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CHANGE RECORD

When the quality of the products changes, the QuID is updated and the SQO is updated. A line is added to this table and the version of the SQO document is the same than that of the REFERENCE QUID. The third column specifies which sections or sub-sections have been updated.

Issue	Date	§	Description of Change	Authors	Validated By
1.0	07/09/2020	All	Creation of the document	R. Castaño-Primo B. Pfeil	
2.2	30/08/2022	All	Update to latest QuID (2.2) and SOCAT and GLODAP product versions (2022). Updated accuracy numbers, references. Minor text edits. Changes in depth histograms (added 500-m bin and percentages) and time distributions (color-coded by version).	R. Castaño-Primo	S. Tarot
2.3	21/02/2024	All	Updated figures and references to SOCATv2023 and GLODAPv2.2023	R. Castaño-Primo	S. Tarot
2.4	02/10/2024	All	Updated figures and references to SOCATv2024	C. S. Landa	S. Tarot

Contents

Executive summary

This document summarizes the quality in terms of space and time coverage for the Copernicus Marine Service product INSITU_GLO_BGC_CARBON_DISCRETE_MY_013_050. It is based on the community-produced data products SOCAT (Surface Ocean CO2 Atlas) and GLODAP (GLobal Ocean Data Analysis Project). Only variables from the observation datasets are considered in this document, not from the gridded datasets. Gridded files are based on the observation datasets, at different grid sizes and time scales, and their quality assessment would be the same.

This document shows results from the latest versions of SOCAT (SOCATv2024) and GLODAP (GLODAPv2.2023), published in June 2024 and October 2023. Barring extraordinary circumstances, subsequent newer versions have more recent data from repeat transects and moorings, and a slightly better geographical cover from some new platforms. However, the QC procedures and the quality of the data flagged as good remains unchanged between versions.

To improve the readability of this document the variables from the cmems_obs-ins_glo_bgc-car_my_glodap-obs_irr dataset do not get their own section individually. The variables are grouped based on themes (physical oceanography, nutrients, organic carbon). Within a theme they are often measured together and have similar geographic and temporal distributions. All the GLODAP variables figures follow the same pattern: a map to show geographical distribution of the observations, a display of the depth coverage, another for time coverage on a year basis.

For additional information regarding the in-depth validation of this product, the calculation of the assessment metrics presented in this product other detailed information in quality and noticeable events please refer to the reference QuID document (CMEMS-INS-QUID-013-050), Bakker *et al* (2016, 2022), Lauvset *et al* (2016, 2024).

Important notice:

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.

GLODAP evaluates the quality of measurements and adjustments using the metric of *internal inter-cruise consistency*, which is a good approximation to accuracy.

The contents of this document are an assessment based on the best set of observations available for evaluation at the time the operational system was validated. The results presented in this report are what the SOCAT and GLODAP communities report in terms of accuracy and internal consistency as estimation of error.

1. CO_2 fugacity (FCO2) from dataset SOCAT

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. 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.

The estimated accuracy of the fCO_2 measurements in SOCAT is at least of 10 μatm, with the majority of observations at 5 or 2 μatm of accuracy, depending on the instrumentation used and auxiliary data available.

