is insufficient.

290 For the halogenated transient tracers, comparisons of surface saturation levels and the relationships among the tracers were used to assess the data consistency (Sect. 3.2.5). For salinity and oxygen, CTD and bottle values were merged into a "hybrid" variable prior to the consistency analyses (Sect. 3.2.1).

3.2.1 Merging of sensor and bottle data

Salinity and oxygen data can be obtained by analysis of water samples (bottle data) and/or directly from the CTD sensor 295 pack. These two measurement types are merged and presented as a single variable in the product. The merging was conducted prior to the consistency checks, ensuring their internal calibration in the product. The merging procedures were only applied to the bottle data files, which commonly include values recorded by the CTD at the pressures where the water samples are collected. Whenever both CTD and bottle data were present in a data file, the merging step considered the deviation between the two and calibrated the CTD values if required and possible. Altogether seven scenarios (Table 4) are 300 possible for each of the CTD conductivity and oxygen (O_2) sensor properties individually, in which the fourth never occurred during our analyses but is included to maintain consistency with GLODAPv2. For salinity 48 % of the 23 new cruises included both CTD and bottle data in the original cruise files, and for oxygen 57 % of the new cruises were oxygen was included (14) had both CTD and bottle data (Table 6). For all these cruises the two data types were found to be consistent for both oxygen and salinity. These new data have higher proportion of cruises with both bottle and CTD 305 measurements than GLODAPv2.2022 (39 % for both salinity and oxygen). For oxygen the remaining cruises have only CTD data, while for salinity 22 % have only CTD data and 30 % have only bottle data. Having both CTD and bottle values in the data files is highly preferred as the information is valuable for quality control (bottle misfires, 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) is mislabeled CTD data (i.e., should be CTDOXY) is uncertain. Regardless, all CTD 310 and bottle data for salinity and oxygen were consistent and did not need any further calibration.

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

Case	Description	Salinity	Oxygen
1	No data are available: no action needed.	0	9
2	No bottle values are available: use CTD values.	11	4
3	No CTD values are available: use bottle values.	1	2
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.	11	8
6	The CTD values deviate significantly from bottle values: calibrate CTD values using linear fit and replace missing bottle values with calibrated CTD values.	0	0

| 7 | The CTD values deviate significantly from bottle values, and no good linear fit can be obtained for the cruise: use bottle values and discard CTD values. | 0 | 0 |

3.2.2 Crossover analyses

The crossover analyses were conducted with the MATLAB toolbox prepared by Lauvset and Tanhua (2015) and with GLODAPv2.2022 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. To minimize the effects of natural variability only deep data are used. Either the 1500 or 2000 dbar pressure surface was used as the upper bound, depending on the amount of available data, their variation at different depths, and the region in question. Which one to use was determined on a case-by-case basis by comparing crossovers with the two depth limits and using the one that provided the clearest and most 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 and bottom water formation usually occurs along the Antarctic coasts, where relatively thin nascent dense water plumes flow down the continental slope. We avoid such cases, which are easily recognizable. 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 alkalinity measured on the two cruises 35TH20180611, which is new to this version, and 45CE20170427, which was included in GLODAPv2.2019, is shown in Fig. 3. For alkalinity the offset is determined as the difference, in accordance with the procedures followed for GLODAPv2. The mean weighted offset shows there is no difference between these cruises.

For each of the 23 new cruises, such a crossover comparison was conducted against all possible cruises in GLODAPv2.2021, i.e., all cruises that had stations closer than 2 arcdeg distance to any station for the cruise in question. The summary figure for alkalinity on 35TH20180611 is shown in Fig. 4. The alkalinity data measured on this cruise are on average 1.82 ± 0.40 µmol kg^{-1} higher when compared to the data measured on nearby cruises included in GLODAPv2.2022. This is smaller than the initial minimum adjustment limit for alkalinity of 4 µmol kg^{-1} (Table 3) and as such does not lead to an adjustment of the data in the merged data product. Detailed analyses are performed for every new cruise, and every core variable, to detect potential temporal trends in the offsets. Figure 4 further illustrates that the alkalinity offset is nearly zero also when comparing only with cruises since 2010 and no thus trend is apparent. All other variables also show very high consistency; thus, no adjustment is given to any other variable on cruise 35TH20180611 in GLODAPv2.2022. This is supported by the CANYON-B and CONTENT results (Sect. 3.2.4). Note that adjustments, when applied, are typically

round numbers (e.g., -3 not -3.4 for TCO$_2$ and 0.005 not 0.0047 for pH) to avoid communicating that the ideal adjustments are accurately known.

