

In Situ Thematic Assembly Centre INSITU_GLO_BGC_CARBON_DISCRETE_MY_013_050

Issue: 2.4

Contributors: Rocío Castaño Primo, Benjamin Pfeil

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QUID for INS Product							
INSITU_	GLO	BGC	CARBON	_DISCRETE_	_MY_	_013_	050

CHANGE RECORD

Ref:

Date:

Issue:

When the quality of the products changes, the QuID is updated and a row is added to this table. The third column specifies which sections or sub-sections have been updated. The fourth column should mention the version of the product to which the change applies.

Issue	Date	§	Description of Change	Author	Validated By
1.0	January 2019		Creation of the document	B. Pfeil	
2.0	November 2019	all	Re-written text, made it more similar to other In Situ TAC QuIDs. Added information specific to the product and updated quality information with data provided to CMEMS.	R. Castaño-Primo B. Pfeil	
2.1	September 2020	1.1 3.1 3.3 4.2	Table 1. Removed the end year of the products to make the document more general. Indicated that only good data are available in SOCAT from v2020 until now due to new guidelines for SOCAT data product publication.	R. Castaño-Primo	
2.2	August 2022	all	New QuID format. New product and dataset names. Validation results of SOCATv2022 and GLODAPv2.2022.	R. Castaño-Primo	S. Tarot
2.3	February 2024	all	Updated to SOCATv2023 and GLODAPv2.2023	R. Castaño-Primo	S. Tarot
2.4	October 2024	all	Updated to SOCATv2024	C. S. Landa	S. Tarot



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I EXECUTIVE SUMMARY

I.1 Products covered by this document

This document applies to the product INSITU_GLO_BGC_CARBON_DISCRETE_MY_013_050: the community data products SOCAT (Surface Ocean CO_2 ATlas) and GLODAP (Global Ocean Data Analysis Project), which contain inorganic carbon observations and auxiliary variables, and their gridded fields at different spatial-temporal resolutions

I.2 Summary of the results

While SOCAT and GLODAP are global datasets, their spatial coverage is irregularly distributed. The Indian, Arctic and Southern oceans are particularly lacking with data. Long-term moorings, standard biogeochemical transects, and certain regular shipping routes concentrate many of the observations.

The general trend is an increase in the number of observations in the more recent decades. This increase is much clearer in SOCAT; surface CO_2 instruments are mainly autonomous and being fitted in a larger variety of platforms: commercial and sailing ships, autonomous vehicles... On the other hand, GLODAP data comes from bottle samples, and almost exclusively research vessels.

Both SOCAT and GLODAP are high-quality data products, due to their thorough, expert QC; in the case of GLODAP, bias corrections are performed if necessary. With time the data quality has increased, mostly due to the evolution in measurement methods. In SOCAT the average accuracy of the observations has increased with time. For GLODAP, there is a clear decrease in the need for bias correction in the latest decade.



I.3 Estimated Accuracy Numbers

Estimated accuracy numbers are stated in Table 1 below. For GLODAP, the estimations are for *internal consistency* of the data product, which is a good accuracy estimate. In SOCAT, temperature and salinity are provided for provenance only, and not subjected to rigorous physical oceanography QC. In GLODAP, if temperature is provided, is assumed as good. Therefore, no estimated accuracy is explicitly available for temperature.

Parameter	Estimated Accuracy	Product
Fugacity of carbon dioxide	2 – 10 µatm	SOCAT
Temperature	-	-
Salinity	0.002	GLODAP
Oxygen	0.6%	GLODAP
Nitrate	0.8%	GLODAP
Silicate	1.0%	GLODAP
Phosphate	1.0%	GLODAP
Dissolved inorganic carbon	2.8 μmol kg-1	GLODAP
Total alkalinity	2.3 μmol kg-1	GLODAP
рН	0.0082	GLODAP

Table 1: EAN for the variables included in the product



II PRODUCTION SYSTEM DESCRIPTION

The Copernicus Marine In Situ Thematic Assembly Centre (In Situ TAC) is a distributed system built on the existing activities and services developed previously within the EC supported projects and EuroGOOS Regional alliances (ROOSes). The In Situ TAC provides the interface between centres, distributing In Situ measurements from national and international observing systems. In situ products provided within Copernicus Marine Service include temperature and salinity, currents, sea level, biogeochemical, waves, and since April 2019, inorganic carbon, in global and regional scales.