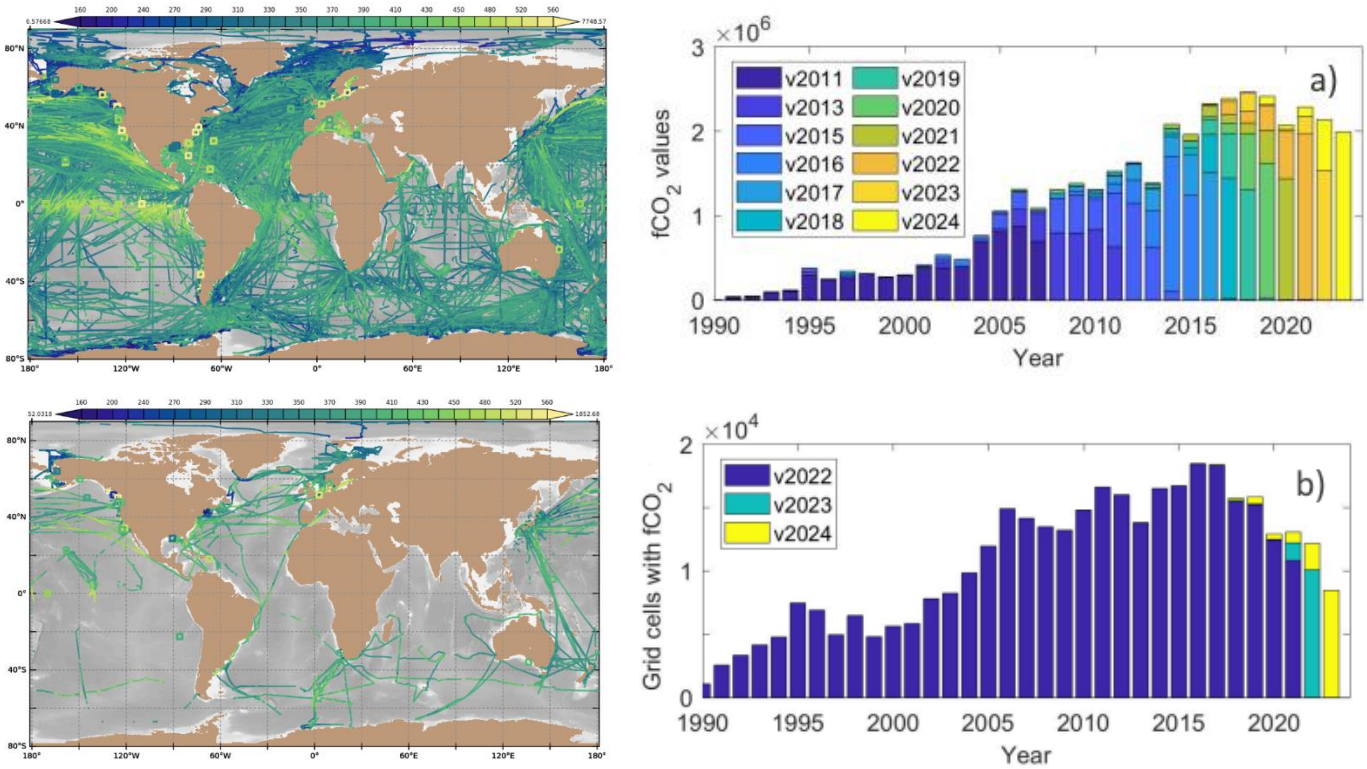


Figure 1: Geographical distribution of fCO_2 observations in the full SOCAT dataset (top left), and the new data submitted for v2024 (bottom left). From SOCAT Live Access Server. Time series of the number of fCO_2 observations in SOCAT with an estimated accuracy below 5 μatm, by version (top right) and number of monthly 1x1 degree cells with fCO_2 observations (bottom right). From SOCATv2024 release poster (Bakker et al. 2024).

2. Temperature (TEMP) and Salinity (PSAL) from dataset 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.

The world maps show (Figure 2) the distribution of stations in black marker; red markers show the stations with valid variable values. 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 with variable frequency. Not shown, the geographical distribution of samples has not changed significantly since v2 (2018).

The depth histograms show: a) the total of possible cast x 500 m depth bin combinations (white), the distribution of actual samples in 500 m bins and the percentage over the total (blue), and 50-m-bin distributions (light purple). 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 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.

The estimated accuracy of salinity is better than 0.002. Temperature is assumed to be of good quality and the instrument to be properly calibrated.

