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Open Access Earth System Science Data Discussions

GLODAPv2.2022: the latest version of 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. GLODAPv2.2022 is an update of the previous version, GLODAPv2.2021 (Lauvset et al., 2021). The major changes are as follows: data from 96 new cruises were added, data coverage was extended until 2021, and for the first time we performed secondary quality control on all sulphur hexafluoride (SF_6) data. In addition, a number of changes were made to data included in GLODAPv2.2021. These changes affect specifically the SF_6 data, which are now subjected to secondary quality control, and carbon data measured onboard the RV *Knorr* in the Indian Ocean in 1994-1995 which are now adjusted using CRM measurements made at the time. GLODAPv2.2022 includes measurements from almost 1.4 million water samples from the global oceans collected on 1085 cruises. The data for the now 13 GLODAP core variables (salinity, oxygen, nitrate, silicate, phosphate, dissolved inorganic carbon, total alkalinity, pH, 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 96 new cruises were derived by comparing those data with the data from the 989 quality controlled cruises in the GLODAPv2.2021 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 (https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2022/, last access: 15 August 2022). 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/10.25921/1f4w-0t92 (Lauvset et al., 2022). 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 GLODAPv2.2022 methods and provides a broad overview of the secondary quality control procedures and results.

1 Introduction

The oceans mitigate climate change by absorbing both atmospheric CO_2 corresponding to a significant fraction of anthropogenic CO_2 emissions (Friedlingstein et al., 2019; Gruber et al., 2019) and most of the excess heat in the Earth system caused by the enhanced greenhouse effect (Cheng et al., 2017; Cheng et al., 2020). The objective of GLODAP (Global Ocean Data Analysis Project, www.glodap.info, last access: 27 June 2022) 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,

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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 sulphur hexafluoride (SF_6).

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

Table 1. Variables in the GLODAPv2.2022 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)		

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Variable	Units	Product file name	WOCE flag name[a]	2nd QC flag name[b]	WHP-exchange name
Potential density anomaly, ref 2000 dbar	kg m^{-3}	sigma2	(salinityf)		
Potential density anomaly, ref 3000 dbar	kg m^{-3}	sigma3	(salinityf)		
Potential density anomaly, ref 4000 dbar	kg m^{-3}	sigma4	(salinityf)		
Neutral density anomaly	kg m^{-3}	gamma	(salinityf)		
Oxygen	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)		
$\delta^{13}C$	‰	c13	c13f	c13qc	DELC13
$\Delta^{14}C$	‰	c14	c14f		DELC14
$\Delta^{14}C$ counting error	‰	c14err			C14ERR
^{3}H	TU	h3	h3f		TRITIUM
^{3}H counting error	TU	h3err			TRITER
$\delta^{3}He$	%	he3	he3f		DELHE3
^{3}He counting error	%	he3err			DELHER
He	nmol kg^{-1}	he	hef		HELIUM
He counting error	nmol kg^{-1}	heerr			HELIER

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Variable	Units	Product file name	WOCE flag name[a]	2nd QC flag name[b]	WHP-exchange name
Ne	nmol kg^{-1}	neon	neonf		NEON
Ne counting error	nmol kg^{-1}	neonerr			NEONER
$\delta^{18}O$	‰	o18	o18f		DELO18
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) and 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). 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, 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 is 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

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Centers for Environmental Information (NCEI) (https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2022/cruise_table_v2022.html, last access: 15 August 2022).

This most recent GLODAPv2.2022 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, 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) where 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, and we anticipate that GLODAPv3 will become available a few years thereafter (pending funding). In the interim, the fourth intermediate update is presented here, which adds data from 96 cruises to the last update, GLODAPv2.2021 (Lauvset et al., 2021).

2 Key features of the update

GLODAPv2.2022 contains data from 1085 cruises covering the global ocean from 1972 to 2021, compared to 989 for the period 1972-2020 for the previous GLODAPv2.2021 (Lauvset et al., 2021). Information about the 96 cruises added to this version is provided in Table A1 in the Appendix. Cruise sampling locations are shown alongside those of GLODAPv2.2021 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

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variables. For example, cruises with only seawater CO_2 chemistry or transient tracer data are still included even without accompanying nutrient data due to their value towards computation of 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 2003 to 2021, with the majority being more recent than 2018. The largest data contribution come from the Coastal Ocean Data Analysis Product in North America (CODAP-NA, Jiang et al., 2021), which is a comprehensive compilation of carefully quality assessed coastal carbon data covering all continental shelves of North America, from Alaska to Mexico in the west and from Canada to the Caribbean in the east. Another large addition are the 29 new cruises from the RV *Keifu Maru II* and RV *Ryofu Maru III* in the western North Pacific (Oka et al., 2018; Oka et al., 2017). In the Arctic Ocean we update the timeseries from Weather Station M in the Norwegian Sea with an additional 10 years of data, and add five new Arctic cruises from RV *Healy*. In the Indian Ocean the 2019 repeat of GO-SHIP line I08N by the RV *Mirai* is included. In addition, we are for the first time including the cruises in the GEOTRACES intermediate data product where seawater CO_2 chemistry data are available (https://www.geotraces.org/geotraces-intermediate-data-product-2021/, last access: 23 June 2022). The GEOTRACES mission is "to identify processes and quantify fluxes that control the distributions of key trace elements and isotopes in the ocean, and to establish the sensitivity of these distributions to changing environmental conditions", but several cruises that measure trace elements and isotopes also measure CO_2 chemistry and these have now been included in GLODAPv2. All new data in GLODAPv2.2022 include seawater CO_2 chemistry, and additionally, 10 new cruises include halogenated transient tracers.

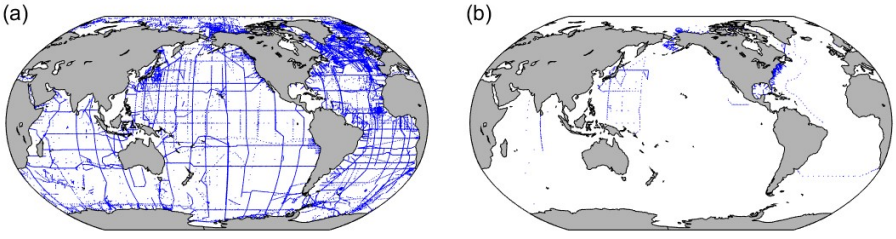

Figure 1. Location of stations in (a) GLODAPv2.2021 and for (b) the new data added in this update.

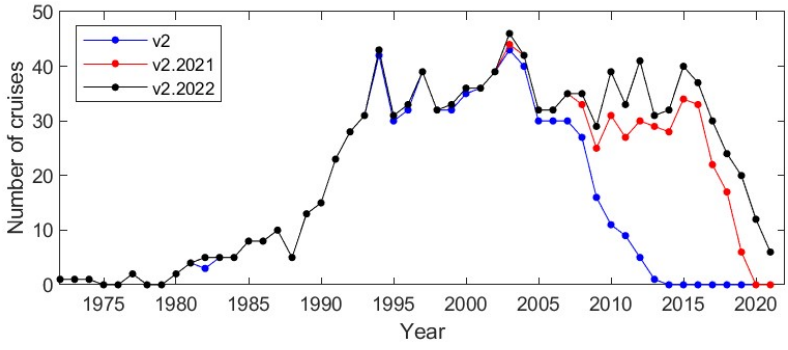

Figure 2. Number of cruises per year in GLODAPv2, GLODAPv2.2021, and GLODAPv2.2022.

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 GLODAPv2.2021 and previous versions, aiming to ensure the consistency of the data from

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the 96 new cruises with the previous release of the GLODAP data product (in this case, the GLODAPv2.2021 adjusted data product). For the first time we also apply secondary QC routines to SF_6 data, thus increasing the number of core variables from 12 to 13.

For GLODAPv2.2021 we added a basin identifier to the product files, where 1 is the Atlantic Ocean, 4 the Arctic 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). The basin identifiers are unchanged in GLODAPv2.2022 and added to the product files 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. Note that there is no overlap between the regional files nor for our basin identifiers, and cruises in the Southern Ocean are placed in the basin where most of the data were collected. As in GLODAPv2.2021 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

Data from the 96 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 : 9 August 2022), the CLIVAR and Carbon Hydrographic Data Office (https://cchdo.ucsd.edu, last access: 27 June 2022), and PANGAEA (https://pangaea.de, last access: 27 June 2022). Each cruise is identified by an expedition code (EXPOCODE). The EXPOCODE is guaranteed to be unique and constructed by combining the country code and platform code with the date of departure in the format YYYYMMDD. The country and platform codes were taken from the ICES (International Council for the Exploration of the Sea) library (https://vocab.ices.dk/, last access 27 June 2022).

