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Synthesis of data products for ocean carbonate chemistry

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Abstract. As the largest active carbon reservoir on Earth, the ocean is a cornerstone of the global carbon cycle, playing a pivotal role in modulating ocean health and regulating climate. Understanding these crucial roles requires access to a broad array of data products documenting the changing chemistry of the global ocean as a vast and interconnected system. This review article provides a comprehensive overview of 60 existing ocean carbonate chemistry data products, encompassing compilations of cruise datasets, derived gap-filled data products, model simulations, and compilations thereof. It is intended to help researchers identify and access data products that best align with their research objectives, thereby advancing our understanding of the ocean's evolving carbonate chemistry.

https://doi.org/10.5194/essd-2025-255
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1 Introduction

Since the onset of the Industrial Revolution in 1750, human activities, such as the burning of fossil fuels, cement production, and land-use change, have emitted ~2600 Gt carbon dioxide (CO_2) into the atmosphere, causing the atmospheric CO_2 levels to increase by ~50% (DeVries, 2022; Friedlingstein et al., 2025; Tans and Keeling, 2025). The global carbon cycle, encompassing the exchange of CO_2 among the atmosphere, oceans, terrestrial ecosystems, and geosphere, plays a critical role in regulating atmospheric CO_2 levels (Archer, 2010; DeVries, 2022; Holzer and DeVries, 2022). As the largest dynamic CO_2 reservoir, the ocean holds approximately 45 times the amount of carbon found in the atmosphere currently and actively exchanges it with the air above and sediments below. On timescales from decades to millennia, the ocean imposes a dominant control over atmospheric CO_2 levels (Revelle and Suess, 1957; Broecker, 1982; Archer et al., 2009; DeVries, 2022).

The ocean currently absorbs about a quarter of human-caused CO_2 emissions (Sabine et al., 2004; Gruber et al., 2019a; Carroll et al., 2022; Crisp et al., 2022; Terhaar et al., 2022a; Gruber et al., 2023; DeVries et al., 2023; Müller et al., 2023; Schimel and Carroll, 2024). The chemistry of the ocean has been shifting as a result of atmospheric CO_2 uptake (Feely et al., 2023; Ma et al., 2023; Müller et al., 2023; Fassbender et al., 2023; Keppler et al., 2023; Jiang et al., 2023; Müller and Gruber, 2024). Since the beginning of the Industrial Revolution, the dissolved inorganic carbon (DIC) content in the surface ocean has risen from 1690 to 1730 Gt of Carbon, and in the subsurface ocean from 35,400 to 35,560 Gt C (Sabine et al., 2004; Müller et al, 2023). This seemingly small increase of 0.5% belies a significant depletion of the oceans' buffer capacity (DeVries, 2022).

As CO_2 enters seawater, a portion of it reacts with water to form carbonic acid. This is the first in a series of rapid acid-base reactions that release protons and decrease the availability of carbonate ions, which are building materials that many marine organisms, such as mollusks, crustaceans, and corals, use to construct their shells and skeletons (Gattuso and Hansson, 2011). This process, termed as "ocean acidification (OA)", has already decreased surface ocean pH by roughly 0.11 (~30% increase in acidity) since 1750 (Orr et al., 2005; Jiang et al., 2019; Kwiatkowski et al., 2020; Jiang et al., 2023; IPCC, 2023). In the subsurface ocean, the trends of some acidification parameters, e.g., pH and hydrogen ion content ($[H^+]$), can be even greater due to the increasing sensitivity of $[H^+]$ to changes in DIC with depth (Chen et al., 2017; Fassbender et al., 2023; Müller and Gruber, 2024). This ongoing acidification threatens critical ocean ecosystem services, including food security, fisheries, aquaculture, and the broader Blue Economy, for billions of people globally (Cooley and Doney, 2009; Doney et al., 2020).

In some parts of the ocean, OA is driven not only by the uptake of carbon but also by other processes (Delaigue et al., 2024), for example via alkalinity changes driven by freshening of the Arctic Ocean (Terhaar et al., 2021a) or changes in the carbon and alkalinity export from Arctic rivers (Terhaar et al., 2019; Qi et al., 2022; Bertin et al. 2023). Local anthropogenic inputs through rivers or from air pollution also lead to OA (e.g. Sarma et al, 2015; Sridvi and Sarma, 2021). In addition, coastal eutrophication and hypoxia could cause enhanced OA in oxygen-depleted bottom water due to weakened seawater buffer capacity by biologically induced CO_2 (Cai et al. 2011). If anthropogenic CO_2 emissions continue without mitigation, as per the shared socioeconomic pathway (SSP5-8.5)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

scenario, surface ocean pH could decrease by a further 0.3 to 0.4 by 2100, equivalent to a 100–150% increase in acidity (Kwiatkowski et al., 2020; Jiang et al., 2023). If society, however, succeeds at reducing emissions, the future acidity level becomes highly uncertain as it sensitively depends on the transient response of the Earth system and the amount of reductions of non-CO_2 radiative agents (Terhaar et al., 2023).

In summary, monitoring ocean carbonate chemistry is essential for (a) tracking the evolving ocean carbon sink, and (b) understanding ocean acidification and its ecological impacts. Additionally, monitoring ocean carbonate chemistry is crucial when considering marine carbon dioxide removal (mCDR) strategies such as ocean alkalinity enhancement (OAE), artificial upwelling, ocean fertilization and electrochemical ocean CO_2 removal (Kheshgi, 1995; Bach et al., 2019; Schimel and Carroll, 2024; Oschlies et al., 2025). The ocean's vast and interconnected nature necessitates that data from individual oceanographic cruises be meticulously preserved, subject to rigorous quality control, and uniformly formatted to promote their usability (Brett et al., 2020; Schoderer et al., 2024). Following the methodology established by Lange et al. (2023), we have curated an exhaustive catalogue of synthesis products pertaining to ocean carbonate chemistry, including cruise data compilations, gridded gap-filled data products, and other derived data products. This compilation spans both global and regional scales, providing a holistic view of the current state of ocean biogeochemistry data aggregation.

2 Methods

In this paper, data products are defined as outputs that aggregate, quality-control, and transform individual datasets from multiple sources into a unified, structured format to support research, decision-making, or operational needs for specific end users. The data products included in this study were identified through a literature review and discussions with researchers via the Ocean Acidification Information Exchange.

3 Results and Discussion

3.1 Data products for ocean carbonate chemistry

The aim of establishing this catalog of ocean carbonate chemistry data synthesis products is to enhance user access and raise awareness of available resources. The list will be regularly updated to include the latest data synthesis products. Contributors are encouraged to submit new data products through the Ocean Acidification Information Exchange (OAIE) interface: https://www.oainfoexchange.org/members/updates/71585. If preferred, submissions can also be directed via email to noaa.ocads@noaa.gov.