Within the In Situ TAC organization, the carbon Production Unit at IMR (Institute of Marine Research – Norway) functions currently as a global PU independent from the global PU managed by IFREMER. Due to the nature of the REP carbon products as already-existing data products, they are distributed as standalone, independent datasets, with proper attribution given in the metadata by use of DOIs.

The carbon MY product pertaining to this document contains the community data products SOCAT and GLODAP, reformatted to facilitate the access to In Situ TAC users. SOCAT and GLODAP are voluntary efforts of the biogeochemical scientific community that provide harmonized, high-quality data necessary to evaluate and understand the inorganic carbon cycle in the oceans. SOCAT and GLODAP are endorsed by the Global Ocean Observing System (GOOS) and are voluntary contributions to the UN Sustainable Development Goal 14.3: *Life Under Water; minimize and address the impacts of ocean acidification, including through enhanced scientific cooperation at all levels*.

SOCAT (<u>https://socat.info</u>, Bakker *et al.* (2016), Bakker *et al.* (2024)), the Surface Ocean CO2 ATIas, is a synthesis activity for quality-controlled surface ocean fCO₂ measurements by more than 100 contributors from around the globe. It enables quantification of the ocean carbon sink, ocean acidification and the evaluation of ocean biogeochemical models. As such, it is used in the Global Carbon Budget (Friedlingstein *et al.* (2022), <u>https://www.globalcarbonproject.org</u>). Version 1 was released in 2011. Automation has allowed for annual releases since version 4 in 2016.

GLODAP (<u>https://glodap.info</u>, Lauvset *et al.* (2023)) is a high-quality, internally consistent, compilation of ocean interior observations of key carbon and biogeochemical variables, harmonized, quality controlled and bias-corrected. GLODAP data have been used for model evaluation, inventory calculations and calibration of BGC-Argo sensor observations. The first version was released in 2005, with cruises from the WOCE/JGOFS and GEOSECS programs. The second version included those in the first one and data from the CARINA and PACIFICA synthesis. Subsequent versions are extensions of the synthesis product (called in Copernicus Marine Service *OBSERVATIONS*) from GLODAPv2 with data from additional cruises.

Section VII contains the references to articles describing the different data products. The user is strongly encouraged to refer to them for further details and to cite them if they make a heavy use of this product, in addition to the Copernicus citation.



III VALIDATION FRAMEWORK

In this document, we have left out the terms "primary" and "secondary" QC on purpose. The definition of what constitutes primary and secondary is product-dependent (SOCAT/GLODAP/Copernicus Marine Service carbon). In this document, where the three data products converge, it makes the text unnecessarily confusing.

For further details on the QC procedures, please refer to the references in section VII.

III.1 SOCAT

Surface measured fCO_2 data submitted to SOCAT have been initially QCed by their respective data providers prior to submission. Then it first goes through a series of automated QC checks on timestamp (no duplicates), position (calculated ship speeds), and range checks of the variables used to calculate fCO_2 . Then the fCO_2 data points are given WOCE QC flags, where 2 equals good, 3 questionable and 4 bad. Only data points with "good" WOCE flags are published in SOCAT.

Since SOCAT is a global data product, the criteria are ample to allow for a wide range of environmental conditions. Timestamps in non-chronological order or an excessive number of duplicated times or an excessive number of flag 4 data points are causes for the dataset to be sent back to the provider.

The next step in QC is manual, performed by scientists specialized in inorganic carbon, divided in groups of regional expertise. The fCO_2 data are visually inspected and WOCE flags reassigned if necessary. The metadata provided is reviewed for completeness, and additional information is requested if missing. Temperature and salinity are not explicitly QCed; they are provided as supporting information for fCO_2 but shall not be used by themselves.