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 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 in https://exchange-format.readthedocs.io/ (v1.2.0 as of 2022-03-22, last access: 16 June 2022); 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, and the identification of the group and person who prepared the file. The latter follows a convention of including the division/group, the institution, 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 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 in https://exchange-format.readthedocs.io/en/latest/parameters.html (v1.2.0 as of 2022-03-22, last access: 16 June 2022). For consistency with previous updates, and to ease the use of existing methods and code,

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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 GLODAPv2.2022 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 GLODAPv2.2022 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, 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 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. For this task, the GLODAP primary quality control software

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(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 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 96 new cruises relative to GLODAPv2.2021, 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 May 2022 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 used (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 GLODAPv2.2021. 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 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 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 changed for data previously included in GLODAPv2.2021.

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 GLODAPv2.2021 and GLODAPv2.2020, but in contrast to 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 two previous updates (2020 and 2021) 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). For previous versions we have also used multiple linear regression analyses and deep water averages, broadly following Jutterström et al. (2010), for

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additional information for the secondary QC of salinity, oxygen, nutrients, TCO_2, and TAlk data. 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.

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 pack. These two measurement types are merged and presented as a single variable in the product. The merging was conducted prior to the consistency checks, ensuring their internal calibration in the product. The merging procedures were only applied to the bottle data files, which commonly include values recorded by the CTD at the pressures where the water samples are collected. Whenever both CTD and bottle data were present in a data file, the merging step considered the deviation between the two and calibrated the CTD values if required and possible. Altogether seven scenarios (Table 4) are possible for each of the CTD conductivity and oxygen (O_2) sensor properties individually, in which the fourth never occurred during our analyses but are included to maintain consistency with GLODAPv2. For 39 % of the 96 new cruises both CTD and bottle data were included in the original cruise files for salinity and oxygen and for all these cruises the two data types were found to be consistent. These new data have a lower proportion of cruises with both bottle and CTD measurements than GLODAPv2.2021 (75 % and 63 % respectively for salinity and oxygen). For salinity the remaining 61 % have only CTD data, while for oxygen 30 % have only CTD data and 21 % 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 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) is mislabeled CTD data (i.e., should be CTDOXY) is uncertain. Regardless, all CTD and bottle data for salinity were consistent and did not need any further calibration, and only 3 out of the 96 cruises required calibration of the oxygen data.

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	7
2	No bottle values are available: use CTD values.	58	30
3	No CTD values are available: use bottle values.	0	19
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.	38	37
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

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3.2.2 Crossover analyses

The crossover analyses were conducted with the MATLAB toolbox prepared by Lauvset and Tanhua (2015) and with GLODAPv2.2021 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 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 silicate measured on the two cruises 49UF20190207, which is new to this version, and 49RY20110515, which was included in GLODAPv2, is shown in Fig. 3. For silicate the offset is determined as the ratio, in accordance with the procedures followed for GLODAPv2. The silicate values from 49UF20190207 are slightly higher, with a weighed mean offset of 1.02 ± 0.01 compared to those measured on 49RY20110515.

For each of the 96 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 silicate on 49UF20190207 is shown in Fig. 4. The silicate data measured on this cruise are 1.01 ± 0.00 higher when compared to the data measured on nearby cruises included in GLODAPv2.2021. This is smaller than the initial minimum adjustment limit for silicate of 2 % (Table 3) and as such does not automatically lead to an adjustment of the data in the merged data product. However, in this case the offset, while small, is very consistent and present in silicate data from many different cruises. Since we have also been able to identify a cause of the offset (see Sect. 4) an adjustment of 1 % has been applied. All other variables show very high consistency, thus, no adjustment is given to any other variable on cruise 49UF20190207 in GLODAPv2.2021. 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.

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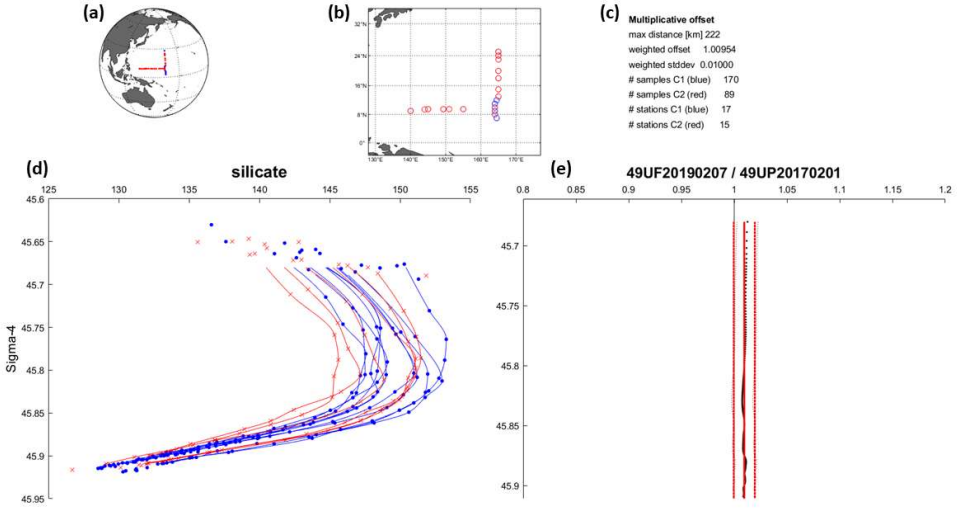

365 **Figure 3.** Example crossover figure, for silicate for cruises 49UF20190207 (blue) and 49RY20110515 (red), as was generated during the crossover analysis. Panel **(a)** shows all station positions for the two cruises and **(b)** shows the specific stations used for the crossover analysis. Panel **(d)** shows the data of silicate (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.
370 Panel **(e)** shows the mean silicate 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)**.

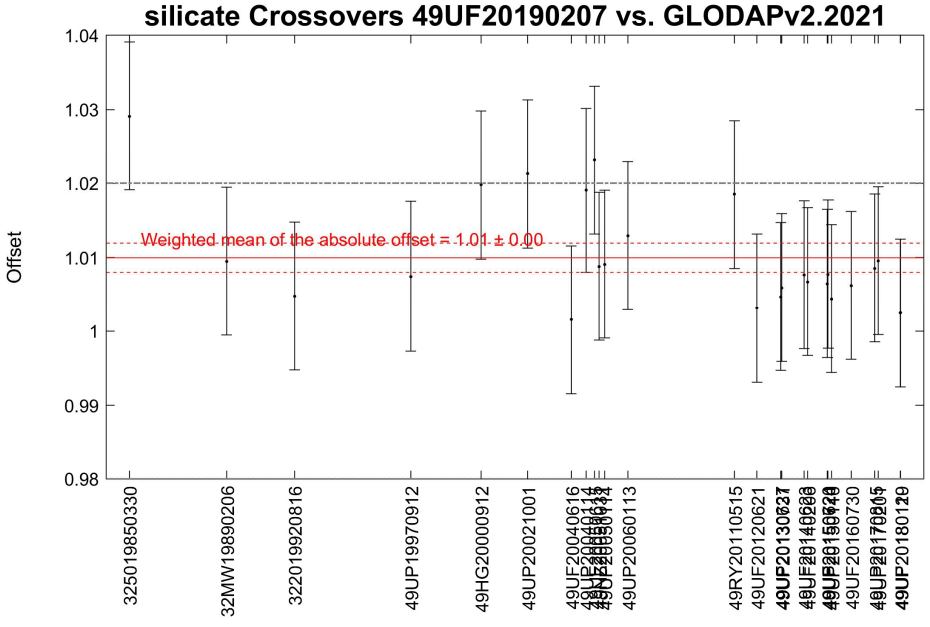

Figure 4. Example summary figure, for silicate crossovers for 49UF20190207 versus the cruises in GLODAPv2.2021 (with cruise EXPOCODE listed on the x axis sorted according to year the cruise was conducted). The black dots and vertical error bars show the
375 weighted mean offset and standard deviation for each crossover (as a ratio). The weighted mean and standard deviation of all these offsets are shown in the red lines and are 1.01 ± 0.00. The dashed black lines are the reference line for a ±2 % offset.