These products are organized based on end-user needs:

1. Cruise data compilations (no interpolation or extrapolation).
2. Time-series data products (no interpolation or extrapolation).
3. Derived gap-filled (interpolated) products for the surface ocean, starting with products offering a

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Preprint. Discussion started: 15 May 2025

climatological snapshot of the ocean, followed by those showing temporal changes.

4. Derived gap-filled (interpolated) products for the interior ocean, also starting with products offering a climatological snapshot of the ocean, followed by those showing temporal changes.
5. Multi-product analyses of 3 and 4. These compilations also include hindcast model simulations of the ocean carbon cycle and biogeochemistry.
6. Model and hybrid data products projecting ocean carbon variables into the future [Note: Here the term "model" refers to ocean biogeochemical models (Fennel et al., 2022). If a statistical model or machine learning model is used for gap filling, the product is not categorized as a model output product in this compilation.]

Each section includes numbered descriptions of each data product in that class, as well as a summary table of the data products with corresponding IDs so the user can easily jump to the associated product description. Although some data products, such as Surface Ocean CO_2 Atlas (SOCAT) and Lamont-Doherty Earth Observatory (LDEO) surface partial pressure of carbon dioxide ($p$$CO_2$) Database report only one ocean carbonate variable, i.e., fugacity of carbon dioxide ($f$$CO_2$), they provide a foundation from which additional variables can be derived using empirical algorithms. For instance, total alkalinity content (TA) can be estimated from salinity and temperature and other factors (Lee et al., 2006) and by neural network approaches such as those developed by Velo et al. (2013) and Broullón et al. (2019). Beyond TA, neural network algorithms have been extended to estimate dissolved inorganic carbon (DIC) as demonstrated by Broullón et al. (2020), and even the full marine carbonate system (MCS) through frameworks like CANYON-B/CONTENT (Bittig et al., 2018) and Empirical Seawater Property Estimation Routines (ESPERs) (Carter et al., 2021). While these methods primarily employ neural networks, both Velo et al. (2013) and Carter et al. (2021) provide alternative estimation approaches based on local interpolation, through their 3-dimensional moving window multilinear regression algorithm (3DwMLR) and locally interpolated regression (LIR) methods, respectively. Utilizing such derived data, the complete suite of ocean carbonate parameters can then be calculated using computer software, such as CO2SYS (Lewis and Wallace, 1998; van Heuven et al., 2011; Orr et al., 2018; Sharp et al., 2023) or its Python implementation PyCO2SYS (Humphreys et al., 2022). An in-depth explanation of the methods employed for these calculations can be found in the Supplementary material of Jiang et al. (2022a).

3.1.1 Cruise data compilations (no interpolation or extrapolation):

The data compilations described in this section standardize datasets collected from individual research vessels, ships of opportunity (SOOP), and unmanned platforms, presenting them in a uniform format for easy access. These datasets typically undergo both primary QC (identifying outliers and obvious errors within an individual cruise dataset) and secondary QC (objectively comparing data from one cruise against another or a previously synthesized dataset to quantify systematic differences in reported values).

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

1) **SOCAT:** The Surface Ocean CO_2 Atlas (SOCAT) represents the most extensive collection of observational ocean CO_2 data for the global surface ocean (Bakker et al., 2016). It features fugacity of carbon dioxide (fCO_2) measurements from both the open ocean and the coastal ocean, predominantly sourced from research vessels, SOOP, and autonomous platforms including fixed moorings and autonomous surface vehicles (ASVs). Since 2013, SOCAT has been updated annually, and assigned dataset flags indicating uncertainty and completeness of metadata. SOCAT is also available as a gridded product. To access the latest version of the SOCAT data product (with 40 million data points), visit https://socat.info/.

2) **LDEO Surface pCO_2 Database:** Dr. Taro Takahashi [Lamont Doherty Earth Observatory (LDEO), Palisades, New York] started synthesizing global surface ocean CO_2 data in 1997, compiling three decades of observations (~250,000 measurements) to create inaugural monthly global surface pCO_2 maps (Takahashi et al., 1997; Takahashi et al., 2002). The most recent version (V2019) expanded this dataset to approximately 14.2 million surface water pCO_2 measurements spanning from 1957–2019. Distinct from the SOCAT database, the LDEO database reports pCO_2, instead of fCO_2, exclusively from equilibrator-CO_2 analyzer systems, with an average estimated uncertainty of ± 2.5 µatm. The database is also interpolated onto a global surface ocean 4° x 5° grid for a reference year 2000 (Takahashi et al., 2009) and 2010 (Fay et al. 2024). Access to the LDEO surface pCO_2 database (Version 2019) is provided by the Ocean Carbon and Acidification Data System (OCADS) with the DOI: "10.3334/CDIAC/otg.ndp088(v2015)", accessible at: https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0160492.html. Additionally, there is a dedicated webpage at OCADS for the LDEO Database: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/LDEO_Underway_Database/.

3) **GLODAPv2:** The Global Ocean Data Analysis Project Version 2 (GLODAPv2) aggregates biogeochemical data collected from discrete bottle samples, offering extensive global coverage from the surface to depths (Key et al., 2015; Olsen et al., 2016; Lauvset et al., 2024). While GLODAP is primarily a product for basin-scale repeat hydrography data, it also includes coastal datasets and observations from a few time-series. The GLODAPv2 data product provides rigorously quality-controlled measurements for 14 essential oceanographic variables: temperature, salinity, dissolved oxygen, nitrate, silicate, phosphate, dissolved inorganic carbon (DIC), total alkalinity (TA), pH, chlorofluorocarbons (CFC-11, CFC-12, CFC-113), carbon tetrachloride (CCl_4), and sulfur hexafluoride (SF_6). These variables, excluding temperature, undergo both primary and secondary quality control procedures to detect outliers and adjust for significant measurement biases. GLODAPv2 was first published in 2016 and has been updated annually through a living data process in Earth System Science Data since 2019. For these updates, new data (including historical data not previously included in the data product) are quality controlled and adjusted to the 2016 version (Olsen et al., 2019; Olsen et al., 2020; Lauvset et al., 2021; Lauvset et al., 2022; Lauvset et al., 2024). Since the global repeat hydrography programs operate with decadal repetitions, the aim is to produce a completely new version of GLODAP, where all cruise datasets will be reevaluated, every

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

decade. Release of the GLODAPv3 data product is planned for 2026. For more information on the secondary quality control process, refer to Tanhua et al. (2010) and Lauvset and Tanhua (2015). GLODAPv2 offers two kind of products: the collection of quality controlled data from discrete bottle samples taken at sampling location (Key et al., 2015; Olsen et al., 2016; Olsen et al., 2019; Olsen et al., 2020; Lauvset et al., 2021; Lauvset et al., 2022; Lauvset et al., 2024), and a gridded product, interpolated to a 1°x1° grid and the 33 standard depth levels of WOA (World Ocean Atlas) (Lauvset et al., 2016). All versions of the GLODAPv2 data product can be accessed at https://glodap.info/.