Part of the manual QC procedure is the assignment of cruise quality flags A-E. These are indicators of the estimated accuracy of fCO_2 in the datasets, from $\leq 2 \mu$ atm for A-B to $\leq 10 \mu$ atm. The criteria for assigning the dataset flag include whether the method follows standard operating procedures (accuracy limits for individual sensors, calibration gasses, etc), the existence of high-quality crossovers and metadata completeness. For Copernicus Marine Service all data with flags A-E is provided, except for the gridded product, which only uses A-D data (2-5 μ atm of fCO₂ accuracy). These flags are untranslatable to Copernicus Marine Service flags, due to the different granularities of the products. If the user is interested in data of a specific accuracy, this information can be found in the metadata list for SOCAT available in Pangaea for all SOCAT versions since v3 to v2019, and the header lines of the original SOCAT data files from v2020 onwards.

III.2 GLODAP

GLODAP deals only with bottle data. The individual cruise data files are converted to WOCE exchange format: a comma-delimited ASCII format for CTD and bottle data from hydrographic cruises. Headers and units are standardized.

A first-step manual QC is performed in all variables except temperature and pressure, which are assumed good if present. It is done by scientists, by visualizing property-property plots of small groups of stations, in search of outliers, and assigning WOCE flags to each observation.

The aim for the second step of QC is to identify and correct any significant biases in the data, while retaining any signal due to time changes. It takes the form of consistency analyses, conducted to identify offsets in the data. All identified offsets are scrutinized by the GLODAP reference group in order to



decide the adjustments to be applied, taken a conservative approach of not applying any when in doubt. The adjustment table is available in https://glodapv2-2023.geomar.de/.

To identify offsets for salinity, oxygen, nutrients, total dissolved inorganic carbon, and total alkalinity crossover comparisons, MLRs, and comparison of deepwater averages were used. For pH, an additional evaluation of the internal consistency of the seawater CO₂ chemistry variables was used whenever possible. For the halogenated transient tracers, examination of surface saturation levels and relationship among the tracers were used to assess the data consistency. For salinity and oxygen, CTD and bottle values were merged into a "hybrid" variable prior to the consistency analyses.

The result of this second step in manual QC is mostly bias corrections, not re-flagging. In some cases, however, outliers were only found during this stage, which granted a change in the QC flag. Only data with WOCE flag 2 (good data) were included in the final product.

III.3 QC flag standardization

The QC flags originally assigned by SOCAT and GLODAP to the individual data points are mapped to the QC flags defined for the Copernicus Marine Service parameters (Table 2).

WOCE	Code	Meaning	Comment		
	0	No QC was performed			
2	1	Good data	All real-time QC tests passed		
3	2	Probably good data	These data should be used with caution		
	3	Bad data that are potentially correctable	These data are not to be used without scientific correction		
4	4	Bad data	Data have failed one or more of the tests		
	5	Value changed	Data may be recovered after transmission error		
	6	Not used			
	7	Nominal value			
	8	Interpolated value	Missing data may be interpolated from neighbouring data in space or time		
	9	Missing value			

 Table 2: Copernicus Marine Service quality control flags



IV VALIDATION RESULTS

IV.1 Spatio-temporal coverage

IV.1.1 SOCAT

The temperature and salinity from the SOCAT dataset are not discussed, only the CO_2 fugacity. Temperature and salinity SST and Salinity are provided in the Copernicus Marine Service product for provenance reasons only, because they are the basis for the fCO_2 calculations, but should not be considered sufficiently robust for use in themselves. The quality control of temperature and salinity required for fCO_2 is not as rigorous as that performed by the physical oceanographers. For TEMP and PSAL data, the reader should refer to other In Situ TAC products.

IV.1.1.1 CO₂ fugacity (FCO2)

The geographical coverage of the SOCAT dataset is shown in Figure 1. The distribution is in general global, with some areas more densely covered than others. The Indian, Arctic and South Pacific oceans are particularly poorly covered. A good amount of data comes from cargo ships (ships of opportunity / voluntary observing ships) on regular lines, which are visible in the maps. All observations from SOCAT come, by definition, from the surface layer only, at a nominal depth of 5 m. fCO_2 measurements date from all the way back to the 1960's (Figure 2). However, the number of observations is very low until the mid 1990's, when it started picking up to the ~2 million observations per year in the late 2010's. The availability of automated systems that allow for relatively hands-off data collection in non-oceanographic vessels and moorings is partly responsible of this increase.