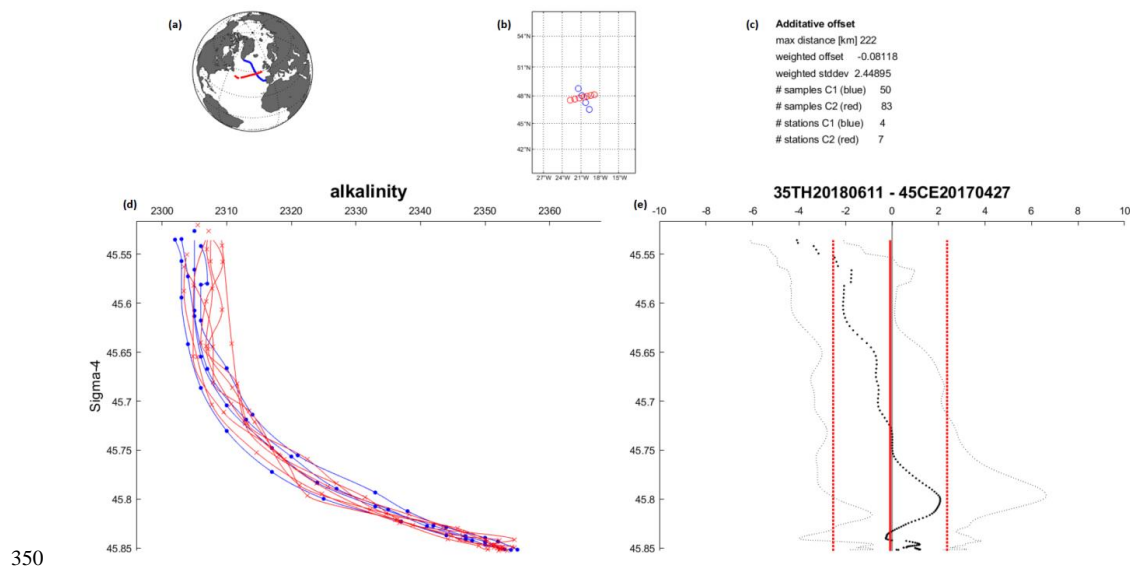



Figure 3. Example crossover figure for alkalinity for cruises 35TH20180611 (blue) and 45CE20170427 (red), as was generated during the crossover analysis. Panel (**a**) shows all station positions for the two cruises, and (**b**) shows the specific stations used for the crossover analysis. Panel (**d**) shows the data of alkalinity (μmol kg^{-1}) below the upper depth limit (in this case 2000 dbar) versus potential density anomaly referenced to 4000 dbar as points and the interpolated profiles as lines. Non-interpolated data either did not meet minimum depth separation requirements (Table 4 in Key et al., 2010) or are the deepest sampling depth. The interpolation does not extrapolate. Panel (**e**) shows the mean alkalinity difference profile (black, dots) with its standard deviation, as well as also the weighted mean offset (straight red lines) and weighted standard deviation. Summary statistics are provided in (**c**).

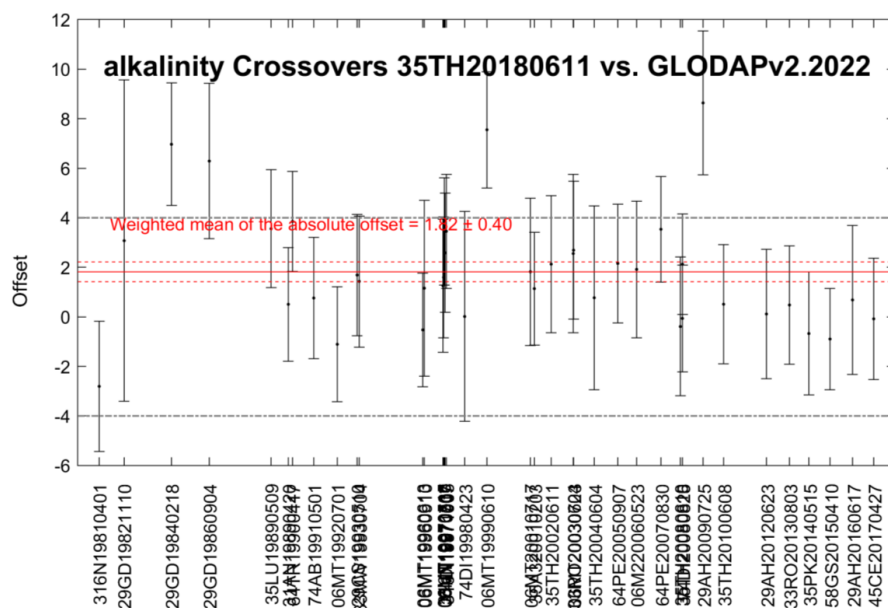



Figure 4. Example summary figure for alkalinity crossovers for 35TH20180611 versus the cruises in GLODAPv2.2022 (with cruise EXPOCODE listed on the x axis sorted according to the year the cruise was conducted). The black dots and vertical error bars show the weighted mean offset and standard deviation for each crossover (as a ratio). The weighted mean and standard deviation of all these offsets are shown in the red lines and are 1.82 ± 0.40. The dashed black lines are the reference line for a ± 4 μmol kg^{-1} offset.

3.2.3 pH scale conversion and quality control

Altogether 12 of the 23 new cruises included measured, spectrophotometric pH data, and none required an adjustment (Sect. 4). All cruises reported pH data on the total scale and at 25 °C. For the one cruise reporting pH on the seawater scale the data were converted following established routines (Olsen et al., 2020). For details on scale and temperature conversions in previous versions of GLODAPv2, we refer to Olsen et al. (2020). In contrast to quality control of pH data in GLODAPv2 (Olsen et al., 2016), the evaluation of the internal consistency of CO_2 system variables has not been used for the secondary quality control of the pH data in the GLODAPv2 updates of 2020 and onwards. For the 12 new cruises with pH in GLODAPv2.2023 only crossover analysis was used, supplemented by CONTENT and CANYON-B comparisons (Sect. 3.2.4). Recent literature has demonstrated that internal consistency evaluation procedures are subject to errors owing to an incomplete understanding of the thermodynamic constants, major ion contents, measurement biases, and potential contribution of organic compounds or other unknown protolytes to alkalinity. These complications lead to pH-dependent offsets in calculated pH compared with cruise spectrophotometric pH measurements (Álvarez et al., 2020; Carter et al., 2018; Fong and Dickson, 2019, Takeshita et al., 2020). The pH-dependent offsets may be interpreted as biases and generate false corrections (Álvarez et al., 2020; García-Ibáñez et al., 2022). The offsets are particularly strong at pH levels below 7.7, where calculated and measured pH values are different by on average between 0.01 and 0.02. For the North Pacific this is a problem as pH values below 7.7 can occur at the depths used during the QC (>1500 dbar for this region; Olsen et al., 2016). Since any correction, which may be an artifact, would be applied to the full profiles, we use a minimum adjustment of 0.02 for the North Pacific pH data in the merged product files. Elsewhere, the inconsistencies that may have arisen are smaller, since deep pH is typically higher than 7.7 (Lauvset et al., 2020), and at such levels the difference between calculated and measured pH is less than 0.01 on average (Álvarez et al., 2020; Carter et al., 2018). Outside the North Pacific, we believe, that the pH data are consistent to within 0.01. Avoiding CO_2 chemistry internal consistency considerations for these intermediate products helps to reduce the problem, but since the reference dataset (as also used for the generation of the CANYON-B and CONTENT algorithms) may have these issues, a future full re-evaluation, envisioned for GLODAPv3, is needed to address the problem completely.