4) **JOA Suite:** The Java OceanAtlas (JOA) Suite offers both a user-friendly application and a library of ocean profile data curated by Jim Swift (Scripps Institution of Oceanography, La Jolla, California, USA). Similar to GLODAPv2, this data product serves as a comprehensive repository of quality-controlled discrete bottle based measurements (and limited CTD), spanning from the surface to the depths of the global ocean. Unlike GLODAPv2, no offset corrections were applied to the JOA data product. The JOA data product encompasses a range of oceanographic variables including temperature, salinity, dissolved oxygen, DIC, TA, silicate, phosphate, nitrate, nitrite, CFC-11, CFC-12, SF_6, and CTD parameters associated with the water sample data. To access the JOA application and data, visit: https://joa.ucsd.edu/. Currently, there is not a peer-reviewed paper or public-accessible report for this data product. Cite the data product itself as: “Swift, J. (2022), Java OceanAtlas Data, https://joa.ucsd.edu/Data_homepage”, or cite the entire JOA Suite as: “Swift, J. and Osborne, J. (2022), The Java OceanAtlas Suite, https://joa.ucsd.edu”.

5) **WOD:** In addition to the GLODAPv2 and JOA Suite, users can also access historical and recent original biogeochemical data collected from discrete bottle samples in a uniform format and units, along with their originator quality control (QC) flags, through the World Ocean Database (WOD) (Mishonov et al., 2024). Like the JOA Suite, these measured data remain unaltered. The WOD allows users to filter and subset data with specific variables, platforms, institutions, projects, regions, or time periods (Garcia et al., 2024). Users can visualize sampling locations on a “distribution plot” and access a cruise list for all selected data and variables. Users also have the option of exporting data in NetCDF or Comma-Separated Values (CSV) formats. Additionally, all data in the WOD are reproducible and traceable to their original sources archived at NOAA’s National Centers for Environmental Information (NCEI) for long-term preservation. The WOD is accessible at https://www.ncei.noaa.gov/products/world-ocean-database.

6) **SNAPO-CO_2:** Metzl et al. (2024) aggregated over 44,400 measurements of DIC and TA from a series of research cruises and ships of opportunity (SOOP) across various oceanic regions in 1993-2022, under the aegis of several French research programs, to create a product called “Service National d’Analyse des Paramètres Océaniques du CO_2 (SNAPO-CO_2)”. The majority of the samples were analyzed by the Service National d’Analyse des Paramètres Océaniques du CO_2 (SNAPO-CO_2) at the LOCEAN laboratory in Paris, France. Sampling was performed either from CTD-rosette casts (Niskin bottles) or collected from the ship’s flow-through system (intake at roughly 5m depth). DIC and TA determinations were conducted

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Preprint. Discussion started: 15 May 2025

Open Access Earth System Science Data Discussions

simultaneously through potentiometric titration in a closed-cell setup, calibrated with certified reference material to achieve an accuracy of ± 4 µmol kg^{-1} for both parameters, as per Edmond (1970). This methodology was also applied for real-time measurements during OISO cruises, with data from the South Indian Ocean for 1998–2018 included in this compilation. The data is split into two sets — one for the global ocean and coastal zones, and another for the Mediterranean Sea — both accessible in the same format: https://doi.org/10.17882/95414. Additionally, this data product is available at OCADS (DOI: "10.25921/ptyh-0y90"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0285681.html (Metzl et al., 2023)

7) **Arctic Ocean anthropogenic carbon estimates:** This dataset includes anthropogenic carbon estimates in the Arctic Ocean based on measurements of transient tracers, such as CFC-12 and SF_6 (Terhaar et al., 2020; Tanhua et al., 2009). Using the transient time distribution (TTD) method, anthropogenic carbon estimates were estimated at measurement locations across all basins of the Arctic Ocean between 1983 and 2005. In addition to these estimates, adjusted estimates of anthropogenic carbon at these locations are provided that account for differences in the saturation of transient tracers and anthropogenic carbon in Arctic Ocean surface waters that caused anthropogenic carbon estimates to be biased low (Terhaar et al., 2020). It is recommended to use the adjusted estimates. This dataset can be accessed at https://doi.org/10.17882/103920 (Terhaar et al., 2024).

8) **CODAP-NA:** Jiang et al. (2021) curated and synthesized two decades of discrete measurements of carbonate system variables, dissolved oxygen, and nutrient chemistry data from the North American continental shelves to generate the first version of Coastal Ocean Data Analysis Data Product in North America (CODAP-NA). The 2021 release encompasses 3,391 oceanographic profiles from 61 research cruises spanning the North American continental shelves from Alaska to Mexico in the west and from Canada to the Caribbean in the east. It includes 14 key variables, including temperature, salinity, DO, DIC, TA, pH, carbonate ion, fCO_2, silicate, phosphate, nitrate, all of which have undergone rigorous quality control. Note that certain datasets meeting the GLODAPv2 QC standards are also included in the GLODAPv2 since its 2022 release. CODAP-NA is available at OCADS (DOI: "10.25921/531n-c230"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0219960.html (Jiang et al., 2020).

9) **AZMP Carbon:** Gibb et al. (2023) compiled carbonate parameters data from the Canadian Atlantic Zone Monitoring Program (AZMP Carbon) since 2014. More than 100 seagoing missions are represented in this dataset. The sample strategy corresponds generally to full-depth water samples mostly collected along standardised hydrographic sections. The majority of these data were collected as part of the Atlantic Zone Monitoring Program (AZMP) of Fisheries and Oceans Canada (DFO). Implemented in 1998, the AZMP aims to characterize and understand the causes of oceanic variability at the seasonal, inter-annual and decadal scales in support of, among other things, fisheries management in the Atlantic Zone (including the Gulf of St. Lawrence, the Scotian shelf and the Newfoundland and Labrador shelf). Since 2014, a minimum

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

of two of the three following carbonate parameters, TA, DIC and pH, are also acquired by the program at standardised hydrographic stations across the zone (sampled up to three times a year). Each measurement is completed with corresponding temperature, salinity and, when available, nutrients and dissolved oxygen concentration data. This dataset also includes samples collected as part of ships of opportunity, fishing and other scientific trips. The entire dataset comprises 19,531 discrete samples [last updated 21 August 2024]. Among this number, 18,085 have at least two of the three carbonate system parameters (e.g., TA, DIC and pH), allowing the derivation of other parameters such as the saturation state relative to aragonite and calcite (Ω_{arg} and Ω_{cal}) and partial pressure of CO_2 (pCO_2, in µatm) using the CO2SYS program modified for Python (https://github.com/mvdh7/PyCO2SYS/tree/v1.2.1, last access: 8 January 2023; Humphreys et al., 2020). The full dataset of measured and derived parameters is available from the Federated Research Data Repository: https://doi.org/10.20383/102.0673 (Cyr et al., 2022) and is updated annually.