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3.2.3 pH scale conversion and quality control

Altogether 60 of the 96 new cruises included measured, spectrophotometric, pH data, and only one required an adjustment (Sect. 4). We also excluded (flag -777) pH on one cruise as a result of the QC work. All except one cruise 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), 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 60 new cruises with pH in GLODAPv2.2022 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 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 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 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

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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 49UF20190207 are presented in Fig. 5. The CANYON-B and CONTENT results confirmed the crossover comparisons for silicate discussed in Sect. 3.2.2 showing an inconsistency of 1.01. 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).

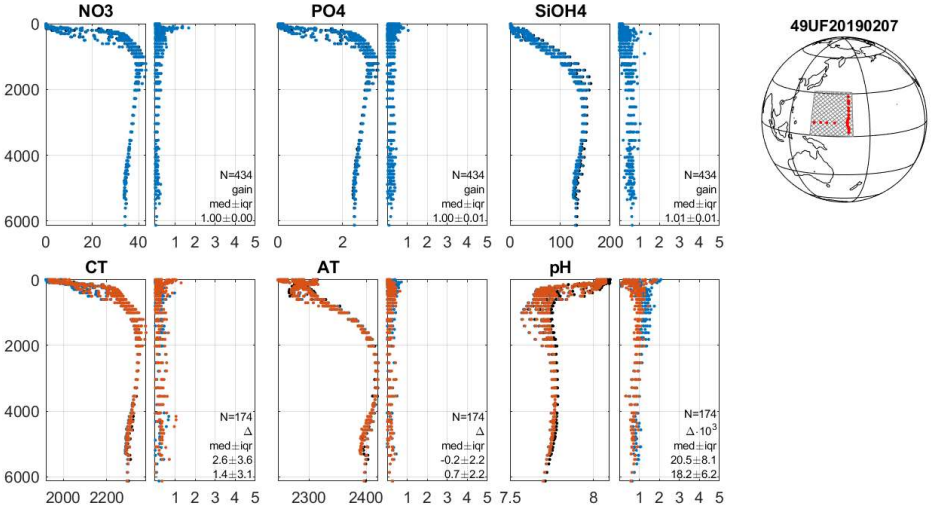

Figure 5. Example summary figure for CANYON-B and CONTENT analyses for 49UF20190207. Any data from regions where CONTENT and CANYON-B were not trained are excluded. The top row shows the nutrients and the bottom row the seawater CO_2 chemistry variables. All are shown versus sampling pressure (dbar) 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) inspection of surface saturation levels and evaluation of relationships between the tracers for each cruise were used to identify biases, rather than crossover analyses. Crossover analysis is of limited value for these variables given their transient nature and low contents

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445 at depth. As for GLODAPv2, the procedures were the same as those applied for CARINA (Jeansson et al., 2010; 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
450 SF_6 with that of CFC-12 and also consider the correlation between SF_6 and CFC-12 in the ocean interior. 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., 2022) 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
455 allowable range, and only apply adjustments if all lines of evidence suggest it is warranted. In GLODAPv2.2022 no adjustment smaller than 10 % has been applied.

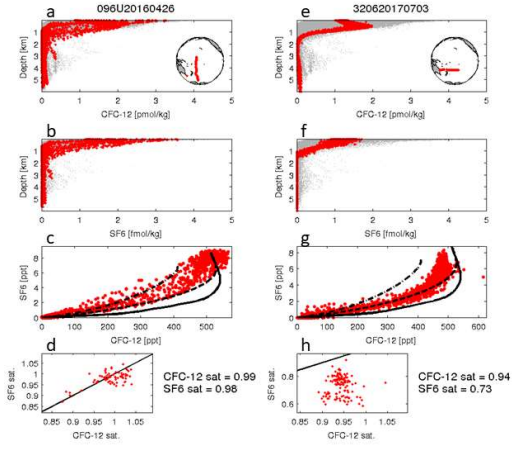

Figure 6. Example of plots used as basis for the SF_6 QC procedure. Shown are results for cruises 096U20160426 (left) and 320620170703 (right). a, e) CFC-12 versus pressure for the specific cruise (red), together with all data from the corresponding GLODAP region (Pacific
460 in this case, grey). b, f) Same as upper row, but for SF_6. c, g) CFC-12 versus SF_6 (red dots), here the measured contents have been converted into atmospheric mixing ratios. Solid black line: atmospheric time history of CFC-12 vs. that of SF_6. Dotted lines: CFC-12 vs. 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.

465 As TTD, we use an inverse Gaussian function, which can be described by two parameters, the mean age (Γ) and the width (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
470 corresponding SF_6 value increases with the Δ/Γ ratio of the TTD and it also increases with decreasing saturation (α). As range for the expected SF_6 to CFC-12 relation we use the TTD with Δ/Γ = 0.5 and α = 1 as lower boundary and the TTD with Δ/Γ = 0.5 and 80 % saturation as 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 boundary (see results for cruise 096U20160426 in Fig. 6). A
475 few exceptions are found for cruises in the Southern Ocean, as has already been shown in Stöven et al. (2015). Note that in

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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 GLODAPv2.2022 was created by updating cruises, and correcting known issues, in the GLODAPv2.2021 merged file, and then appending a merged and bias-corrected file containing the 96 new cruises—sorted according to EXPOCODE, station, and pressure—to this updated GLODAPv2.2021 file. GLODAP cruise numbers were assigned consecutively, starting from 4001, so they can be distinguished from the GLODAPv2.2021 cruises, which ended at 3043. 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).

3.3.1 Updates and corrections for GLODAPv2.2021

For GLODAPv2.2022 we made several updates to cruises included in GLODAPv2.2021 (and earlier versions). The major updates were (i) to perform secondary quality control on all SF_6 data (see Sect. 3.2.5), and (ii) to apply small adjustments to TCO_2 and TAlk data measured onboard the RV *Knorr* in 1994-1995 (EXPOCODES 316N199*, Table A2). These adjustments are derived from offsets in the CRM measurements which were previously reported, but never applied to the seawater measurements (pers. comm. C. Sabine and D. Wallace; Johnson et al., 2002). These offsets are lower than the minimum adjustment limits defined for GLODAP. Applying these adjustments achieves procedural consistency with other CO_2 chemistry data that are usually corrected for CRM offsets before being subjected to secondary QC.

For TAlk the original CRM offsets were derived from Table 2 in Millero et al. (1998), who reported repeated CRM measurements on different titration cells for each cruise. The mean measured CRM value across all cells was calculated and compared to the published reference value for the same batch, and, if necessary, the offsets obtained from multiple CRM batches measured on one cruise were averaged. For TCO_2 the original CRM offsets were calculated from Table 3 in Johnson et al. (1998), who reported offsets for two measurement systems, which were here averaged. Johnson et al. (2002) report that their TCO_2 measurements were affected by changes in pipette volumes, which they were able to correct for in the CRM measurements. However, these volume corrections were most likely not applied to the seawater measurements (pers. comm. D. Wallace; Johnson et al., 2002) and we therefore use the CRM offsets reported before correcting for the changes in pipette volume. For both TAlk and TCO_2 we calculate and use the mean CRM offset across all Indian Ocean cruises on the RV *Knorr* from 1994-1995 (-3.5 µmol kg^{-1} for TAlk and 1.7 µmol kg^{-1} for TCO_2) as a bulk adjustment value for the seawater measurements on these cruises. The GLODAP policy for avoiding small adjustments does not apply in this instance because there is a documented reason for the adjustment beyond improving internal consistency of the GLODAPv2 data product. Encouragingly, we also note that applying these adjustments improves the consistency with more recent (post-2000) Indian ocean data in GLODAPv2: For TAlk the mean absolute offset decreased from 2.8 µmol kg^{-1} for the unadjusted data to -0.7 µmol kg^{-1} for the adjusted data, while for TCO_2 the mean absolute offset decreased from -2.3 µmol kg^{-1} for the unadjusted data to -0.6 µmol kg^{-1} for the adjusted data respectively.

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, several minor omissions and errors have been identified and corrected:

- Corrected an error in the QC flagging of calculated CO_2 chemistry variables when fCO_2 was used as one of the inputs (changed from 1 to 0).