3.2.4 CANYON-B and CONTENT analyses

CANYON-B and CONTENT (Bittig et al., 2018) were used to support decisions regarding the application of adjustments (or not). CANYON-B is a neural network for estimating nutrients and seawater CO_2 chemistry variables from temperature, salinity, and oxygen content. CONTENT additionally considers the consistency among the estimated CO_2 chemistry variables to further refine them. These approaches were developed using the data included in the GLODAPv2 data product (i.e., the 2016 version without any more recent updates). 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 nonlinear relationships in the underlying neural network. For example, if elevated nutrient values measured on a cruise are not due to a measurement bias, but actual aging of the water masses that have been sampled and as such accompanied by a decrease in oxygen content, the measured values and the CANYON-B estimates are likely to 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 which form the basis of our analyses. Specifically, we gave no weight to comparisons in which the crossover analyses had suggested that the salinity and/or O_2 data were biased as this would lead to error in the predicted values. We also considered the uncertainties of the CANYON-B and CONTENT estimates. These uncertainties are determined for each predicted value, and for each comparison the ratio of the difference (between measured and predicted values) to the local uncertainty was used to gauge the comparability. As an example, the CANYON-B and CONTENT analyses of the data obtained for 35TH20180611 are presented in Fig. 5. The CANYON-B and CONTENT results confirmed the crossover comparisons for alkalinity discussed in Sect. 3.2.2 showing an inconsistency of only 1.3-1.4. 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).

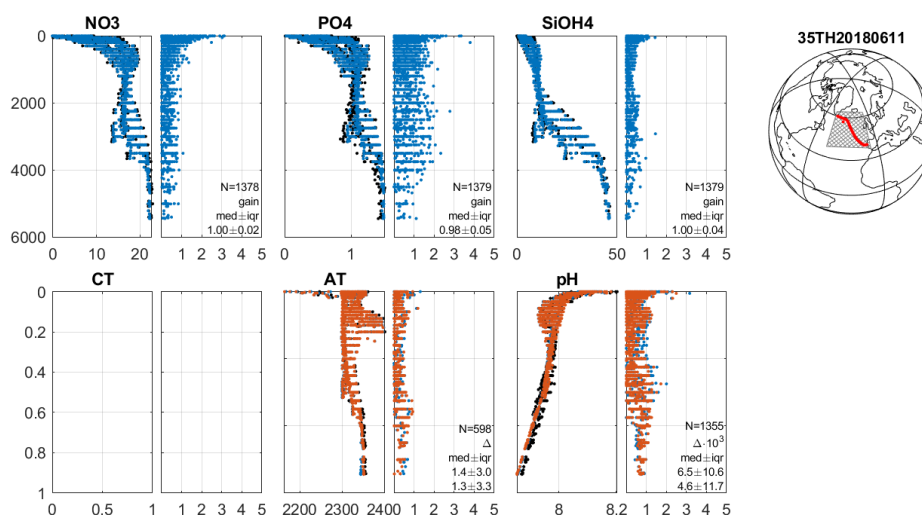



Figure 5. Example summary figure for CANYON-B and CONTENT analyses for 35TH20180611. Any data from regions where CONTENT and CANYON-B were not trained are excluded. The top row shows the nutrients and the bottom row the seawater CO_2 chemistry variables. All are shown versus sampling pressure (dbar), and the unit is micromoles per kilogram (μmol kg^{-1}) for all except pH, which is on the total scale at in situ temperature and pressure. 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 and CONTENT uncertainty estimate, which is determined for each estimated value. These values are used to gauge the comparability; a value below 1 indicates a good match, as it means that the difference between measured and estimated values is less than the uncertainty of the latter. The statistics in each panel are for all data deeper than 500 dbar, and N is the number of samples considered. A multiplicative adjustment and its interquartile range are given for the nutrients. For the seawater CO_2 chemistry variables the numbers in 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.

Another advantage of the CANYON-B and CONTENT comparisons 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 temperature, salinity, and O_2 data are available. Cases of strong differences between measured and estimated values are always examined. This has helped us to identify primary QC issues for some cruises and variables, for example a case of an inverted pH profile on cruise 32PO20130829, which was identified and amended in GLODAPv2.2020.

3.2.5 Halogenated transient tracers and SF$_6$

For the halogenated transient tracers (CFC-11, CFC-12, CFC-113, and CCl$_4$; CFCs for short) an inspection of surface saturation levels and an evaluation of relationships between the tracers for each cruise were used to identify biases, rather

than crossover analyses. Crossover analysis is of limited value for these variables given their transient nature and low contents at depth. As for GLODAPv2, the procedures were the same as those applied for CARINA (Jeansson et al., 2010;
430   Steinfeldt et al., 2010).

Beginning with GLODAPv2.2022, we have performed secondary quality control for SF_6 data, as this tracer is increasingly being measured and has proven a valuable addition to CFCs. The procedure is mainly based on comparisons with the quality-controlled CFC-12 data, which are available for all cruises with SF_6 measurements. We compare the surface saturation of SF_6 with that of CFC-12 and also consider the correlation between SF_6 and CFC-12 in the ocean interior.
435   Typically, this relation shows some scatter and does not follow a distinct curve (Fig. 6). However, for a given CFC-12 value the SF_6 content should fall into a certain range, and this range can be estimated by the transit time distribution (TTD; Hall et al., 2002) method. Note that we are not trying to adjust SF_6 to perfectly correlate with CFC-12 as that would severely decrease the value of SF_6 as an independent constraint on ocean circulation. We merely confirm that the SF_6 content is within an allowable range and only apply adjustments if all lines of evidence suggest it is warranted. In GLODAPv2.2023,
440   as in GLODAPv2.2022, no adjustment smaller than 10 % has been applied.

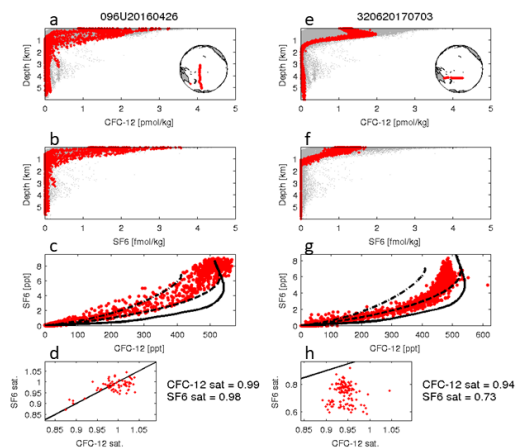



Figure 6. Example of plots used as basis for the SF_6 QC procedure. Shown are results for cruises 096U20160426 (left) and 320620170703 (right). a, e) CFC-12 versus pressure for the specific cruise (red), together with all data from the corresponding GLODAP region (Pacific in this case, grey). b, f) Same as upper row but for SF_6. c, g) CFC-12 versus SF_6 (red dots), here the measured contents have been
445   converted into atmospheric mixing ratios. Solid black line: atmospheric time history of CFC-12 versus that of SF_6. Dotted lines: CFC-12 versus SF_6 derived from the TTD method for two different sets of TTD parameters. d, h) CFC-12 vs. SF_6 saturation for the surface layer (P<20 dbar), where the numbers give the mean saturation.