10) **MOCHA**: Kennedy et al. (2023) curated a comprehensive coastal ocean data product called "Multistressor Observations of Coastal Hypoxia and Acidification (MOCHA)", encompassing temperature, salinity, dissolved oxygen, ocean carbonate variables (TA, DIC, pH, pCO_2, fCO_2), nutrients, and chlorophyll measurements from the full water column along the U.S. west coast. The synthesis integrates observations from 71 different sources, including high-resolution autonomous sensors, synoptic oceanographic cruises, and shoreline samples. The MOCHA synthesis spans from the shoreline to well-beyond the continental shelf and incorporates observations from CODAP-NA, CalCOFI, and other large-scale oceanographic cruises to facilitate linking nearshore, high-resolution observations to broader oceanographic conditions. It boasts 15.9 million temperature readings, 5.0 million salinity measurements, 3.9 million dissolved oxygen records, and 2.3 million pH measurements, along with 8,368 dissolved inorganic carbon, 10,144 total alkalinity, and 505,000 pCO_2/fCO_2 measurements, with limited additional chlorophyll and nutrient observations. To reduce the computational load from high-resolution sensors, the synthesis is also available as a "daily aggregated" dataset, with all data sources averaged by day, location, and depth. All data in the MOCHA synthesis product has been quality controlled to a "plausible and reasonable" standard, but researchers requiring high-precision coastal data may need to apply additional QC tests. The data product is available at OCADS (DOI: "10.25921/2vve-fh39"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0277984.html, while the methods and product are described in Kennedy et al. (2024).

11) **ARIOS:** The Acidification in the Rias and the Iberian Continental Shelf (ARIOS) project involved compiling and analyzing the historical record of carbon system measurements and associated parameters conducted by the Instituto de Investigaciones Mariñas (IIM-CSIC) in Vigo, Spain. This dataset comprises 3,343 oceanographic stations and 17,653 discrete samples, combining measurements of pH, alkalinity, and other physical (pressure, temperature and salinity) and biogeochemical parameters (dissolved oxygen, nitrate, phosphate, and silicate) off the northwestern Iberian Peninsula from June 1976 to September 2018

(Padin et al., 2020). The oceanography cruises funded by 24 projects were primarily carried out in the Ría de Vigo coastal inlet, but also in an area ranging from the Bay of Biscay to the Portuguese coast. Robust seasonal cycles and long-term trends were calculated along a longitudinal section, gathering data from the coastal and oceanic zone of the Iberian upwelling system. The pH in the surface waters of these separated regions, which were highly variable due to intense photosynthesis and the remineralization of organic matter, showed an interannual acidification ranging from 0.0012 to 0.0039 yr^{-1} that increased towards the coastline and interior embayments. A synthesis paper is available at https://doi.org/10.5194/essd-12-2647-2020 (Padin et al., 2020), and the data product is available at https://doi.org/10.20350/digitalCSIC/12498 (Pérez et al., 2020).

12) **Marine inorganic carbon chemistry observations in the northern Gulf of Alaska:** Monacci et al. (2023) compiled a data product of discrete seawater samples collected each May and September over a 10-year period from 2008 to 2017 along the long-term hydrographic line in the Gulf of Alaska (GAK Line). Samples were collected from a sampling rosette on a profiling CTD. Data variables include profiled seawater temperature, salinity, and dissolved oxygen. Discrete sample variables include dissolved oxygen (i.e., Winkler titrations), macronutrients (nitrate, nitrite, phosphate, silicic acid), dissolved inorganic carbon (DIC), and total alkalinity (TA). The repeat hydrographic cruises were funded by the Alaska Ocean Observing System (AOOS), the Exxon Valdez Oil Spill Trustee Council (EVOS), Gulf Watch Alaska, and the North Pacific Research Board (NPRB) and were mostly conducted aboard the United States Fish and Wildlife Service (USFWS) R/V Tiĝlax̂. All carbonate parameters were analysed at the Ocean Acidification Research Center (OARC) at the University of Alaska Fairbanks (UAF). This data product is available at OCADS (DOI: 10.25921/x9sg-9b08): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0277034.html (Monacci et al., 2023), and the synthesis paper can be accessed at https://doi.org/10.5194/essd-16-647-2024 (Monacci et al., 2024).

13) **Coral Reef Carbonate Chemistry Off the Florida Keys:** Palacio-Castro et al. (2023) compiled discrete seawater samples from 38 permanent stations located along 10 inshore-offshore transects at the Florida Coral Reef. These samples were collected as part of NOAA's National Coral Reef Monitoring Program (NCRMP) and the South Florida Ecosystem Restoration Research (SFER) cruises. Sampling efforts commenced in 2010, with every two months collections initiated in 2015, resulting in a total of 47 sampling cruises and 1,538 discrete seawater samples. For all samples, a minimum of two of the carbonate equilibrium parameters (TA, DIC) were measured, in addition to salinity and temperature. The aragonite saturation state (Ω_{Ar}), partial pressure of CO_2 (pCO_2) and pH were derived from the measured parameters using the R package seacarb (Gattuso et al., 2021a). The time series analysis provides insight into the dynamic carbonate conditions spanning the inshore to offshore gradients, encompassing four distinct regions of the Florida Coral Reef: Biscayne Bay, the Upper Keys, Middle Keys, and Lower Keys. The findings underscore significant variability in the seasonality and interannual trends of surface carbonate

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Preprint. Discussion started: 15 May 2025

chemistry across different regions and reef zones. Data is available at NCEI (DOI: "10.25921/vfz0-dg77"): https://www.ncei.noaa.gov/access/metadata/landing-page/bin/iso?id=gov.noaa.nodc:NCRMP-CO3-Atlantic (Manzello et al., 2018).