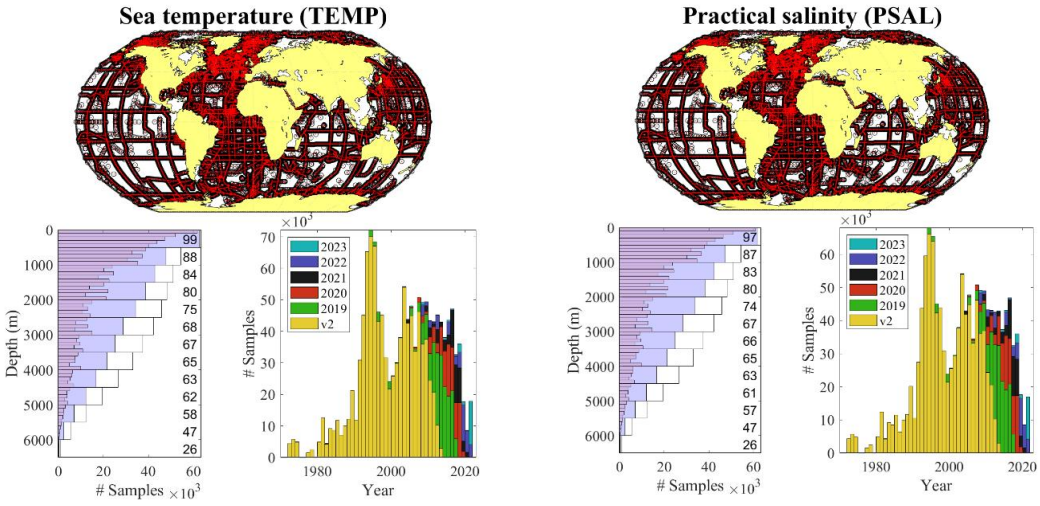
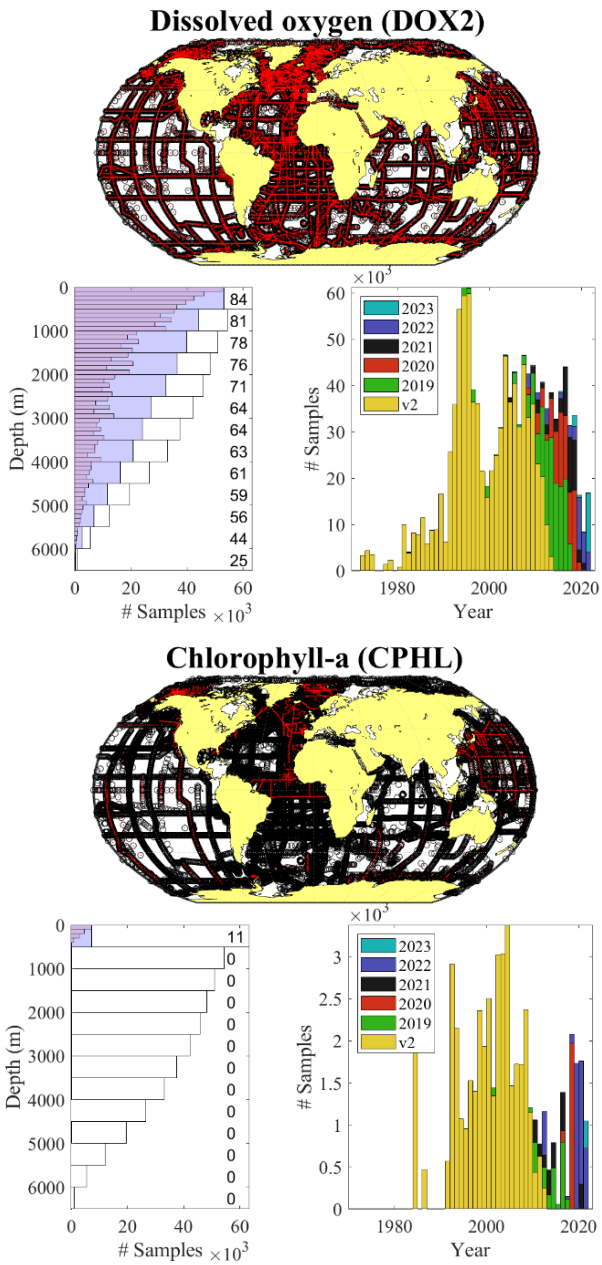


Figure 2: Global geographic, vertical and temporal distribution of sea temperature (left) and practical salinity (right) for v2 and from 2019 to 2023.