As TTD, we use an inverse Gaussian function, which can be described by two parameters: the mean age (Γ) and the width
450   (Δ) (Hall et al., 2002). Typically, the ratios of Δ/Γ are chosen as a fixed parameter, and Γ is varied. Here, we use a range of Γ between 0 and 2000 years and two values for Δ/Γ: 0.5 and 2. This range of TTD parameters reproduces simultaneous observation of different tracers, like CFC-12 and SF_6, when calculating the tracer contents from the TTD and the atmospheric mixing ratio (Steinfeldt et al., 2009). Typically, for the same CFC-12 value derived from the TTD, the corresponding SF_6 value increases with the Δ/Γ ratio of the TTD, and it also increases with decreasing saturation (α). As
455   range for the expected SF_6 to CFC-12 relation we use the TTD with $\Delta/\Gamma = 0.5$ and $\alpha = 1$ as the lower boundary and the TTD with $\Delta/\Gamma = 0.5$ and 80 % saturation as the upper boundary. In some cases, like deep water formation or an ice-covered region, the tracer saturation might be lower, as the minimum of 65 % from Steinfeldt et al. (2009) indicates, but the majority of the data is actually located between our assumed lower and upper boundaries (see results for cruise 096U20160426 in

Fig. 6). A few exceptions are found for cruises in the Southern Ocean, as has already been shown in Stöven et al. (2015).
460   Note that in 1996, a SF_6 release experiment was performed in the Greenland Sea (Watson et al., 1999). This leads to a large
excess of SF_6 compared to CFC-12 in the Nordic Seas, which is clearly visible in our analyses and hampers the quality
control of the SF_6 data in this region.

3.3 Merged product generation

The merged product file for GLODAPv2.2023 was created by updating cruises and correcting known issues in the
465   GLODAPv2.2022 merged file and then appending a merged and bias-corrected file containing the 23 new cruises—sorted
according to EXPOCODE, station, and pressure—to this updated GLODAPv2.2022 file. GLODAP cruise numbers were
assigned consecutively, starting from 5001, so they can be distinguished from the GLODAPv2.2022 cruises, which ended
at 4096. The merging was otherwise performed following the procedures used for previous GLODAP versions (Olsen et
al., 2019; Olsen et al., 2020; Lauvset et al., 2021).

470   **3.3.1 Updates and corrections for GLODAPv2.2022**

For GLODAPv2.2023 we made some minor updates to cruises included in GLODAPv2.2022 (and earlier versions).
Table A2 in the Appendix shows a list of the cruises that have been updated, as well as what the update consists of. In
addition a small amount of duplicate data points were removed, and we fixed some rounding errors which resulted in the
combination of station, cast, and bottle numbers not being unique for several cruises.

475   **4 Secondary quality control results and adjustments**

The secondary QC has five possible outcomes which 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 text below. Some
cruises were not applicable for full secondary QC. Specifically, in some cases data were too shallow or geographically too
isolated for full and conclusive consistency analyses. In other cases, the results of these analyses were inconclusive, but we
480   have no reason to believe that the data in question are of poor quality. 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 on individual measurements. For example, interpolated (salinity, oxygen,
485   nutrients) or calculated (TCO_2, TAlk, pH) values, which have a primary QC flag of 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).

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, are consistent with the rest of the dataset and should not be adjusted.	0/1[a]
The data are of good quality but are biased: adjust by adding (for salinity, TCO_2, TAlk, pH) or by multiplying (for oxygen, nutrients, CFCs) the adjustment value	Adjustment value
The data have not been 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

490   [a]The value of 0 is used for variables with additive adjustments (salinity, TCO$_2$, TAlk, pH) and 1 for variables with multiplicative adjustments (for oxygen, nutrients, CFCs). This is mathematically equivalent to 'no adjustment' in both cases

Table 6. Summary of secondary QC results for the 23 new cruises, in number of cruises per result and per variable.

	Sal.	Oxy.	NO$_3$	Si	PO$_4$	TCO$_2$	TAlk	pH	CFC-11	CFC-12	CFC-113	CCl$_4$	SF$_6$
With data	23	14	20	17	20	22	22	12	7	8	5	0	7
No data	0	9	3	6	3	1	1	11	16	15	18	96	16
Unadjusted[a]	12	10	8	6	10	12	12	8	7	7	5	0	6
Adjusted[b]	0	0	2	4	0	0	1	0	0	0	0	0	1
-888[c]	11	4	10	7	10	10	9	4	0	1	0	0	0
-666[d]	0	0	0	0	0	0	0	0	0	0	0	0	0
-777[e]	0	0	0	0	0	0	0	0	0	1	0	0	0

[a]The data are included in the data product file as is, with a secondary QC flag of 1.
495   [b]The adjusted data are included in the data product file with a secondary QC flag of 1.
[c]Data appear of good quality but have not been subjected to full secondary QC. They are included in data product with a secondary QC flag of 0.
[d]Data are of uncertain quality and suspended until full secondary QC has been carried out; they are excluded from the data product.
[e]Data are of poor quality and excluded from the data product.

500   The secondary QC actions for the 13 core variables and the distribution of adjustments applied on the 23 new cruises are summarized in Table 6 and Fig. 7, respectively. No salinity, oxygen, TCO$_2$, pH, or phosphate data were adjusted. Out of the 22 cruises with TAlk, data from only 1 was adjustedFor nitrate data from 2 out of 20 cruises were adjusted, and for silicate 4 out of 17 cruises were adjusted. For the CFCs, no cruises required adjustment. Of the 23 new cruises in GLODAPv2.2022 seven include SF$_6$, and one required an adjustment. Overall, the magnitudes of the various adjustments

505   applied are small, and the tendency observed during the production of the three previous updates remains, namely that the large majority of recent cruises are consistent with earlier releases of the GLODAP data product. However, the new crossover and inversion analysis of all pH data in the northwestern Pacific that was planned following the release of GLODAPv2.2020 has not yet been performed. Such an analysis is planned for the next full update of GLODAP, i.e., GLODAPv3. Therefore, the conclusion from GLODAPv2.2020 remains that some caution should be exercised if looking

510   at trends in ocean pH in the northwestern Pacific using GLODAPv2.2023 or earlier versions.