14) **Salish cruise data package and multi-stressor data product:** Alin et al. (2021) compiled data from 35 individual cruise data sets that sampled marine waters of the southern Salish Sea and northern Washington coast (USA) during 2008–2018. These data sets were collected in support of research and monitoring efforts of the University of Washington Puget Sound Regional Synthesis Model (2008–2013), Washington Ocean Acidification Center (WOAC, 2014–present), NOAA Ocean Acidification Observing Network, Northwest Association of Networked Ocean Observing Systems, and NOAA Pacific Marine Environmental Laboratory. Ongoing seasonal sampling occurred during April, July, and September for Puget Sound cruises has occurred under WOAC support since 2014 and most frequently during May and October for Sound-to-Sea cruises, which sample from Puget Sound through the Strait of Juan de Fuca to the northern Washington coast. The Salish cruise data package contains observations from a total of 715 oceanographic profiles, with > 7490 sensor measurements of temperature, salinity, and oxygen; ≥ 6070 measurements of discrete oxygen and nutrient (nitrate, phosphate, silicate, ammonium, nitrite) samples; and ≥ 4462 measurements of inorganic carbon variables (DIC and TA). Alin et al. (2023) published a follow-on data product based on the Salish cruise data package, which only included the 3971 samples with complete information for temperature, salinity, oxygen, nutrients, DIC, and TA. To facilitate applications of this data product to understanding multi-stressor ocean conditions in Pacific Northwest marine waters by various end users, Alin et al. (2023) also included the most commonly used calculated carbonate system parameters in this data product (pH_{total}, fCO_2, pCO_2, Ω_{Ar}, Ω_{Ca}). The data package is available at OCADS (DOI: "10.25921/zgk5-ep63"): https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/SalishCruise_DataPackage.html. The multi-stressor data product is available at: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/SalishCruises_DataProduct.html. Two synthesis papers describing the data package and interpreting the data product can be found at: https://essd.copernicus.org/articles/16/837/2024/ (Alin et al. 2024a) and https://bg.copernicus.org/articles/21/1639/2024/ (Alin et al. 2024b).

Table 1. Ocean carbonate chemistry data products out of cruise data compilations (no gridding or gap filling).

No.	Name	Open or coastal ocean	Surface or water column	Discrete bottle or continuous	Highlights	Reference
1	SOCAT	Open + Coastal	Surface	Continuous	The largest collection of surface ocean carbon observations	Bakker et al. (2016)
2	LDEO Surface pCO_2 Database	Open + Coastal	Surface	Continuous	The LDEO database reports pCO_2 exclusively from equilibrator-CO_2 analyzer systems	Takahashi et al. 2017

3	GLODAPv2	Open ocean	Water column	Discrete bottle	Adjustments are applied by comparing data in the deep ocean (>2000 m) using a crossover and inversion method as described by Johnson et al (2001).	Lauvset et al. (2024)
4	JOA Suite	Open ocean	Water column	Discrete bottle	Similar to GLODAPv2, with no adjustments	Swift (2022)
5	WOD	Open ocean	Water column	Discrete bottle	Similar to GLODAPv2, with no adjustments	Mishonov et al. (2024)
6	SNAPO-CO_2	Open + Coastal	Water column	Discrete bottle and semi-continuous	A compilation of cruises from multiple French initiatives	Metzl et al. (2024)
7	Arctic Ocean anthropogenic carbon estimates	Open ocean	water column	Discrete bottle (normalized to year 2005)	Observation-based estimates of anthropogenic carbon in the Arctic Ocean	Tanhua et al. (2009); Terhaar et al. (2020)
8	CODAP-NA	Coastal ocean	Water column	Discrete bottle	Similar to GLODAPv2, but for the coastal ocean	Jiang et al. (2021)
9	AZMP Carbon	Continental Shelf and slope	Water column	Discrete bottle	A compilation of cruises from the Atlantic Zone Monitoring Program (AZMP) since 2014	Gibb et al. (2023)
10	MOCHA	Coastal ocean	Water column	Discrete bottle + Continuous	U.S. West Coast	Kennedy et al. (2024)
11	ARIOS	Coastal ocean	Water column	Discrete bottle	An OA Database for the Galician Upwelling Ecosystem off the NW Iberian Peninsula from 1976 to 2018	Padin et al., (2020)
12	Marine inorganic carbon chemistry observations in the northern Gulf of Alaska	Coastal ocean	Water column	Discrete bottle	A synthesis of twenty cruises from 2008 to 2017 on the Gulf of Alaska (GAK) Line	Monacci et al. (2023)
13	Coral Reef Carbonate Chemistry Off the Florida Keys	Coastal / regional	Water column	Discrete bottle	Temporal trends of DIC, TA, pCO_2, pH, Ω_{arag}, in different areas of the Florida Keys	Palacio-Castro et al. (2023)
14	Salish cruise data package and multi-stressor data product	Coastal / estuarine	Water column	Discrete bottle	A data compilation and multi-stressor (ocean acidification, hypoxia, temperature) data product based on cruises from 2002 to 2018 in the southern Salish Sea and Washington coast	Alin et al. (2021, 2023)

3.1.2 Time-series data products (no interpolation or extrapolation):

The time-series data products described in this section include observations collected at regular time intervals, over a sustained period, and at fixed locations. The data often represent changes in a particular oceanographic variable over time, such as temperature, salinity, TA and DIC. The list below includes both climate-quality time-series data products compiled at selected stations, and data products compiling time-series measurements at multiple locations. Additionally, some hydrographic sections are measured regularly enough to warrant being called a time series, e.g., Line P (Freeland, 2007), sections in the northwest Pacific (Ishii et al., 2011a), the OVIDE lines (Mercier et al., 2024). Measurements from these sections are typically included in cruise data compilations (3.1.1) and are not listed separately here.

15) **BATS**: The Bermuda Atlantic Time-series Study (BATS) observations and data products extend to forty years of observations of DIC and TA and ocean acidification indicators, and constitute the longest continuous record of warming, salinification, ocean deoxygenation, and ocean acidification in the open ocean (Bates and Johnson, 2023). The sustained observations at the BATS site began in October 1988, approximately 80 km to the south-east of Bermuda (https://bios.asu.edu/bats). The program comprises monthly cruises with CTD, water-column biogeochemical sampling and rate measurements (e.g., primary and export production) plus additional cruises in the spring period and annual transects between the Gulf Stream and Puerto Rico. CO_2-carbonate chemistry sampling includes full-depth bottle DIC and alkalinity data (including additional surface measurements going back to 1983 collected at the Hydrostation S site). Hydrostation S is located ~25 km south-east of Bermuda (https://bios.asu.edu/research/projects/hydrostation-s) and began in 1954 with biweekly cruises each year. Underway fCO$_2$ /pCO$_2$ data collected from the R/V *Atlantic Explorer* that supports the BATS and Hydrostation S sites constitutes part of the annual data submission to SOCAT. The BATS project page at the Biological and Chemical Oceanography Data Management Office (BCO-DMO) includes metadata and data streams (https://demo.bco-dmo.org/project/2124). Hydrostation S data and DOIs are also available at BCO-DMO (https://www.bco-dmo.org/project/859583).