Figure 1: Geographical distribution of fCO₂ observations in the full SOCAT dataset (top), and the new data submitted for v2O24 (bottom). From <u>SOCAT Live Access Server</u>





Figure 2: Time series of the number of fCO_2 observations in SOCAT with an estimated accuracy below 5 μ atm by version (a) and number of monthly 1x1 degree cells with fCO_2 observations (b). From SOCATv2024 release poster (Bakker et al. 2024).

IV.1.2 GLODAP

GLODAP consists of open ocean (not coastal) physical and biogeochemical variables from the ocean interior. Spatial and temporal coverage of temperature and salinity are similar, and representative of the maximum data distribution in GLODAP.

Each variable has three figures attached: The world maps show the distribution of stations in black marker; red markers show the stations with valid variable values. The depth histogram shows: a) the total number of possible cast x 500 m depth bin combinations (white), the distribution of actual samples in 500-m bins (blue) and the percentage over the total, and 50-m-bin distributions (light purple). The time series is a histogram of the number of samples per year, color-coded by GLODAP version, starting with v2, released in 2016.

IV.1.2.1 Temperature (TEMP) and Salinity (PSAL)

Their spatio-temporal coverage are similar, and representative of the maximum data distribution in GLODAP (Figure 3). While the observations are distributed globally, the North Atlantic and the Northeast Pacific off the coast of Japan are more densely sampled. The Indian, Pacific, and Arctic oceans are more sparsely observed. A large fraction of the stations is distributed along reference transects that are visited



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with variable frequency. Not shown, the geographical distribution of samples has not changed significantly since v2 (2018).

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GLODAP is a bottle-file based dataset, hence the 50-m depth distribution shows peaks at certain reference depths: 1000, 2000 m etc. For variables measured using sensors (temperature, some of the salinity and oxygen) the value used in GLODAP is the one recorded in the bottle file, not the full cast. Surface layers have better sampling coverage than deeper zones and with a finer resolution. The deepest layers are the least sampled, at around 25% for temperature and salinity.

GLODAP contains observations from the early 1970's until present. Distinctive peaks in the time series correspond to large international sampling programs like GEOSECS (1970's), WOCE/JGOFS (1990's), CLIVAR and GO-SHIP (2000's). From the data distribution of the latest 5 versions, we see there is a lag of a couple of years between sampling and inclusion in GLODAP, so apparent declines in sampling may be artificial. The effect of the COVID-19 pandemic is clearer in v2.2023, with a rebound in the number of measurements, after the decline from 2019.



Figure 3: Geographical distribution of stations, depth and time distribution of observations for temperature and salinity. Detailed explanation of the subplots in section IV.1.2



IV.1.2.2 Dissolved oxygen (DOX2) and Chlorophyll-a (CPHL)

Dissolved oxygen data (either from bottle samples or sensors) is commonly measured in standard biogeochemical sampling setups, and its coverage follows closely the GLODAP coverage, in time and both space dimensions (Figure 4); in comparison the surface layers are less sampled, but the coverage is very similar in the deeper ocean.

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Chlorophyll-a from bottle samples, however, is measured much less frequently, focusing exclusively in the surface layers, where the live phytoplankton exists. The spatial distribution is patchy, with large areas almost devoid of measurements like the northwestern and southern Atlantic, the Indian and Arctic oceans. The time distribution pattern is slightly different from that of other GLODAP variables: early 90s and 2000s are the maximum in temporal distribution of values, with very few da ta until 1990 and during the 2010's. The number of data points increases significantly again towards the 2020's.



Figure 4: Geographical distribution of stations, depth and time distribution of observations for dissolved oxygen and Chlorophyll a. Detailed explanation of the subplots in section IV.1.2



IV.1.2.3 Inorganic nutrients Nitrate (NTAW), Nitrite (NTIW), Phosphate (PHOW) and Silicate (SLCW)

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The data coverage of the principal nutrients (nitrate, phosphate and silicate) is slightly less comprehensive but follows closely that of the total GLODAP observations (Figure 5). Nitrite deviates from the general distribution more than the other nutrients. The main geographical gaps are found in Agulhas return current (southwest Indian Ocean) and around Australia and the Indonesian archipelago. The time series shows the gap between sampling and data publishing.