For the nutrients, adjustments were applied to maintain consistency with data included in GLODAPv2.2022 and earlier versions. An alternative goal for the adjustments would be maintaining consistency with data from cruises that employed reference materials (RMNS) 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

515   would require a re-evaluation of the entire dataset, this will not occur until the next full update of GLODAP. 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.

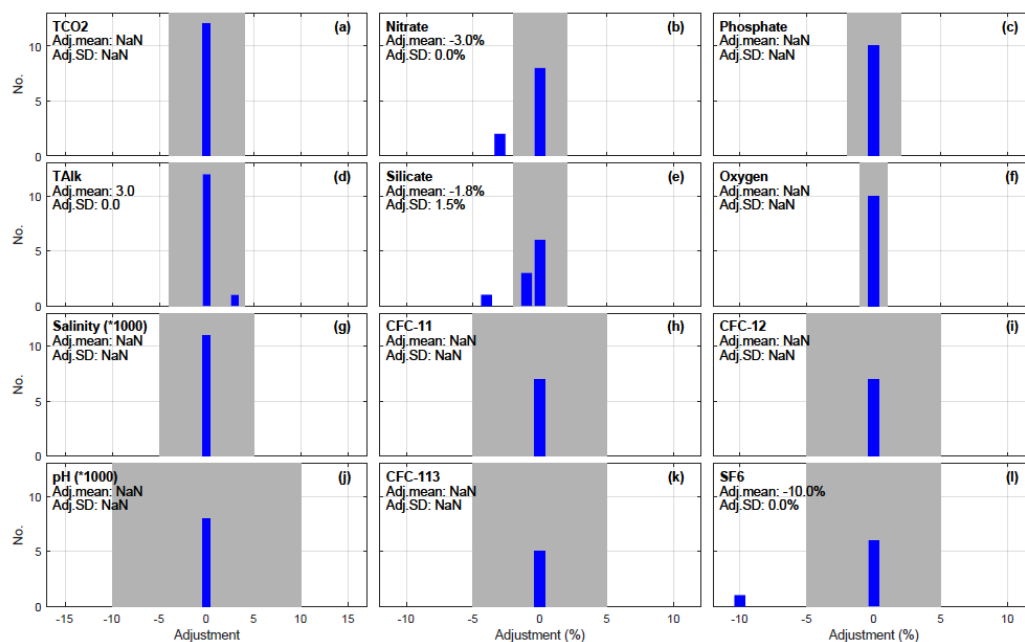



Figure 7. Distribution of applied adjustments for each core variable that received secondary QC, in micromoles per kilogram (μmol kg^{-1}) for TCO$_2$ and TAlk and unitless for salinity and pH (but multiplied by 1000 in both cases so a common x axis can be used), while for the other properties adjustments are given in percent ((adjustment ratio-1)x100). Grey areas depict the initial minimum adjustment limits. The figure includes numbers for data subjected to secondary quality control only. Note also that the y-axis scale is set to render the number of adjustments visible, so the bar showing zero offset (the 0 bar) for each variable is cut off (see Table 6 for these numbers).

The improvement in data consistency resulting from 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. 3.2.5). 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 can be substantial improvements when the adjustments are applied.

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 GLODAPv2.2022 (Fig. 8 in Lauvset et al., 2022). Most TCO$_2$ and TAlk data from the 1970s needed an adjustment, but this fraction steadily declines until only a small percentage is adjusted in recent years. This is encouraging and demonstrates the value of standardizing sampling and measurement practices (Dickson et al., 2007), the widespread use of CRMs (Dickson et al., 2003), and instrument automation. The pH adjustment frequency also has a downward trend; however, there remain issues with the pH adjustments, and this is a topic for future development in GLODAP, with the support from the Ocean Carbon & Biogeochemistry (OCB) Ocean Carbonate System Intercomparison Forum (OCSIF, https://www.us-ocb.org/ocean-carbonate-system-intercomparison-forum/, last accessed: 7 Sep 2023) 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., 2010),

availability of RMNS (Aoyama et al., 2012; Ota et al., 2010), and the Scientific Committee on Oceanic Research (SCOR) working group no. 147 – towards comparability of global oceanic nutrient data (COMPONUT; https://scor-int.org/group/147/, last accessed: 16 October 2023). 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.

Table 7. Improvements resulting from quality control of the 23 new cruises, per basin and for the global dataset. The values in the table are the weighted mean of the absolute offset of unadjusted and adjusted data versus GLODAPv2.2022. The total number of valid crossovers in the global ocean for the variable in question is n. The values in this table represent the inter-cruise consistency in the GLODAPv2.2023 product.

	ARCTIC			ATLANTIC			INDIAN			PACIFIC			GLOBAL			n (global)
	Unadj		Adj	Unadj		Adj	Unadj		Adj	Unadj		Adj	Unadj		Adj	
Sal (x1000)	2.7	=>	2.7	4.0	=>	4.0	NA	=>	NA	1.4	=>	1.4	2.0	=>	2.0	462
Oxy (%)	1.1	=>	1.1	0.8	=>	0.8	NA	=>	NA	0.5	=>	0.5	0.6	=>	0.6	393
NO_3 (%)	1.4	=>	1.4	1.5	=>	1.5	NA	=>	NA	1.4	=>	0.5	1.4	=>	0.8	207
Si (%)	8.1	=>	8.1	5.1	=>	5.1	NA	=>	NA	1.2	=>	0.6	1.5	=>	1.0	357
PO_4 (%)	3.7	=>	3.7	1.9	=>	1.9	NA	=>	NA	0.9	=>	0.9	1.0	=>	1.0	348
TCO_2 (µmol/kg)	2.8	=>	2.8	5.8	=>	5.8	NA	=>	NA	1.8	=>	1.8	2.8	=>	2.8	176
TAlk (µmol/kg)	4.7	=>	4.7	2.5	=>	2.5	NA	=>	NA	2.9	=>	2.0	2.9	=>	2.3	202
pH (x1000)	8.8	=>	8.8	9.7	=>	9.7	NA	=>	NA	6.5	=>	6.3	8.2	=>	8.2	142