16) **HOT:** The Hawaii Ocean Time-series (HOT) CO_2 measurement program documents 35+ years of inorganic carbon dynamics in the open waters of the central North Pacific. Since October 1988, full ocean depth profiles of DIC and TA have been analyzed, and direct measurements of pH have been made over most of this longest-running Pacific Ocean time-series study. The overall scientific mission of HOT has been to sustain observations of the variability of hydrological and ecological properties, elemental cycling, heat fluxes, and circulation of the North Pacific Subtropical Gyre (NPSG). The program is based on shipboard observations and experiments conducted on ~10 expeditions per annum to Station ALOHA (22.75°N, 158°W). HOT program background information and details of sampling strategy may be found in Karl and Lukas (1996) and Karl et al. (2001). Results from the HOT CO_2 measurement program may be found in Winn et al. (1994, 1998), Dore et al. (2003, 2009, 2014), and Knor et al. (2023). The HOT project page, metadata, data streams and data identifiers are listed at https://www.bco-dmo.org/project/2101. A surface ocean data product that includes CO2SYS-calculated values of pCO$_2$, carbonate mineral saturation states and other derived quantities may be found at https://hahana.soest.hawaii.edu/hot/hotco2/hotco2.html and https://doi.org/10.5281/zenodo.15060930. A MAPCO$_2$ system on the Woods Hole Oceanographic Institution Hawaii Ocean Time-series Site mooring (WHOTS; https://www.soest.hawaii.edu/whots/) has provided a near-continuous record of surface pCO$_2$ since 2004, and is anchored by the longer high-accuracy

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Preprint. Discussion started: 15 May 2025

HOT ship-based program (see Sutton et al. 2019 and Knor et al. 2023). These synergistic measurements have contributed to global ocean carbon observation networks (e.g., the newly released SOCATv22), which have improved our ability to characterize natural and anthropogenic drivers of ocean carbon uptake and acidification.

17) **ESTOC:** The European Station for Time Series in the Ocean (ESTOC) began carbon dioxide monitoring in October 1995, providing a 30-year record on total alkalinity (TA), pH, and dissolved inorganic carbon (DIC). This dataset represents the longest continuous monthly record of warming, rising carbon dioxide levels, and acidification in the eastern North Atlantic (González-Dávila and Santana-Casiano, 2023). ESTOC is located 100 km north of the Canary Islands archipelago (https://plocan.eu/en/installations/ocean-observatory). The program includes a ship-based observation system, measuring physical, chemical, and biological parameters throughout the 3,670-meter water column. It also features a moored platform for surface meteorological and oceanic observations as well as subsurface measurements, maintained by the Canary Island Oceanic Platform (PLOCAN, https://plocan.eu/en) and the University of Las Palmas de Gran Canaria (https://iocag.ulpgc.es/research/research-units/quima). Carbon dioxide system measurements include full-depth bottle sampling for photometric pH, total alkalinity, and DIC, conducted monthly from 1995 to 2008, every two months until 2018, and semiannually in recent years due to limited ship time, timed to coincide with moored structure maintenance. ESTOC is also visited every two weeks by a volunteer observing ship, ES-SOOP-CanOA (https://meta.icos-cp.eu/resources/stations/OS_687B), part of the European Research Infrastructure ICOS (https://www.icos-cp.eu/observations/ocean/stations), which provides real-time surface data on carbon dioxide fluxes and ocean acidification. The program also includes the CO_2-ESTOC oceanographic buoy (https://meta.icos-cp.eu/labeling/). The full dataset with DOIs is accessible on Pangaea (González-Dávila and Santana-Casiano, 2023).

18) **Point B Time-series:** The Point B time series documents the carbonate chemistry at a coastal site of the Bay of Villefranche (43.686200N 7.314800E) in Villefranche-sur-mer, France, northwestern Mediterranean Sea. Since January 2007, seawater is sampled weekly at 1 and 50 m, and analyzed for total dissolved inorganic carbon and total alkalinity (Kapsenberg et al., 2017). Salinity and temperature are extracted from CTD profiles. Parameters of the carbonate system such as pH (total hydrogen ion scale) are calculated using the R package seacarb. Data are available at Pangaea: https://doi.org/10.1594/PANGAEA.727120 (Gattuso et al., 2021b).

19) **Ny-Ålesund Time-series:** The Ny-Ålesund time series documents the carbonate chemistry at a coastal site of Kongsfjorden, Spitsbergen (78.930660N 11.920030E) during the period 2015-2021. It is the first high-frequency (1 hour), multi-year (6 years) dataset of salinity, temperature, dissolved inorganic carbon, total alkalinity, pCO$_2$, and pH in the High-Arctic Ocean (Gattuso et al., 2023a). Data are available at Pangaea: https://doi.org//10.1594/PANGAEA.957028 (Gattuso et al., 2023b).

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

20) **SPOTS:** The Synthesis Product for Ocean Time-Series (SPOTS) is a ship-based biogeochemical pilot, aiming at regularly providing high quality data from fixed time-series stations with consistent format and semantics (Lange et al., 2024a). The pilot includes data from 12 fixed ship-based time-series programs with a focus on the Global Ocean Observing System's biogeochemical essential ocean variables. These stations represent unique marine environments across a variety of spatiotemporal resolutions and ranges, with data from 1983 to 2021. While implementing the FAIR Principles (Wilkinson et al., 2016) and open data, Lange et al. also improved the metadata of the time-series stations to interoperate with the IOC-UNESCO Ocean Data and Information System (ODIS). Additionally, an extensive quality assessment resulted in enhanced intra- and inter-station comparability. Altogether, SPOTS' pilot increased the readiness of biogeochemical time-series (Lange et al., 2023) and facilitates a variety of applications that benefit from the collective value of biogeochemical time-series observations. Data are available at https://www.bco-dmo.org/dataset/896862 with the DOI "10.26008/1912/bco-dmo.896862.2" (Lange et al., 2024b).

21) **Autonomous pCO$_2$ and pH time series from 40 surface buoys:** Sutton et al. (2019) established a living dataset comprising 40 individual autonomous moored surface ocean pCO$_2$ time series established between 2004 and 2013, 17 of them also include autonomous pH measurements. These time series characterize a wide range of surface-ocean carbonate conditions, across a variety of environments, including 17 oceanic and 13 coastal locations, as well as 10 coral reefs. The dataset serves as a significant resource for assessing the natural variability of surface ocean carbonate chemistry across diverse regions. Data are available at OCADS (DOI "10.7289/v5db8043"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0173932.html (Sutton et al., 2018). Additionally, there is a dedicated webpage at OCADS for this project: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/Moorings/ndp097.html.

Table 2. Time-series based ocean carbonate chemistry data synthesis products.