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- CFC-12 data were added to cruise 06M320150501
- Missing bottle number were added to cruises 29AH20160617 and 29HE20190406
- For cruise 316N19831007 the WOCE flag on TAlk was changed from 2 to 0
- Oxygen concentrations of 49UP19970912 have been adjusted 1.5% upward
- pH values of 49HG19960807 have been adjusted downward by 0.05
- The timeseries from Weather Station M in the Norwegian Sea was updated with data from 2008-2021
- In addition to DOIs for all original data files, DOIs for the included data products (CODAP-NA and GEOTRACES) have been added to the product files.
- An extra column "G2expocode" has been added, listing the EXPOCODE for each entry

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 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, 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). Prominent examples for this version are the CODAP-NA data (Jiang et al., 2021), which as a primarily coastal data set typically has quite shallow sampling depths that rendered conclusive secondary QC impossible. As a consequence, most, but not all, of these data are included with a secondary QC flag of 0.

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

[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

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Table 6. Summary of secondary QC results for the 96 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	96	90	91	92	93	93	94	60	5	6	1	0	2
No data	0	6	5	4	3	3	2	36	91	90	95	96	94
Unadjusted[a]	35	33	33	5	33	35	34	28	3	4	1	0	2
Adjusted[b]	0	2	0	29	1	0	1	1	1	1	0	0	0
-888[c]	61	55	58	58	58	58	59	30	1	1	0	0	0
-666[d]	0	0	0	0	1	0	0	0	0	0	0	0	0
-777[e]	0	0	0	0	0	0	0	1	0	0	0	0	0

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

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

[c]Data appear of good quality but have not been subjected to full secondary QC. They are included in data product with a secondary QC flag of 0.

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

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

The secondary QC actions for the 13 core variables and the distribution of adjustments applied on the 96 new cruises are summarized in Table 6 and Fig. 7, respectively. For most variables only a small fraction of the data were adjusted: no salinity, TCO_2 or nitrate data, 1.1 % TAlk data and phosphate data, 2.2 % of oxygen data, and 31 % of silicate data. The large percentage of silicate data requiring adjustment in this version is due to a consistent 1 % offset in the silicate data from the Japan Meteorological Agency (JMA) after 2018 (compared to older data from JMA). This offset has been traced to a change in the batch of Merck silicate standard solution used. In GLODAPv2.2022 this offset has been corrected by adjusting the new data (after 2018) to be consistent with the older data. For the CFCs, CFC-11 required adjustment for 1 out of the 5 new cruises, and CFC-12 required adjustment on 1 out of 6 new cruises. For the total of 82 cruises with SF_6 data in GLODAPv2.2022 two cruises (06MT20060712 and 325020080826) could not be subjected to secondary quality control (-888) and 5 cruises received an upward adjustment (see example for cruise 320620170703 in Fig. 6). The magnitude of the adjustment was calculated using the saturation of CFC-12 as a benchmark. Additionally, for two cruises (49K619990523 and 58GS20090528), the SF_6 values are out of the TTD derived range, as are the surface saturations. In these cases, the SF_6 data are discarded (QC flag -777). Of the 96 new cruises in GLODAPv2.2022 only 2 include SF_6 and neither required an adjustment. Overall, the magnitudes of the various adjustments 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. 60 out of the 96 new cruises included measured pH data, but only one received an adjustment (and one was flagged -777). 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 at trends in ocean pH in the northwestern Pacific using GLODAPv2.2022 or earlier versions.

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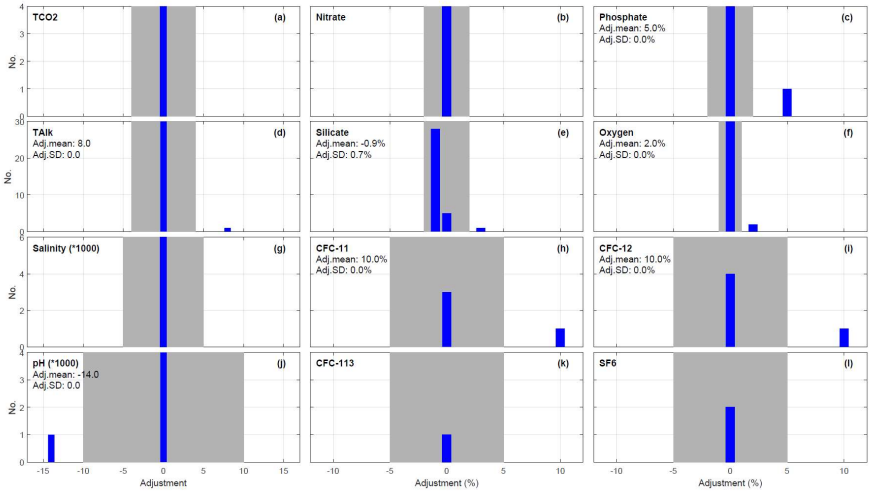

Figure 7. Distribution of applied adjustments for each core variable that received secondary QC, in micromoles per kilogram (µmol kg^{-1}) for TCO_2 and TAlk and unitless for salinity and pH (but multiplied by 1000 in both cases so a common x axis can be used), while for the other properties adjustments 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).

For the nutrients, adjustments were applied to maintain consistency with data included in GLODAPv2.2021 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 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.

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 are substantial improvements when the adjustments are applied. For example, oxygen, silicate and phosphate in the Atlantic Ocean all show a considerable improvement.

Table 7. Improvements resulting from quality control of the 96 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 GLODAPv2.2021. 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 GLODAPv2.2022 product.

	ARCTIC			ATLANTIC			INDIAN			PACIFIC			GLOBAL			
	Unadj		Adj	Unadj		Adj	Unadj		Adj	Unadj		Adj	Unadj		Adj	*n* (global)
Sal (x1000)	NA	=>	NA	4.6	=>	4.6	0.7	=>	0.7	1.2	=>	1.2	1.3	=>	1.3	1105

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Oxy (%)	NA	=>	NA	1.5	=>	0.8	0.5	=>	0.5	0.4	=>	0.4	0.5	=>	0.4	1064
NO_3 (%)	NA	=>	NA	1.7	=>	1.7	0.7	=>	0.7	0.4	=>	0.4	0.4	=>	0.4	940
Si (%)	NA	=>	NA	3.0	=>	2.6	0.9	=>	0.9	1.4	=>	0.6	1.4	=>	0.6	916
PO_4 (%)	NA	=>	NA	2.0	=>	1.1	0.7	=>	0.7	0.7	=>	0.7	0.7	=>	0.7	936
TCO_2 (µmol/kg)	NA	=>	NA	7.3	=>	7.3	2.0	=>	2.0	1.8	=>	1.8	2.4	=>	2.4	544
TAlk (µmol/kg)	NA	=>	NA	4.5	=>	3.1	5.2	=>	5.2	1.8	=>	1.8	1.9	=>	1.8	515
pH (x1000)	NA	=>	NA	11.6	=>	11.6	NA	=>	NA	5.5	=>	5.3	5.5	=>	5.4	462

NA: not available

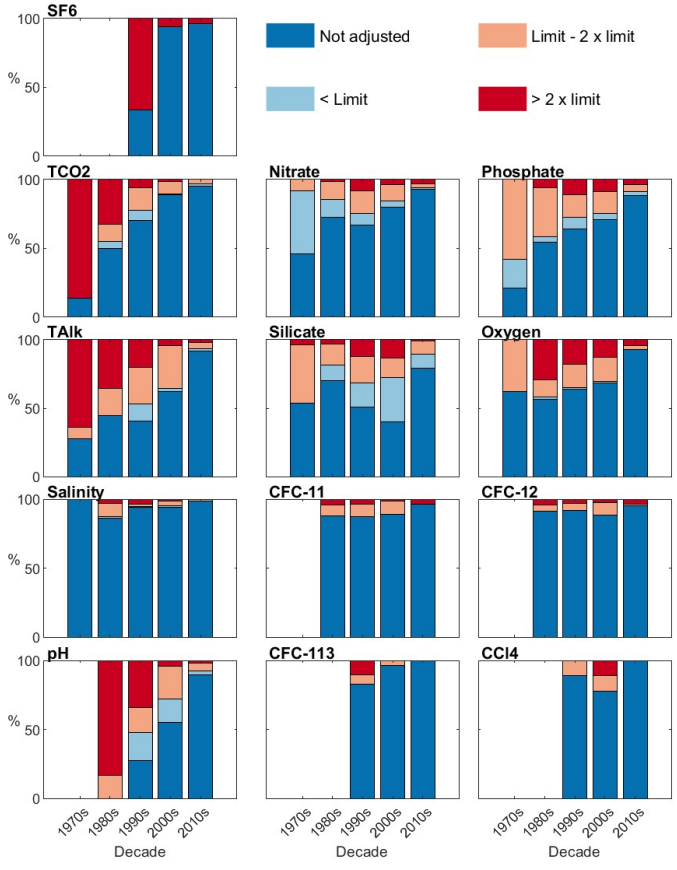

Figure 8. Magnitude of applied adjustments relative to minimum adjustment limits (Table 3) per decade for the 1085 cruises included in GLODAPv2.2022.