NA: not available

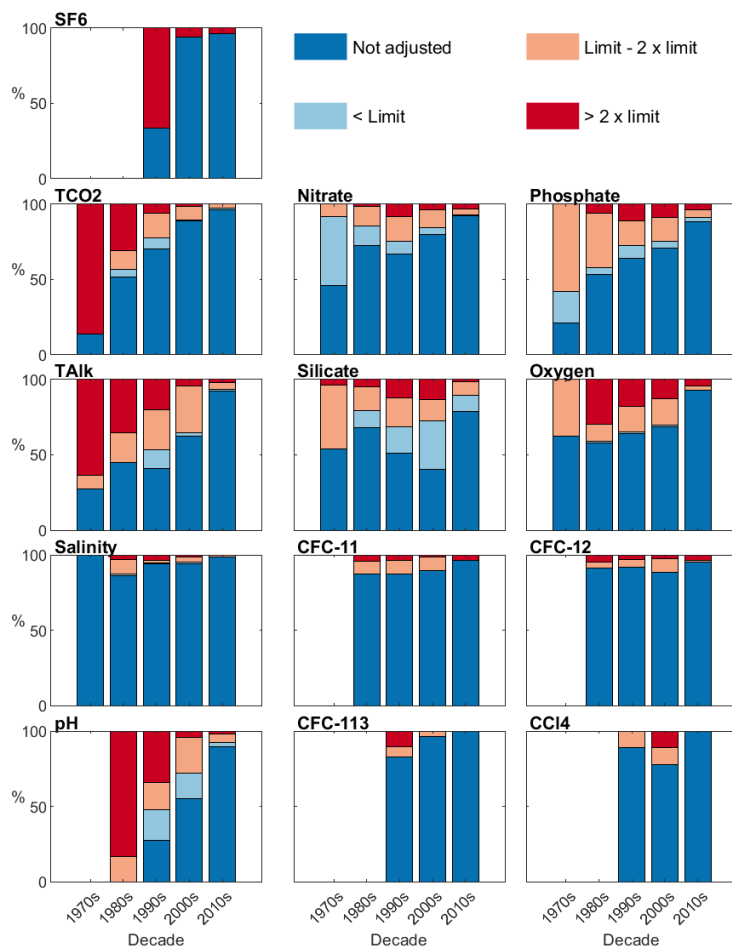



Figure 8. Magnitude of applied adjustments relative to minimum adjustment limits (Table 3) per decade for the 1108 cruises included in GLODAPv2.2023.

5 Data availability

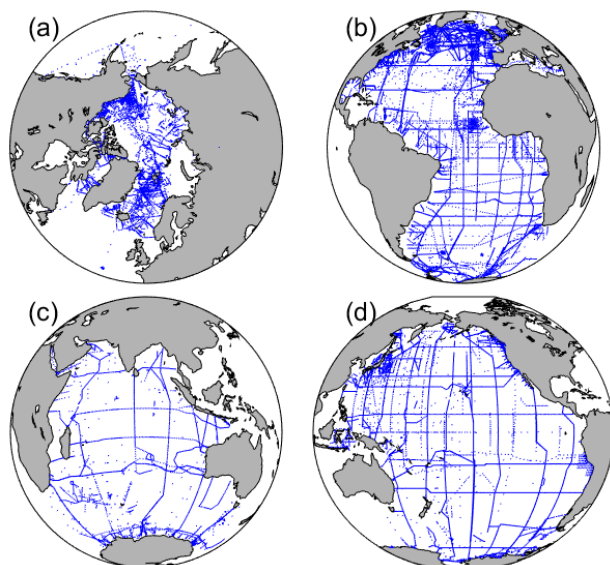
The GLODAPv2.2023 merged and adjusted data product is archived at the OCADS of NOAA NCEI (https://doi.org/10.25921/zyrq-ht66, Lauvset et al., 2023). These data and ancillary information are also available via our web pages and https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2023/ (last access: 12 October 2023). 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). The data product is also made available as an Ocean Data View (ODV) file which can be easily explored using the "webODV Explore" online data service (https://explore.webodv.awi.de/, last access: 27 October 2023). 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 variables are listed in Table 1. As well as being included in the .csv and .mat files, lookup tables for matching the EXPOCODE and DOI of a cruise with GLODAP cruise number are provided with the data files. A "known issues

document" accompanies the data files and provides an overview of known errors and omissions in the data product files. It
570   is regularly updated, and users are encouraged to inform us whenever any new issues are identified.

All material produced during the secondary QC is available via the online GLODAP adjustment table hosted by GEOMAR,
Kiel, Germany, at https://glodapv2-2023.geomar.de/ (last access: 15 August 2022) and can also be accessed through
www.glodap.info (last access: 7 Sep 2023). 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.

575   The original cruise files, with updated flags determined during additional primary GLODAP QC, are available through the
GLODAPv2.2023 cruise summary table (CST) hosted by OCADS: https://www.ncei.noaa.gov/access/ocean-carbon-
acidification-data-system/oceans/GLODAPv2_2023/cruise_table_v2023.html (last access: 12 October 2023). Each of
these files has been assigned a DOI, which is included in the data product files but not listed here. The CST also provides
brief information on each cruise and access to metadata, cruise reports, and its adjustment table entry.

580   While GLODAPv2.2023 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 both the cruise DOI and any articles where the data are described as well as, preferably,
contacting principal investigators to explore opportunities for collaboration and co-authorship. To this end, DOIs are
provided in the product files, as well as relevant articles and principal investigator names in the cruise summary table.

585   Contacting principal investigators comes with the additional benefit that the principal investigators often possess expert
insight into the data and/or specific 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.

590   **Figure 9.** Locations of stations included in the (a) Arctic, (b) Atlantic, (c) Indian, and (d) Pacific ocean product files for the complete
GLODAPv2.2023 dataset.