No.	Name	Open or coastal ocean	Surface or water column	Discrete bottle or autonomous	Highlights	Reference
15	BATS	Open	Top 4600 m	CTD profiles, discrete bottle data from hydrocast, rate measurements (primary, export and bacterial production), biomass and other biological measurements, underway measurements	One of the longest continuous record of warming, salinification, ocean deoxygenation, and ocean acidification in the open ocean	Bates and Johnson (2020, 2023)
16	HOT	Open	Top 4500 m	Discrete Bottle for shipboard measurements; sensor measurements on WHOTS mooring	35+ years of inorganic carbon dynamics in the open waters of the central North Pacific	Dore et al. (2009)

17	ESTOC	Open	Top 3570m	Discrete Bottle for shipboard measurements; sensor measurements on ESTOC mooring	The longest continuous monthly record of warming, rising carbon dioxide levels, and OA in the eastern North Atlantic	González-Davila and Santana-Casiano (2023)
18	Point B Time-series	Coastal	5 and 50 m	CTD profiles, discrete bottle data	Carbonate chemistry at a coastal site of the Bay of Villefranche, France	Kapsenberg et al. (2017)
19	Ny-Ålesund Time-series	Coastal	12 m	CTD, discrete bottle data, sensor measurements at the COSYNA/MOSES-AWIPEV underwater observatory	Carbonate chemistry at a coastal site of Kongsfjorden, Spitsbergen	Gattuso et al. (2023)
20	SPOTS	Open + Coastal	Water column	Discrete	The pilot includes biogeochemical data from 12 fixed ship-based time series programs	Lange et al. (2024a), Lange et al. (2024b)
21	Autonomous *p*CO_2 and pH time series from 40 surface buoys	Open + Coastal	Surface	Autonomous	Based on 40 moored surface *p*CO_2 time series, with 17 of them containing pH	Sutton et al. (2019)

3.1.3 Gridded and derived data products - Surface:

This section describes gridded data products that have been derived from observations through interpolation and gap-filling procedures, and depict the surface ocean. Note that this compilation focuses primarily on data products with global coverage, acknowledging that many regional gap-filled products became available in recent years and shall be include in future updates:

22) **Updated Takahashi delta *f*CO_2 and flux climatology:** Following on previous climatologies published by the late Taro Takahashi in 1997 and 2009, Fay et al. (2024) created a legacy climatology using his methodology and the updated SOCAT database of observations. This product provides 12 months of delta *f*CO_2values and corresponding fluxes for a base year of 2010 at 4° x 5° resolution subsequently subgridded to 1° x 1° resolution and near-global coverage. This climatology represents the mean of ocean conditions over the last four decades and is distinctive relative to many other mechanistic machine learning approaches in that it interpolates in time and space using only the available *f*CO_2 data and a surface water advection scheme rather than using proxy variables for gap filling. It uses the median of observations to determine a reference year of 2010 and fluxes are provided using air-sea partial pressure differences and inputs from the SeaFlux product (Fay et al., 2021). The climatology product is available at OCADS (DOI: "10.25921/295g-sn13"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0282251.html. The related manuscript is available at ESSD: https://doi.org/10.5194/essd-16-2123-2024 (Fay et al., 2024).

23) **MPI-ULB-SOM-FFN:** Landschützer et al. (2020a) created a uniform pCO$_2$ climatology combining open and coastal oceans. It is a monthly climatological gridded global surface ocean pCO$_2$ data product without adjusting for a specific reference year. Developed on a higher-resolution 0.25° × 0.25° global surface-ocean grid, this product is the result of combining two neural network-based pCO$_2$ products: the open ocean product described below (i.e., Landschützer et al. 2016) and the coastal product created by Laruelle et al (2017). Consequently, it represents coastal zones better. Data collected between 1998 and 2015 from the SOCAT database (Version 5) were used to create this data product. The merged climatology is available at OCADS (DOI: "10.25921/qb25-f418"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0209633.html. Additionally, there is a dedicated web page at OCADS for this project: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/MPI-ULB-SOM_FFN_clim.html.

24) **VLIZ-SOM-FFN:** Landschützer et al. (2016) employed the Self-Organizing Map-Feed-Forward Network (SOM-FFN) neural network method designed by Landschützer et al. (2013) to map the sea surface pCO$_2$ from the Surface Ocean CO$_2$ Atlas (SOCAT; see above No. 1) (Bakker et al., 2014) to generate monthly pCO$_2$ fields on a 1° x 1° global surface ocean grid, covering the period from 1982 to near present. It is based on the gridded pCO$_2$ measurements from SOCAT and is updated regularly. The creation of the pCO$_2$ fields involve a two-step neural network approach, which has been extensively detailed and validated in previous works by Landschützer et al. (2013, 2014, 2016). In the initial step, the global ocean is clustered into biogeochemical provinces, and subsequently, the non-linear relationship between CO$_2$ driver variables and gridded data from SOCAT (Bakker et al. 2016) is reconstructed. Air-sea CO$_2$ fluxes are also computed based on the air-sea pCO$_2$ difference, utilizing a bulk gas transfer formulation as described by Landschützer et al. (2013, 2014, 2016). The product is available at OCADS (DOI: "10.7289/v5z899n6"): https://www.ncei.noaa.gov/data/oceans/ ncei/ocads/metadata/0160558.html. Additionally, there is a dedicated page at OCADS for this project: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/SPCO2_1982_present_ETH_SOM_FFN.html.

25) **JMA-MLR:** Iida et al. (2021) developed a monthly data product for inorganic carbon variables on a 1° × 1° global surface ocean grid for the period 1993–2018. Variables include dissolved inorganic carbon (DIC), total alkalinity (TA), CO$_2$ partial pressure (pCO$_2$), sea-air CO$_2$ flux, pH, and aragonite saturation state (Ω_{arag}). They leveraged data products such as SOCAT.v2019 (Bakker et al., 2016) and GLODAPv2.2019 (Olsen et al., 2019), as well as satellite-based variables, including sea-surface dynamic height (SSDH), mixed layer depth (MLD), and chlorophyll-a. The product is updated annually using the latest SOCAT and GLODAPv2 data. The data product can be accessed at: https://www.data.jma.go.jp/kaiyou/english/co2_flux/co2_flux_data_en.html.