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

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to GLODAPv2.2021 (Fig. 7 in Lauvset et al., 2021). Most TCO_2 and TAlk data from the 1970s needed an adjustment, but this fraction steadily declines until only a small percentage is adjusted in recent years. This is encouraging and demonstrates the value of standardizing sampling and measurement practices (Dickson et al., 2007), the widespread use of CRMs (Dickson et al., 2003), and instrument automation. The pH adjustment frequency also has a downward trend; however, there remain issues with the pH adjustments and this is a topic for future development in GLODAP, with the support from the OCB Ocean Carbonate System Intercomparison Forum (OCSIF, https://www.us-ocb.org/ocean-carbonate-system-intercomparison-forum/, last accessed: 27 June 2022) 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 #147, towards comparability of global oceanic nutrient data (COMPONUT). For silicate, the fraction of cruises receiving adjustments peaks in the 1990s and 2000s. This is related to the 2 % offset between US and Japanese cruises in the Pacific Ocean that was revealed during production of GLODAPv2 and discussed in Olsen et al. (2016). For salinity and the halogenated transient tracers, the number of adjusted cruises is small in every decade.

5 Data availability

The GLODAPv2.2022 merged and adjusted data product is archived at the OCADS of NOAA NCEI (Lauvset et al., 2022). 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_2022/ (last access: 15 August 2022). 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: 15 August 2022). Regional subsets are available for the Arctic, Atlantic, Pacific, and Indian oceans. There are no data overlaps between regional subsets and each cruise exists in only one basin file even if data from that cruise crosses basin boundaries. The station locations in each basin file are shown in Fig. 9. The product file variables are listed in Table 1. 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 is 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 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.

All material produced during the secondary QC is available via the online GLODAP adjustment table hosted by GEOMAR, Kiel, Germany at https://glodapv2-2022.geomar.de/ (last access: 15 August 2022), and can also be accessed through www.glodap.info (last access: 27 June 2022). 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.

The original cruise files, with updated flags determined during additional primary GLODAP QC, are available through the GLODAPv2.2022 cruise summary table (CST) hosted by OCADS: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2022/cruise_table_v2022.html (last access: 15 August 2022). 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.

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While GLODAPv2.2022 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, and relevant articles and principal investigator names 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 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.

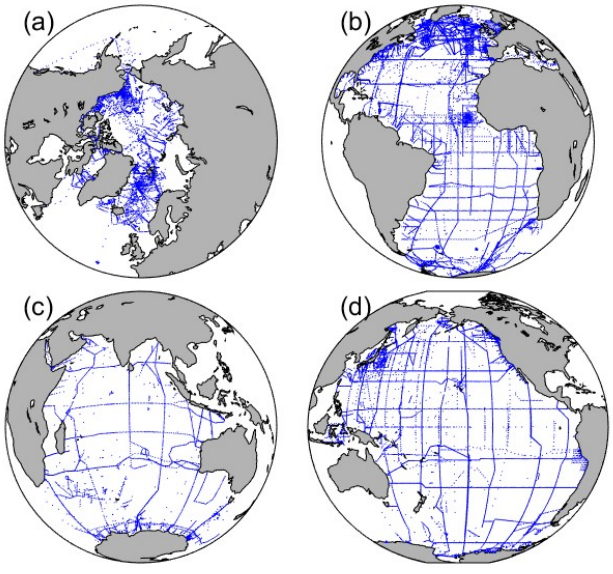

Figure 9. Locations of stations included in the (a) Arctic, (b) Atlantic, (c) Indian, and (d) Pacific ocean product files for the complete GLODAPv2.2022 dataset.

6 Summary

GLODAPv2.2022 is an update of GLODAPv2.2021. Data from 96 new cruises have been added to supplement the earlier release and extend temporal coverage by 1 year. GLODAP now includes 48 years, 1972–2021, of global interior ocean biogeochemical data from 1085 cruises. The total number of data records is 1 381 248 (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 is the simultaneous availability of data for all four transient tracer species and SF_6. In GLODAPv2.2022 there are 98 951 records with SF_6 data, and 427 913 records with at least one transient tracer or SF_6. A total of 2 % (27 906) 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.

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Table 8. Table listing the number of data points in GLODAPv2.2022, 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	168 330
CFC-11, CFC-12, CFC-113, CCl_4, and SF_6	926
At least one transient tracer species or SF_6	427 913
SF_6	98 951
Two out of the three CO_2 chemistry core variables (TCO_2, TAlk, pH)	448 024
Measured fCO_2	33 844
Salinity, oxygen, nitrate, silicate, and phosphate	861 650
Salinity and oxygen	1 165 389
No salinity	27 906
Total in GLODAPv2.2022	1 381 248

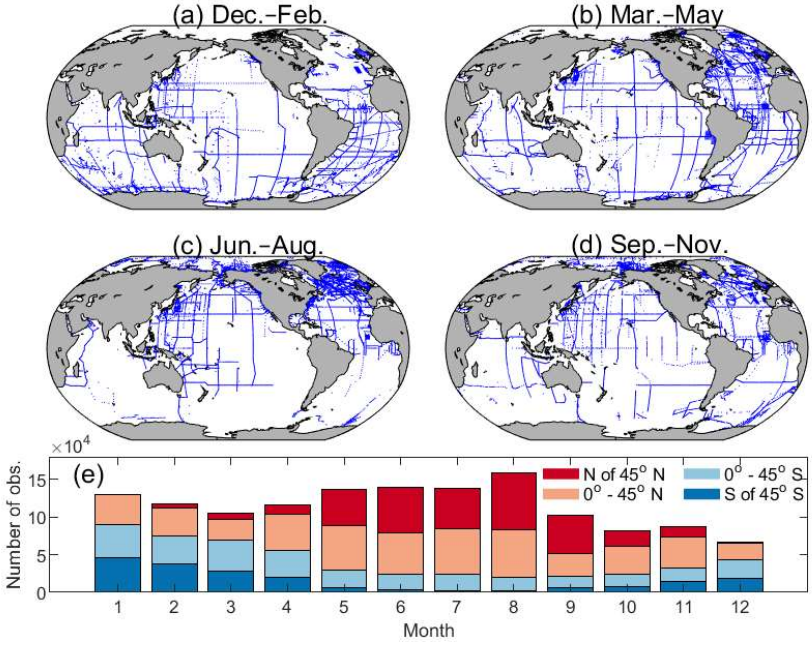

Figure 10. Distribution of data in GLODAPv2.2022 in (a) December–February, (b) March–May, (c) June–August, and (d) September–November, as well as (e) number of observations for each month in four latitude bands.

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 poleward 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

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observations stabilizes and even increases between 5000 and 6000 m; the latter is a zone where the volume of each depth surface decreases sharply (Weatherall et al., 2015). In the deep trenches, i.e., areas deeper than ~ 6000 m, both number and density of observations are low.

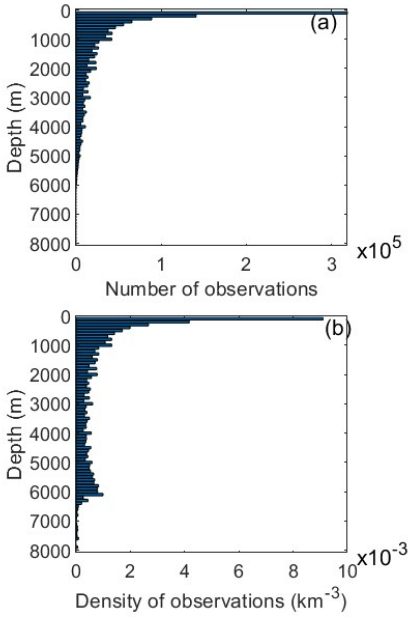

Figure 11. Number (a) and density (b) of observations in 100 m depth layers. The latter was calculated by dividing the number of observations in each layer by its global volume calculated from ETOPO2 (National Geophysical Data Center, 2006). For example, in the layer between 0 and 100 m there are on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

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.