6 Summary

GLODAPv2.2023 is an update of GLODAPv2.2022. Data from 23 new cruises have been added to supplement the earlier release. GLODAP now includes 48 years, 1972–2021, of global interior ocean biogeochemical data from 1108 cruises. The total number of data records is 1 402 829 (Table 8). Records with measurements for all 13 core variables (salinity, oxygen, nitrate, silicate, phosphate, TCO_2, TAlk, pH, CFC-11, CFC-12, CFC-113, CCl_4 and SF_6) are very rare (174), and requiring only two out of the three core seawater CO_2 chemistry variables, in addition to all the other core variables, is still very rare with only 636 records (Table 8). A major limiting factor to having all core variables together is the simultaneous availability of data for all four transient tracer species and SF_6. In GLODAPv2.2023 there are 103 791 records with SF_6 data, and 433 932 records with at least one transient tracer or SF_6. A total of 2 % (28 777) of all data records do not have salinity. There are several reasons for this, the main one being the inability to vertically interpolate due to a separation that is too large between measured samples. Other reasons for missing salinity include salinity not being reported, and missing depth or pressure which leads to all other variables being set to -999, but not the removal of that line in the data product.

Table 8. Table listing the number of data points in GLODAPv2.2023, as well as the number of data with various combinations of variables.

Variables	Number of records
All core (salinity, oxygen, nitrate, silicate, phosphate, TCO_2, TAlk, pH, CFC-11, CFC-12, CFC-113, CCl_4, and SF_6)	174
All core except SF_6	2029
Salinity, oxygen, nitrate, silicate, phosphate, CFC-11, CFC-12, CFC-113, CCl_4, and SF_6 plus two of TCO_2, TAlk, and pH	636
salinity, oxygen, nitrate, silicate, phosphate, TCO_2, TAlk, pH	172 554
CFC-11, CFC-12, CFC-113, CCl_4, and SF_6	926
At least one transient tracer species or SF_6	433 932
SF_6	103 791
Two out of the three CO_2 chemistry core variables (TCO_2, TAlk, pH)	460 274
Measured fCO_2	35 387
Salinity, oxygen, nitrate, silicate, and phosphate	873 641
Salinity and oxygen	1 182 940
No salinity	28 777
Total in GLODAPv2.2023	1 402 829

As for previous versions there is a bias toward 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 (Fig. 10). These tendencies are strongest for the Arctic and Antarctic regions and reflect the harsh conditions during winter months which make fieldwork difficult. The upper 100 m is the best-sampled part of the global ocean, both in terms of number (Fig. 11a) and density (Fig. 11b) of observations. The number of observations steadily declines with depth. In part, this is caused by the reduction in ocean volume towards greater depths. Below 1000 m the density of observations stabilizes and even increases between 5000 and 6000 m; the latter is a zone where the volume of each depth surface decreases sharply (Weatherall et al., 2015). In the deep trenches, i.e., areas deeper than ~ 6000 m, both the number and density of observations are low.

Except for salinity and oxygen, the core data were collected exclusively through chemical analyses of collected water samples. The data of the 13 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.

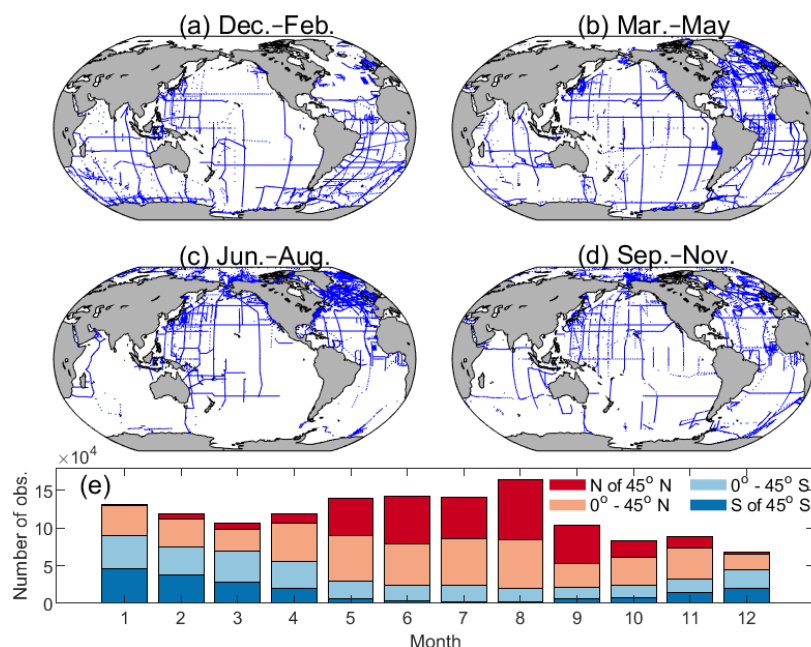



Figure 10. Distribution of data in GLODAPv2.2023 in (a) December–February, (b) March–May, (c) June–August, and (d) September–November, as well as (e) number of observations for each month in four latitude bands.

The consistency analyses were conducted by comparing the data from the 23 new cruises to the previous data product GLODAPv2.2022. 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://glodapv2-2023.geomar.de/ (last access: 15 August 2022) lists all applied adjustments and provides a brief justification for each. The consistency analyses rely on deep ocean data (>1500 or 2000 dbar depending on region), but supplementary CANYON-B and CONTENT analyses consider data below 500 dbar. Data consistency for cruises with exclusively shallow sampling was not examined. All new pH data for this version were comprehensively reviewed using crossover analysis, and only one required adjustment. Regardless, full reanalysis of all available pH data, particularly in the North Pacific, will be conducted for GLODAPv3.

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

The primary WOCE QC flags in the product files are simplified (e.g., all questionable and bad data were removed). For salinity, oxygen, and the nutrients, any data flagged 0 are interpolated rather than measured. For TCO_2, TAlk, pH, and fCO$_2$ any data flags of 0 indicate that the values were calculated from two other measured seawater CO_2 variables. Finally, while questionable (WOCE flag = 3) and bad (WOCE flag = 4) data have been excluded from the product files, some may have gone unnoticed through our analyses. Users of the data product are encouraged to report on any data that appear suspicious.