3. Oxygen (DOX2) and Chlorophyll-a (CPHL) from dataset GLODAP



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; in comparison the surface layers are less sampled, but the coverage is very similar in the deeper ocean (Figure 3, top).

Chlorophyll-a from bottle samples (Figure 3, bottom), 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.

The estimated accuracy of oxygen in GLODAP is of 0.6%. The data on chlorophyll-a has not been bias corrected and its accuracy cannot be ascertained.

Figure 3: Global geographic, vertical and temporal distribution of dissolved Oxygne (top) and Chlorophyll-a (bottom) for v2 and from 2019 to 2023.

4. Nutrients - Nitrate/Nitrite (NTAW/NTIW), Phosphate (PHOW) & Silicate (SLCW) from dataset GLODAP

The data coverage of the principal nutrients (nitrate, phosphate and silicate) is slightly less comprehensive but follows closely that of the total GLODAP observations. 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

The estimated accuracy of nitrate, phosphate and silicate is of 0.8, 1.0, 1.0% respectively.

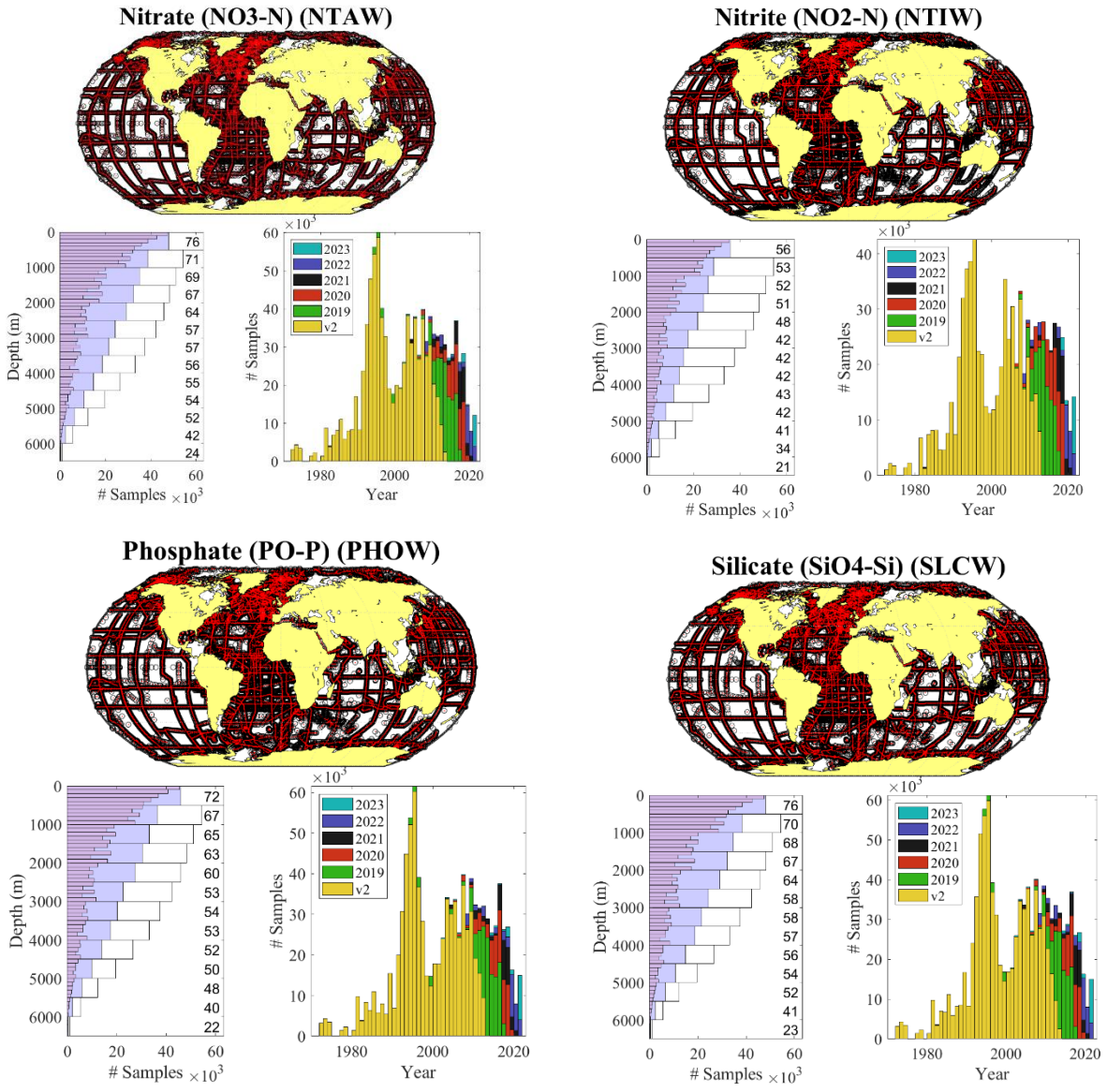
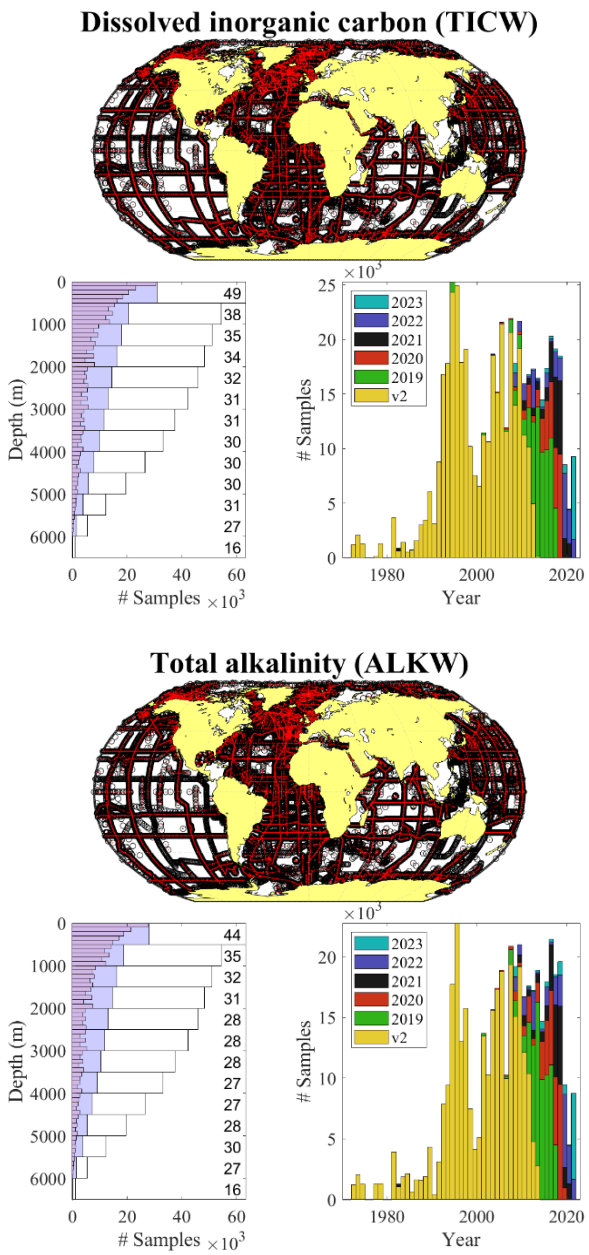


Figure 4: Global geographic, vertical and temporal distribution of Nitrate (top left) and Nitrite (top right), Phosphate (bottom left), Sillicate (bottom right) for v2 and from 2019 to 2023.

5. Dissolved Inorganic Carbon (TICW) & Total Alkalinity (ALKW) from dataset GLODAP



Similarly to nutrients and oxygen, these two variables were sampled less often than temperature and salinity; however the spatial and temporal distribution (Figure 5) follows the general sampling distribution of GLODAP, too. The main spatial gaps are around Australia and the Indonesian archipelago, and a transect in the tropical Pacific.