The consistency analyses were conducted by comparing the data from the 96 new cruises to the previous data product GLODAPv2.2021. 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. For GLODAPv2.2022 a special case are the RV *Knorr* cruises in 1994-1995 where the adjustment reflects offsets in CRM measurements that have not previously been corrected for. The adjustment table at https://glodapv2-2022.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

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was not examined. All new pH data for this version were comprehensively reviewed using crossover analysis, and only one required adjustment while another had to be flagged bad (-777) and removed from the product. 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 $\delta^{13}C$, the QC results by Becker et al. (2016) for the North Atlantic were applied, and a secondary QC flag was therefore added to this variable.

The primary WOCE QC flags in the product files are simplified (e.g., all questionable and bad data were removed). For salinity, oxygen, and the nutrients, any data flagged 0 are interpolated rather than measured. For TCO_2, TAlk, pH, and fCO_2 any data flags of 0 indicate that the values were calculated from two other measured seawater CO_2 variables. Finally, while questionable (WOCE flag = 3) and bad (WOCE flag = 4) data have been excluded from the product files, some may have gone unnoticed through our analyses. Users are encouraged to report on any data that appear suspicious.

Based on the initial minimum adjustment limits and the improvement of the consistency resulting from the adjustments (Table 7), the data subjected to consistency analyses are believed to be consistent to better than 0.005 in salinity, 1 % in oxygen, 2 % in nitrate, 2 % in silicate, 2 % in phosphate, 4 μmol kg^{-1} in TCO_2, 4 μmol kg^{-1} in TAlk, and 5 % for the halogenated transient tracers and SF_6. For pH, the consistency among all data is estimated as 0.01–0.02, depending on region. As mentioned above, the included fCO_2 data have not been subjected to quality control, therefore no consistency estimate is given for this variable. This should be conducted in future efforts.

7 Author contributions.

SKL and TT led the team that produced this update. RMK, AK, BP, and SDJ compiled the original data files. NL conducted the primary and secondary QC analyses. HCB conducted the CANYON-B and CONTENT analyses. CS manages the adjustment table e-infrastructure. AK maintains the GLODAPv2 webpages at NCEI/OCADS. JDM was responsible for identifying the small offsets in the historical Indian Ocean data. LQJ, RAF, BRC, SRA, and LB conducted CODAP-NA QC efforts prior to ingestion into GLODAP. TT, RS, and EJ performed the secondary QC on all transient tracers. All authors contributed to the interpretation of the secondary QC results and made decisions on whether to apply adjustments. Many conducted ancillary QC analyses. SKL updated the living data manuscript with contributions from all authors.

8 Competing interests

The authors declare that they have no competing interests.

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Figure captions

Figure 1. Location of stations in (a) GLODAPv2.2021 and for (b) the new data added in this update.

Figure 2. Number of cruises per year in GLODAPv2, GLODAPv2.2021, and GLODAPv2.2022.

Figure 3. Example crossover figure, for silicate for cruises 49UF20190207 (blue) and 49RY20110515 (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 silicate (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 silicate 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 silicate crossovers for 49UF20190207 versus the cruises in GLODAPv2.2021 (with cruise EXPOCODE 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 (as a ratio). The weighted mean and standard deviation of all these offsets are shown in the red lines and are 1.01 ± 0.00. The dashed black lines are the reference line for a ±2 % offset.

Figure 5. Example summary figure for CANYON-B and CONTENT analyses for 49UF20190207. 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.

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 converted into atmospheric mixing ratios. Solid black line: atmospheric time history of CFC-12 vs. that of SF_6. Dotted lines: CFC-12 vs. 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.

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).

Figure 8. Magnitude of applied adjustments relative to minimum adjustment limits (Table 3) per decade for the 1085 cruises included in GLODAPv2.2022.

Figure 9. Locations of stations included in the (a) Arctic, (b) Atlantic, (c) Indian, and (d) Pacific ocean product files for the complete GLODAPv2.2022 dataset.

Figure 10. Distribution of data in GLODAPv2.2022 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.

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

Appendix A. Supplementary tables

Table A1. Cruises included in GLODAPv2.2022 that did not appear in GLODAPv2.2021. 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_2022/cruise_table_v2022.html (last access: 15 August 2022).

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No	EXPOCODE	Region	Alias	Start	End	Ship
4001	18DD20100720	Salish Sea	2.010.036	20100720	20100817	*John P. Tully*
4002	18DD20110621	Salish Sea	2.011.009	20110621	20110625	*John P. Tully*
4003	18DL20150710	Arctic	ArcticNet1502	20150710	20150820	*CCGS Amundsen*
4004	18DL20150905	Arctic	ArcticNet1503	20150905	20151001	*CCGS Amundsen*
4005	18DL20200722	Atlantic	AZOMP, AR07W	20200722	20200811	*Amundsen*
4006	18VT20030902	Salish Sea	2.003.029	20030902	20030906	*Vector*
4007	18VT20031201	Salish Sea	2.003.041	20031201	20031206	*Vector*
4008	18VT20100403	Salish Sea	2.010.016	20100403	20100406	*Vector*
4009	18VT20100805	Salish Sea	2.010.057	20110805	20110808	*Vector*
4010	18VT20101029	Salish Sea	2.010.073	20101029	20101102	*Vector*
4011	18VT20110404	Salish Sea	2.011.028	20110404	20110411	*Vector*
4012	18VT20110805	Salish Sea	2.011.006	20110805	20110808	*Vector*
4013	18VT20110909	Salish Sea	2011.01	20110909	20110914	*Vector*
4014	18VT20111124	Salish Sea	2.011.076	20111124	20111128	*Vector*
4015	18VT20120401	Salish Sea	2.012.019	20120401	20120405	*Vector*
4016	18VT20120405	Salish Sea	2.012.004	20120405	20120410	*Vector*
4017	18VT20120613	Salish Sea	2.012.005	20120613	20120619	*Vector*
4018	18VT20120714	Salish Sea	2.012.057	20120714	20120717	*Vector*
4019	18VT20120919	Salish Sea	2.012.006	20120919	20120925	*Vector*
4020	316G20120202	Atlantic	DE1202	20120202	20120219	*Delaware*
4021	316N20090614	Pacific	KN195	20090614	20090730	*Knorr*
4022	31FN20090924	Pacific	MF0904	20090924	20091013	*Miller Freeman*
4023	332220120904	Pacific	WCOA2012	20120904	20120917	*Bell M. Shimada*
4024	332220170918	Pacific	SH1709	20170918	20170928	*Bell M. Shimada*
4025	334A20140510	Atlantic	EX1403	20140510	20140517	*Okeanos Explorer*
4026	334B20121026	Atlantic	PC1207	20121026	20121114	*Pisces*
4027	334B20141103	Atlantic	PC1405	20141103	20141121	*Pisces*
4028	334B20160807	Atlantic	PC1604	20160807	20160819	*Pisces*
4029	334B20161018	Atlantic	PC1609	20161018	20161019	*Pisces*
4030	33FA20180624	Pacific	FK180624	20180624	20180713	*Falkor*
4031	33GG20130609	Atlantic	GU1302	20130609	20130623	*Gordon Gunter*
4032	33GG20131113	Atlantic	GU1305	20131113	20131125	*Gordon Gunter*
4033	33GG20140301	Atlantic	GU1401 Leg2	20140301	20140308	*Gordon Gunter*
4034	33GG20150619	Atlantic	GU15-04, ECOA1	20150619	20150723	*Gordon Gunter*
4035	33GG20151012	Atlantic	GU1506 Leg2	20151013	20151024	*Gordon Gunter*
4036	33GG20160521	Atlantic	GU1608 Leg1	20160521	20160602	*Gordon Gunter*
4037	33GG20160607	Atlantic	GU1608 Leg2	20160607	20160612	*Gordon Gunter*
4038	33GG20170516	Atlantic	GU1701 Leg1	20170517	20170525	*Gordon Gunter*
4039	33GG20170530	Atlantic	GU1701 Leg2	20170530	20170605	*Gordon Gunter*
4040	33GG20170610	Atlantic	GU1702	20170610	20170621	*Gordon Gunter*
4041	33GG20171031	Atlantic	GU1706	20171031	20171111	*Gordon Gunter*
4042	33GG20180822	Atlantic	GU1804	20180822	20180831	*Gordon Gunter*
4043	33H520181102	Atlantic	S11802	20181102	20181112	*Hugh R. Sharp*
4044	33HH20120531	Atlantic	HB1202	20120602	20120613	*Henry B. Bigelow*
4045	33HH20150519	Atlantic	HB1502	20150520	20150602	*Henry B. Bigelow*
4046	33HH20170211	Atlantic	HB1701	20170211	20170223	*Henry B. Bigelow*
4047	33HH20180523	Atlantic	HB1803	20180523	20180604	*Henry B. Bigelow*
4048	33HH20180625	Atlantic	HB-18-04, ECOA2	20180625	20180729	*Henry Bigelow*
4049	33HQ20080329	Pacific	BEST '08 Spring; HLY0802	20080329	20080506	*Healy*
4050	33HQ20080703	Pacific	BEST '08 Summer; HLY0803	20080703	20080731	*Healy*
4051	33HQ20090403	Pacific	HLY0902	20090403	20090512	*Healy*
4052	33HQ20100907	Arctic	HLY1003	20100907	20100927	*Healy*
4053	33HQ20121005	Arctic	HLY1203	20121005	20121025	*Healy*
4054	33HQ20170826	Arctic	HLY1702	20170826	20170915	*Healy*
4055	33HQ20180807	Arctic	HLY1801	20180807	20180824	*Healy*