Figure 5: Geographical distribution of stations, depth and time distribution of observations for nitrate, nitrite, phosphate and silicate. Detailed explanation of the subplots in section IV.1.2







Figure 6: Geographical distribution of stations, depth and time distribution of observations for total alkalinity, dissolved inorganic carbon, pH in situ and at 25°C, 0 bar of pressure (surface). Detailed explanation of the subplots in section IV.1.2

Similarly, to nutrients and oxygen, Dissolved Inorganic Carbon and Total Alkalinity were sampled less often than temperature and salinity; however the spatial and temporal distribution follows the general sampling distribution of GLODAP (Figure 6). pH deviates more from the GLODAP distribution, specially in time and depth. In terms of geographical distribution, observations are more sparse but relatively homogenously distributed in space. The main spatial gaps are around Australia and the Indonesian



archipelago, and a transect in the tropical Pacific. The two pH variables have the same distribution since pH at 25°C, 0 dbar is calculated from *in situ* pH. Both are provided in the total scale. The reason to provide pH at 25°C, 0 dbar is to allow for comparisons unaffected by temperature and pressure.

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While pH measurements date further back than the 1990's, the scale in which they were frequently reported (NBS) has uncertainties large enough that many of those measurements were not included in GLODAP, hence the lack of data points in the first period.

The depth distribution for pH is relatively homogeneous, at around 20% of the potential observations, slightly more frequent in the surface layer, and less in the deepest ones. For Inorganic Carbon and Alkalinity, the sampling is more frequent in the top layers, and it decreases in depth.

IV.1.2.5 Total Dissolved Nitrogen (NT1D), Dissolved Organic Nitrogen (NODW) and Dissolved Organic Carbon (CORG)

These variables are the least sampled of the GLODAP dataset distributed via Copernicus Marine Service. which is clear from their spatio-temporal distribution (Figure).

Total dissolved nitrogen was not sampled before the 2000's, and while there are observations spread among the main oceans, they are particularly scarce in the eastern Pacific compared to the total station distribution. Dissolved organic carbon has a better geographical coverage and the first observations date back to the 1990's. The depth distribution for both variables was rather homogeneous across the water column sampled. Dissolved nitrogen was only sampled in a few cruises, only on the surface layers, and no new data has been added in the recent versions of GLODAP.



Figure 7: Geographical distribution of stations, depth and time distribution of observations for dissolved organic nitrogen and carbon, and total dissolved nitrogen. Detailed explanation of the subplots in section IV.1.2 (conitnues in the next page).





Figure 7: (cont.) Geographical distribution of stations, depth and time distribution of observations for dissolved organic nitrogen and carbon, and total dissolved nitrogen. Detailed explanation of the subplots in section IV.1.2.

IV.2 Quality flag distribution

SOCAT and GLODAP are data products that publish only the data points deemed good after their QC and adjustment processes. Therefore, discussing Quality flag distribution does not apply to the In Situ TAC carbon product.

IV.3 Accuracy

The accuracy values for SOCAT and GLODAP are reflected in the executive summary, Table 1.



V SYSTEM'S NOTICEABLE EVENTS, OUTAGES OR CHANGES

Date	Change/Event description	System version	other
August 2023	GLODAPv2.2023 was released later than the usual period (late summer), which caused that it could not be included in the November 2023 release.		
September 2024	There will be no release of GLODAP in 2024.		

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VI QUALITY CHANGES SINCE PREVIOUS VERSION

No changes in the Quality Control methodologies have happened since the previous version of the product or documentation.

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VII REFERENCES

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• SOCAT synthesis product description:

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• SOCAT QC Cookbook:

Lauvset, S., Currie, K., Metzl. N., Nakaoka, S., Bakker, D., Sullivan, K., Sutton, A., O'Brien, K., Olsen, A. (2018) SOCAT Quality Control Cookbook -For SOCAT version 7. <u>https://www.socat.info/wp-content/uploads/2019/01/2018_SOCAT_QC_Cookbook_for_SOCAT_Version_7.pdf</u>

• SOCAT v2024 (latest version) release poster:

https://socat.info/wp-content/uploads/2024/06/2024_Poster_SOCATv2024.pdf

• GLODAPv2.2023 synthesis product dataset



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• GLODAPv2.2023 synthesis product paper

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• GLODAP gridded climatologies

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