The estimated accuracy of Dissolved Inorganic Carbon is or 2.8 μmol kg^{-1}, while for alkalinity the estimated accuracy is of 2.3 μmol kg^{-1}.

Figure 5: Global geographic, vertical and temporal distribution of Dissolved inorgnaic Carbon (top) and Total Alkalinity (bottom) for v2 and from 2019 to 2023.

6. pH and pH at 25°C, 0 dbar (PHPH/PH25) from dataset GLODAP

These two variables have the same distribution (Figure 6) since pH at 25°C, 0 dbar is calculated from *in situ* pH. Both variables 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.

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 is relatively homogeneous, at around 20% of the potential observations, slightly more frequent in the surface layer, and less in the deepest ones.

The estimated accuracy for pH is 0.0082 units in the total scale.

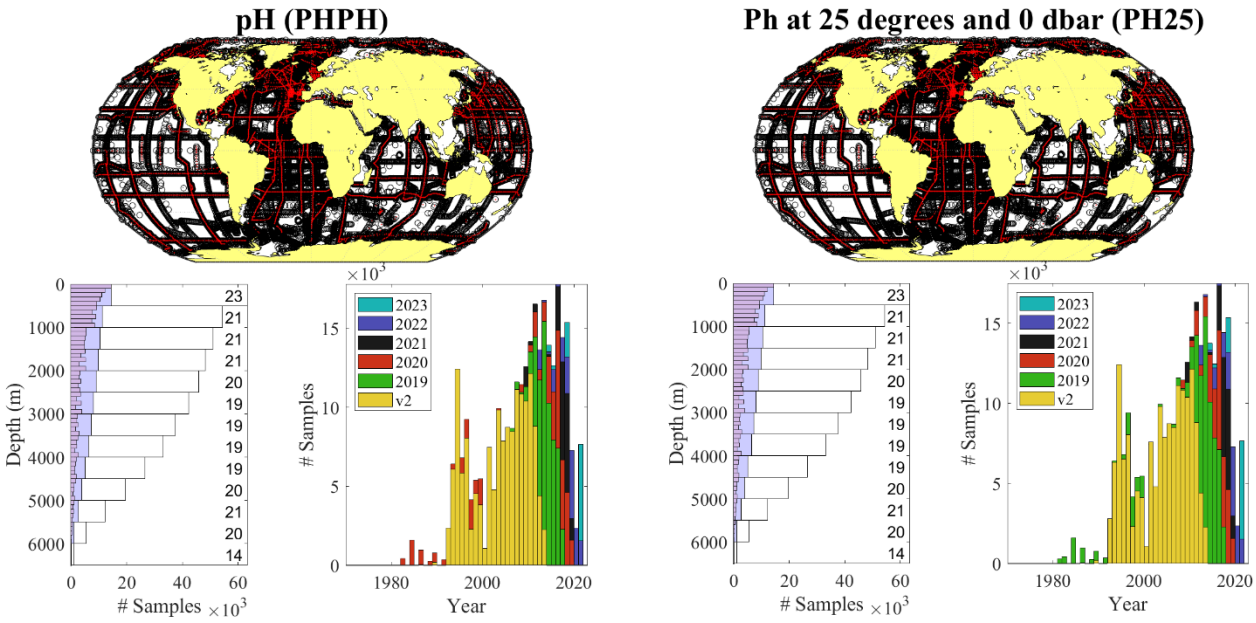
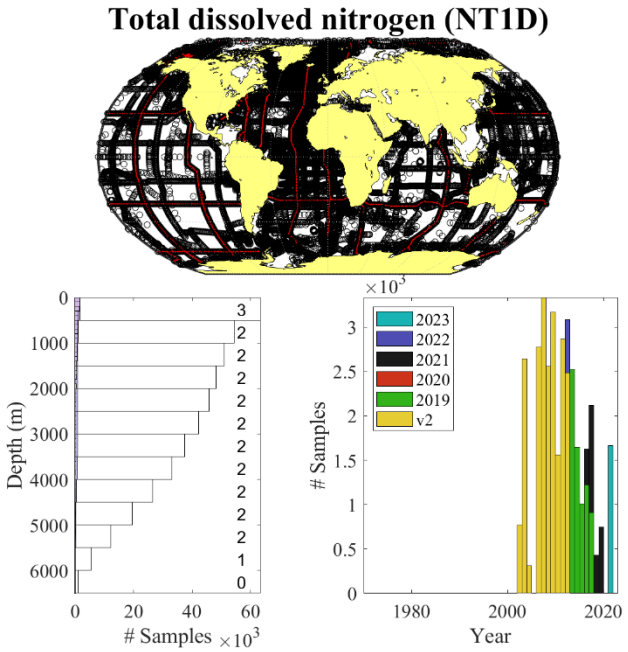