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4056	33HQ20190806	Arctic	HLY1901	20190806	20190822	*Healy*
4057	33RO20120721	Atlantic	RB-12-03, GOMECC2	20120722	20120813	*Ronald H. Brown*
4058	33RO20170718	Atlantic	GOMECC3	20170718	20170820	*Ronald H. Brown*
4059	33WA20141201	Atlantic	WS1418	20141201	20141205	*F.G. Walton Smith*
4060	33WA20150921	Atlantic	WS15264	20150921	20150925	*F.G. Walton Smith*
4061	49HH20091106	Indian	KH09-05	20091106	20100109	*Hakuho Maru*
4062	49NZ20191205	Indian	MR19-04 (Leg 2), GO-SHIP I08N	20191205	20191227	*Mirai*
4063	49UF20190207	Pacific	ks201902	20190207	20190320	*Keifu Maru II*
4064	49UF20190424	Pacific	ks201904	20190424	20190526	*Keifu Maru II*
4065	49UF20190604	Pacific	ks201905	20190604	20190710	*Keifu Maru II*
4066	49UF20190716	Pacific	ks201906	20190716	20190908	*Keifu Maru II*
4067	49UF20190916	Pacific	ks201907	20190916	20191022	*Keifu Maru II*
4068	49UF20200108	Pacific	ks202001	20200108	20200126	*Keifu Maru II*
4069	49UF20200201	Pacific	ks202002	20200201	20200323	*Keifu Maru II*
4070	49UF20200605	Pacific	ks202004	20200605	20200614	*Keifu Maru II*
4071	49UF20200619	Pacific	ks202005	20200619	20200724	*Keifu Maru II*
4072	49UF20200730	Pacific	ks202006	20200730	20200820	*Keifu Maru II*
4073	49UF20201021	Pacific	ks202008	20201021	20201201	*Keifu Maru II*
4074	49UF20210202	Pacific	ks202102	20210202	20210312	*Keifu Maru II*
4075	49UF20210407	Pacific	ks202103	20210407	20210509	*Keifu Maru II*
4076	49UF20210515	Pacific	ks202104	20210515	20210627	*Keifu Maru II*
4077	49UP20181122	Pacific	rf201808to09	20181122	20181225	*Ryofu Maru III*
4078	49UP20190110	Pacific	rf201901	20190110	20190223	*Ryofu Maru III*
4079	49UP20190228	Pacific	rf201902	20190228	20190326	*Ryofu Maru III*
4080	49UP20190408	Pacific	rf201903	20190208	20190511	*Ryofu Maru III*
4081	49UP20190516	Pacific	rf201904	20190516	20190606	*Ryofu Maru III*
4082	49UP20190612	Pacific	rf201905	20190612	20190803	*Ryofu Maru III*
4083	49UP20190811	Pacific	rf201906	20190811	20190926	*Ryofu Maru III*
4084	49UP20191125	Pacific	rf201908	20191125	20191222	*Ryofu Maru III*
4085	49UP20200227	Pacific	rf202002	20200227	20200323	*Ryofu Maru III*
4086	49UP20200605	Pacific	rf202005	20200605	20200715	*Ryofu Maru III*
4087	49UP20200730	Pacific	rf202006	20200730	20200909	*Ryofu Maru III*
4088	49UP20201019	Pacific	rf202008	20201019	20201109	*Ryofu Maru III*
4089	49UP20210113	Pacific	rf202101	20210113	20210223	*Ryofu Maru III*
4090	49UP20210301	Pacific	rf202102	20210301	20210321	*Ryofu Maru III*
4091	49UP20210425	Pacific	rf202104	20210425	20210528	*Ryofu Maru III*
4092	58HB20201110	Atlantic		20201110	20211116	*Hans Brattstrøm*
4093	64PE20100428	Atlantic	PE319	20100428	20100526	*RV Pelagia*
4094	64PE20100611	Atlantic	PE321	20100611	20100708	*RV Pelagia*
4095	740H20111224	Atlantic	JC068	20111224	20120127	*RRS James Cook*
4096	74EQ20101018	Atlantic	D357	20101018	20101122	*RRS Discovery*

Table A2. List of cruises included in GLODAPv2.2021 which have been updated as part of 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_2022/cruise_table_v2022.html (last access: 15 August 2022).

No.	EXPOCODE	Region	Alias	Update	Adjustment
26	06M220090714	Atlantic	CLIVAR AR07W_2009, MSM12_3	Performed 2nd QC on SF6	1.0
55	06MT20030626	Atlantic	06MT591	Performed 2nd QC on SF6	1.0
57	06MT20030831	Atlantic	06MT593	Performed 2nd QC on SF6	1.0
58	06MT20040311	Atlantic	06MT605	Performed 2nd QC on SF6	1.0
62	06MT20060712	Atlantic	MT68_3_2006	Performed 2nd QC on SF6	-888
63	06MT20091026	Atlantic	MT80/1_2009	Performed 2nd QC on SF6	1.0