645 Based on the initial minimum adjustment limits and the improvement in the consistency resulting from the adjustments (Table 7), the data subjected to consistency analyses are believed to be consistent to better than 0.005 in salinity, 1 % in oxygen, 2 % in nitrate, 2 % in silicate, 2 % in phosphate, 4 μmol kg^{-1} in TCO$_2$, 4 μmol kg^{-1} in TAlk, and 5 % for the halogenated transient tracers and SF$_6$. For pH, the consistency among all data is estimated as 0.01–0.02, depending on the region. As mentioned above, the included fCO$_2$ data have not been subjected to quality control; therefore no consistency
650 estimate is given for this variable. This should be conducted in future efforts.

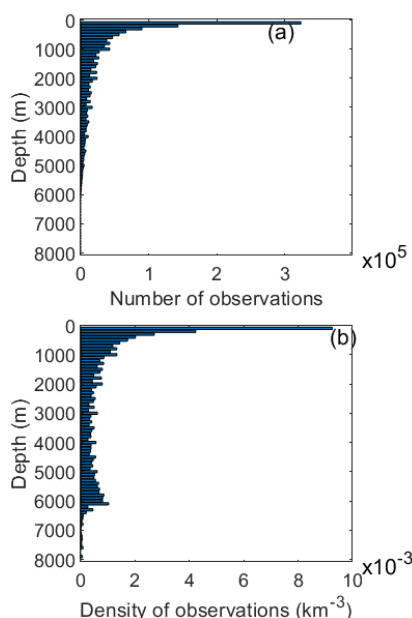



Figure 11. Number (a) and density (b) of observations in 100 m depth layers. The latter was calculated by dividing the number of observations in each layer by its global volume calculated from ETOPO2 (National Geophysical Data Center, 2006). For example, in the layer between 0 and 100 m there are on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

7 Author contributions.

SKL and TT led the team that produced this update. AK compiled the original data files and maintains the GLODAPv2 web pages at NCEI/OCADS. NL conducted the primary and secondary QC analyses. HCB conducted the CANYON-B and CONTENT analyses. CS manages the adjustment table e-infrastructure. TT, RS, and EJ performed the secondary QC on
660 all transient tracers. All authors contributed to the interpretation of the secondary QC results and made decisions on whether to apply adjustments. NL, SKL, HCB, JDM, and MPH made final checks of the data product. Many authors conducted ancillary QC analyses. SKL and NL updated the living data manuscript with contributions from all authors.

8 Competing interests

At least one of the (co-)authors is a member of the editorial board of *Earth System Science Data*. The authors have no other
665 competing interests to declare.

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945 **Appendix A.** Supplementary tables

Table A1. Cruises included in GLODAPv2.2023 that did not appear in GLODAPv2.2022. Complete information on each cruise, such as variables included, and chief scientist and principal investigator names is provided in the cruise summary table at https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2023/cruise_table_v2023.html (last access: 12 October 2023).

No	EXPOCODE	Region	Alias	Start	End	Ship
5001	18DD20150210	Atlantic Ocean	Line P	20150210	20150224	John P. Tully
5002	20HZ20151205	Pacific Ocean	LowpHOX 1_1	20151205	20151209	Cabo de Hornos
5003	20HZ20151227	Pacific Ocean	LowpHOX 1_2	20151127	20151128	Cabo de Hornos
5004	20HZ20180203	Pacific Ocean	LowpHOX 2	20180203	20180206	Cabo de Hornos
5005	325020210316	Atlantic Ocean	A20	20210316	20210416	Thomas G. Thompson
5006	325020210420	Atlantic Ocean	A22	20210420	20210516	Thomas G. Thompson
5007	35TH20180611	Atlantic Ocean	OVIDE 2018, GO_SHIP A25	20180611	20180714	Thalassa
5008	45CE20170206	Atlantic Ocean	CE17002	20170206	20170211	Celtic Explorer
5009	45CE20180210	Atlantic Ocean	CE18001	20180210	20180217	Celtic Explorer
5010	45CV20180128	Atlantic Ocean	CV18001	20180128	20180206	Celtic Voyager
5011	45CV20190109	Atlantic Ocean	CV19001	20190110	20190119	Celtic Voyager
5012	45CE20190524	Atlantic Ocean	CV19005	20190524	20190605	Celtic Explorer
5013	46BS20020215	Atlantic Ocean	IcelandSea; IrmingerSea	20020215	20060529	Arni Fridriksson, Bjarni
5014	49NZ20210713	Pacific Ocean	MR21-04, P01	20210713	20210826	Mirai
5015	49UP20210728	Pacific Ocean	GO-SHIP P03, RF21-06	20210728	20210728	Ryofu Maru III
5016	49UP20210827	Pacific Ocean	GO-SHIP P03, RF21-07	20210827	20210827	Ryofu Maru III
5017	49UP20210920	Pacific Ocean	GO-SHIP P03, RF21-08	20210920	20210920	Ryofu Maru III
5018	58JH20110113	Atlantic Ocean		20110113	20170605	Johan Hjort
5019	58JH20110121	Atlantic Ocean		20110121	20170402	Johan Hjort
5020	58HJ20140110	Arctic Ocean	79N	20140110	20140110	Helmer Hansen
5021	74EQ20191202	Pacific Ocean	DY111	20191202	20200109	Discovery
5022	76XL20080730	Arctic Ocean	CHINARE2008	20080730	20080911	Xuelong
5023	77DN20210725	Arctic Ocean	SAS-Oden2021	20210725	20210920	Oden

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Table A2. List of cruises included in GLODAPv2.2022 which have been updated as part of GLODAPv2.2023. Complete information on each cruise, such as variables included, and chief scientist and principal investigator names is provided in the cruise summary table at https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2023/cruise_table_v2023.html (last access: 12 October 2023).

No.	EXPOCODE	Region	Alias	Update	Adjustment
721	IcelandSea	Atlantic	LN6	Added new data from 2014 until 2019; Added CFC data for entire dataset	
720	IrmingerSea	Atlantic	FX9	Added new data from 2014 until 2019	
1040	33HQ20150809	Arctic	ARC01	Added delC13 and delC14 data	
34	06MT19921227	Atlantic	06MT22_5	Oxygen data	
1002	06AQ20120107	Atlantic	ANTXXVIII-3	SF6 data	-
1109	74EQ20151206	Atlantic	A05.2015	Remove DIC adjustment and recalculate pH and fCO_2	
3	06AQ19870704	Arctic	ARK IV/3	Downward adjustment silicate	0.96
695	74DI20040404	Atlantic	A05	Removed bad fCO2 data and TCO2 calculated from those	

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