Figure 6: Global geographic, vertical and temporal distribution of Dissolved inorgnaic Carbon (top) and Total Alkalinity (bottom) for v2 and from 2019 to 2023.

7. Total Dissolved Nitrogen (NT1D), Dissolved Organic Nitrogen (NODW) & Dissolved Organic Carbon (CORG) from dataset GLODAP



These variables are the least sampled of the GLODAP dataset (Figure 7).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. Both variables in v2.2023 have a significant number of new observations for the last year of sampling (2022). 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. Similarly to Chlorophyll-a, these variables have not been bias corrected in GLODAP and their accuracy cannot be ascertained.

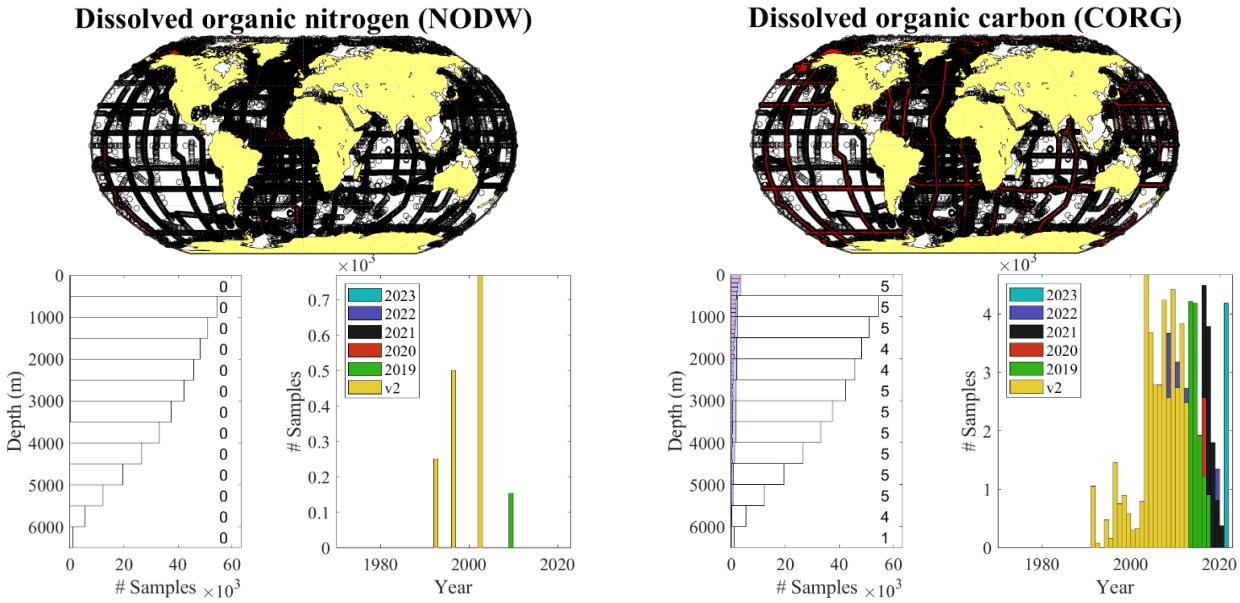


Figure 7: Global geographic, vertical and temporal distribution of Total Dissolved Nitrogen (top), Dissolved Organic Nitrogen (bottom left) and Dissolved Organic Carbon (bottom right) for v2 and from 2019 to 2023.

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