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64	06MT20110405	Atlantic	MT84_3	Performed 2nd QC on SF6	1.0
263	316N20020530	Arctic	NS02, KN166_11	Performed 2nd QC on SF6	1.0
273	318M20091121	Pacific	CLIVAR P06_2009	Performed 2nd QC on SF6	1.0
295	320620110219	Pacific	CLIVAR S04P_2011	Performed 2nd QC on SF6	1.0
307	325020080826	Pacific	CLIVAR_TN224_2008	Performed 2nd QC on SF6	-888
324	32OC20080510	Atlantic	32OC446	Performed 2nd QC on SF6	1.0
329	33AT20120324	Atlantic	CLIVAR_A22_2012	Performed 2nd QC on SF6	1.0
330	33AT20120419	Atlantic	CLIVAR_A20_2012	Performed 2nd QC on SF6	1.0
345	33RO20071215	Pacific	CLIVAR P18_2007	Performed 2nd QC on SF6	1.0
346	33RO20100308	Atlantic	CLIVAR A13.5_2010, RB_07-05	Performed 2nd QC on SF6	1.0
347	33RO20110926	Atlantic	CLIVAR A10_2011 , RB-11-02	Performed 2nd QC on SF6	1.0
355	33RR20090320	Indian	CLIVAR I05_2009	Performed 2nd QC on SF6	1.0
434	49HG19971110	Pacific	NH97	Performed 2nd QC on SF6	1.2
435	49HG19980812	Pacific	NH98	Performed 2nd QC on SF6	1.2
461	49K619990523	Pacific	49EWMI9905_1	Performed 2nd QC on SF6	-777
631	58AA20010527	Arctic	58AA0113, TRACTOR 13	Performed 2nd QC on SF6	1.0
635	58GS20090528	Arctic	SARS09, CLIVAR 75N_2009	Performed 2nd QC on SF6	-777
674	740H20081226	Atlantic	JC30	Performed 2nd QC on SF6	1.0
702	74JC19960720	Arctic	74JC9608	Performed 2nd QC on SF6	1.0
703	74JC20100319	Atlantic	JR239, ANDREX-2	Performed 2nd QC on SF6	1.0
706	77DN20020420	Arctic	77DN0204	Performed 2nd QC on SF6	1.0
708	77DN20050819	Arctic	ODEN05, AOS-2005	Performed 2nd QC on SF6	1.0
724	ZZIC2005SWYD	Arctic	SWITCHYARD	Performed 2nd QC on SF6	1.0
1002	06AQ20120107	Atlantic	ANT-XXVIII/3	Performed 2nd QC on SF6	1.0
1003	06AQ20120614	Arctic	ARK XXVII/1	Performed 2nd QC on SF6	1.0
1005	06AQ20150817	Arctic	PS-94, ARK-XXIX/3	Performed 2nd QC on SF6	1.0
1007	06M220080723	Atlantic	MSM09-1	Performed 2nd QC on SF6	1.0
1008	06M220170104	Atlantic	MSM60-1 SAMOC	Performed 2nd QC on SF6	1.0
1011	06M320150501	Atlantic	M116/1	Performed 2nd QC on SF6	1.0
1012	06M220081031	Atlantic	MSM10/1	Performed 2nd QC on SF6	1.0
1013	06MT20091126	Atlantic	MT80/2	Performed 2nd QC on SF6	1.1
1014	06MT20101014	Atlantic	M83/1	Performed 2nd QC on SF6	1.0
1016	06MT20140317	Atlantic	M105	Performed 2nd QC on SF6	1.0
1020	096U20160426	Pacific	IN2016_V03, P15S	Performed 2nd QC on SF6	1.0
1025	18HU20130507	Atlantic	AR07W_2013	Performed 2nd QC on SF6	1.0
1026	18HU20140502	Atlantic	AR07W_2014	Performed 2nd QC on SF6	1.0
1027	18HU20150504	Atlantic	AR07W_2015	Performed 2nd QC on SF6	1.0
1029	18MF20120601	Atlantic	AR07W_2012	Performed 2nd QC on SF6	1.0
1033	316N20111106	Atlantic	GT11, NAT-11	Performed 2nd QC on SF6	1.0
1035	318M20130321	Pacific		Performed 2nd QC on SF6	1.0
1036	320620140320	Pacific	GO-SHIP P16S_2014	Performed 2nd QC on SF6	1.0
1038	325020131025	Pacific	TGT303, P21_2013	Performed 2nd QC on SF6	1.0
1040	33HQ20150809	Arctic	HLY1502	Performed 2nd QC on SF6	1.0
1041	33RO20130803	Atlantic	A16N_2013	Performed 2nd QC on SF6	1.0
1042	33RO20131223	Atlantic	RB1307, A16S_2013	Performed 2nd QC on SF6	1.0
1043	33RO20150410	Pacific	GO-SHIP P16N_2015 Leg 1	Performed 2nd QC on SF6	1.0

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1044	33RO20150525	Pacific	GO-SHIP P16N_2015 Leg 2	Performed 2nd QC on SF6	1.0
1045	33RO20161119	Pacific	RB1606, GO-SHIP P18_2016	Performed 2nd QC on SF6	1.0
1046	33RR20160208	Indian	I08S_2016	Performed 2nd QC on SF6	1.0
1050	49NZ20121128	Indian	P14S_S04_2012; MR12-05 Leg 2	Performed 2nd QC on SF6	1.0
1051	49NZ20130106	Indian	S04I_2013	Performed 2nd QC on SF6	1.0
1053	49NZ20140717	Pacific	MR14-04, GO-SHIP P01_2014	Performed 2nd QC on SF6	1.0
1054	49NZ20151223	Indian	MR15-05, I10_2015	Performed 2nd QC on SF6	1.0
1055	49NZ20170208	Pacific	MR16-09, P17E	Performed 2nd QC on SF6	1.0
1103	58GS20150410	Atlantic	AR07E_2015	Performed 2nd QC on SF6	1.0
1104	58GS20160802	Arctic	75N_2016	Performed 2nd QC on SF6	1.0
2003	06M220130509	Atlantic	MSM28	Performed 2nd QC on SF6	1.0
2005	06M220150502	Atlantic	MSM42	Performed 2nd QC on SF6	1.0
2006	06M220150525	Atlantic	MSM43	Performed 2nd QC on SF6	1.0
2008	096U20180111	Indian	SR03.2018	Performed 2nd QC on SF6	1.0
2011	29AH20160617	Atlantic	OVIDE-16	Performed 2nd QC on SF6	1.0
2020	316N20101015	Atlantic	KN199-04	Performed 2nd QC on SF6	1.0
2023	316N20150906	Atlantic	Davis Strait 2015	Performed 2nd QC on SF6	1.0
2026	35TH20080825	Atlantic	SUBPOLAR08	Performed 2nd QC on SF6	1.0
2027	45CE20170427	Atlantic	CE17007	Performed 2nd QC on SF6	1.0
3002	06M220160331	Atlantic	MSM53	Performed 2nd QC on SF6	1.0
3003	06MT20160828	Atlantic	M130	Performed 2nd QC on SF6	1.0
3004	06MT20170302	Pacific	M135	Performed 2nd QC on SF6	1.0
3005	06MT20180213	Atlantic	M145	Performed 2nd QC on SF6	1.0
3029	320620170703	Pacific		Performed 2nd QC on SF6	1.2
3030	320620170820	Pacific		Performed 2nd QC on SF6	1.1
3031	320620180309	Pacific	NBP18_02	Performed 2nd QC on SF6	1.0
3033	325020190403	Indian	TN366	Performed 2nd QC on SF6	1.0
3034	33RO20180423	Indian		Performed 2nd QC on SF6	1.0
3041	49NZ20191229	Indian	MR19-04 (Leg 3)	Performed 2nd QC on SF6	1.0
3042	58JH20190515	Arctic	JH2019205	Performed 2nd QC on SF6	1.0
249	316N19941201	Indian	316N145_5	Performed 2nd QC on TCO2	1.7
249	316N19941201	Indian	316N145_5	Performed 2nd QC on TAlk	-3.5
250	316N19950124	Indian	316N145_6	Performed 2nd QC on TCO2	1.7
250	316N19950124	Indian	316N145_6	Performed 2nd QC on TAlk	-3.5
251	316N19950310	Indian	316N145_7	Performed 2nd QC on TCO2	1.7
251	316N19950310	Indian	316N145_7	Performed 2nd QC on TAlk	-3.5
252	316N19950423	Indian	316N145_8	Performed 2nd QC on TCO2	1.7
252	316N19950423	Indian	316N145_8	Performed 2nd QC on TAlk	-3.5
253	316N19950611	Indian	316N145_9	Performed 2nd QC on TCO2	1.7
253	316N19950611	Indian	316N145_9	Performed 2nd QC on TAlk	-3.5
254	316N19950715	Indian	316N145_10	Performed 2nd QC on TCO2	1.7
254	316N19950715	Indian	316N145_10	Performed 2nd QC on TAlk	-3.5
255	316N19950829	Indian	316N145_11, 316N145_12	Performed 2nd QC on TCO2	1.7
255	316N19950829	Indian	316N145_11, 316N145_12	Performed 2nd QC on TAlk	-3.5
256	316N19951111	Indian	316N145_13	Performed 2nd QC on TCO2	1.7
256	316N19951111	Indian	316N145_13	Performed 2nd QC on TAlk	-3.5

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257	316N19951202	Indian	316N145_14, 316N145_15	Performed 2nd QC on TCO2	1.7
257	316N19951202	Indian	316N145_14, 316N145_15	Performed 2nd QC on TAlk	-3.5
433	49HG19960807	Pacific	NH96-2	Performed 2nd QC on pH	-0.05
574	49UP19970912	Pacific	RF97-09	Performed 2nd QC on oxygen	1.015
1011	06M320150501	Atlantic	M116/1	Added CFC-12 data	
656	58P320011031	Arctic	Station M	Added new data from 2008 until 2021	
2011	29AH20160617	Atlantic	OVIDE-16	Added bottle numbers	
2013	29HE20190406	Atlantic	FICARAM_XIX	Added bottle numbers	
239	316N19831007	Atlantic	AJAX	Changed TAlk WOCE flag from 2 to 0	