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

26) OceanSODA-ETHZ:

(a) OceanSODA-ETHZv1 is a monthly gridded global surface ocean data product for multiple ocean carbon variables, including dissolved inorganic carbon (DIC), total alkalinity (TA), partial pressure of carbon dioxide (pCO_2), pH on total scale, and saturation states of aragonite and calcite (Ω_{arag} and Ω_{calc}) (Gregor and Gruber, 2020; Gregor and Gruber, 2021; Gregor and Gruber, 2023; Ma et al., 2023). This dataset is structured on a 1°×1° global surface ocean grid with monthly resolution from 1982–2022, facilitating research on OA over seasonal to decadal scales. The OceanSODA-ETHZ data product was created by extrapolating in time and space the surface ocean observations of fCO_2 from SOCATv2022 (Bakker et al., 2016) and TA from GLODAPv2.2022 using the newly developed Geospatial Random Cluster Ensemble Regression (GRaCER) method (Gregor, 2021). TA and pCO_2 were then used to calculate the remaining parameters of the marine carbonate system with the PyCO2SYS software (Humphreys et al., 2022). Phosphate and silicate from the World Ocean Atlas (2018) product were used (Boyer et al., 2018; Garcia et al., 2018a). The OceanSODA-ETHZ data product is available at OCADS (DOI: "10.25921/m5wx-ja34"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/ metadata/0220059.html.

(b) OceanSODA-ETHZv2 is a surface fCO_2 product with a 0.25° × 0.25° spatial resolution and an 8-day temporal resolution, providing estimates starting from 1982 (Gregor et al., 2024a; Gregor et al., 2024b). The high-resolution outputs are suitable for investigating the shorter- and finer-scale dynamics of surface fCO_2. Despite sharing a name with its predecessor, OceanSODA-ETHZv2 does not provide TA estimates and employs a different methodology, as described in the following steps: 1) The atmospheric trend of CO_2 is removed by subtracting marine boundary layer CO_2 concentrations from SOCAT fCO_2 producing a new target Δ^*CO_2 to reduce the biases at the start and end of the time series. 2) An 8-day seasonal climatology of Δ^*CO_2 is estimated using Gradient Boosted Decision Trees (GBDT), which is later used as a predictor. 3) The non-seasonal thermal component is removed from Δ^*CO_2, resulting in a new target, $\Delta^*CO_2^{nonT}$. 4) The new target is estimated using a feed-forward neural network, with the GBDT as one of the forcing variables. 5) Steps 4 through to 1 are inverted to arrive at fCO_2. 6) Air-sea CO_2 fluxes are computed using ERA5 winds. Data are available at https://doi.org/10.5281/zenodo.11206365 and are updated annually.

27) LDEO-HPD fCO_2 product: The LDEO Hybrid Physics Data (LDEO-HPD) estimates the temporal evolution of surface ocean fCO_2 and air-sea CO_2 exchange, utilizing the strengths of observations and global ocean biogeochemical models (GOBMs) (Gloege et al., 2022). GOBMs are internally consistent, mechanistic representations of the ocean circulation and carbon cycle, and have long been the standard for making spatiotemporally resolved estimates of air-sea CO_2 fluxes. However, there is often a bias between the modelled fCO_2 and available surface ocean measurements (Fay and McKinley 2021). The LDEO-HPD approach trains an eXtreme Gradient Boosting (XGB) algorithm to learn a non-linear relationship between model-data fCO_2 mismatch and observed predictor variables: SST, SSS, chlorophyll concentration, mixed layer depth). The GOBM fCO_2 is then corrected with the predicted model-data misfit to estimate real-world fCO_2 for the observation period (Gloege et al. 2022). The results in reconstructed monthly surface ocean

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

fCO_2 and air-sea CO_2 fluxes on a 1° × 1° grid in the open ocean beginning in 1982. Additional information can be found at oceancarbon.ldeo.columbia.edu. The data product is available at: https://zenodo.org/records/4760205.

28) **LDEO HPD product with extended temporal coverage:** Building on the work of Gloege et al. (2022), the LDEO-HPD product as mentioned above (nr. 25) can be extended back in time to predict *f*CO_2 for all available model years. Bennington et al (2022a) find that the largest component of the GOBM corrections is climatological. The smaller corrections at other timescales suggest either that these are well captured by the GOBMs or the data are insufficient. The dominance of climatological corrections supports the extension of the LDEO-HPD *f*CO_2 product backwards in time. A climatology of model-observation misfits for the best-observed period (2000–present) is applied to the GOBMs for 1959–1981, while an inter-annually varying correction is used for 1982 onward. (Bennington et al 2022a). This results in reconstructed monthly surface ocean *f*CO_2 and air–sea CO_2 fluxes on a 1° × 1° grid covering the open ocean, beginning in 1959. Since 2022, the LDEO-HPD Back in Time product has been included in the annual release of the Global Carbon Budget. Additional information can be found at oceancarbon.ldeo.columbia.edu. The data product can be accessed via Zenodo at https://zenodo.org/records/13891722.

29) **LDEO *f*CO_2 - Residual Method:** A frequently used approach for estimating full-coverage *f*CO_2 is to train a machine learning algorithm on sparse in situ *f*CO_2 data and associated physical and biogeochemical observations. While these associated variables have well-known relationships to *f*CO_2, it is often unclear how they mechanistically drive fCO_2 around the world. The LDEO *f*CO_2-Residual method takes the basic approach and enhances connections between physical understanding and reconstructed *f*CO_2. The novel approach used here includes applying pre-processing to the *f*CO_2 data to remove the direct effect of temperature – a relationship well-documented in literature and lab experiments (Takahashi et al. 2002). This enhances the biogeochemical/physical component of *f*CO_2 in the target variable (now *f*CO_2-Residual) and reduces the complexity that the machine learning must disentangle. The resulting algorithm has physically understandable connections between input data and the output biogeochemical/physical component of *f*CO_2 (Bennington et al. 2022b). This results in reconstructed monthly surface ocean *f*CO_2 and air–sea CO_2 fluxes on a 1° × 1° grid covering the open ocean, beginning in 1982 and extended to the most recent year of available data. Additional information can be found at oceancarbon.ldeo.columbia.edu. The data product can be accessed via Zenodo at https://zenodo.org/records/13941548.

30) **CMEMS-LSCE surface ocean carbon data products**:
(a) **CMEMS-LSCEv1:** Monthly surface ocean *p*CO_2 and air–sea CO_2 fluxes on a 1° × 1° grid in both the open ocean and coastal seas from 1985–2019 were reconstructed by Chau et al., (2022). CMEMS-LSCE is short for Copernicus Marine Environment Monitoring Service - Laboratoire des Sciences du Climat et de l'Environnement. This product is generated from an ensemble-based reconstruction of *p*CO_2 maps trained

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

with gridded data from SOCATv2020 (Bakker et al., 2016). Sea-surface pCO_2 values (converted from the original fCO_2 values in SOCATv2020) were regressed against a set of predictors with non-linear functions, i.e., feed-forward neural network (FFNN) models. The predictors include: sea-surface height (SSH), SST, SSS, MLD, chlorophyll a (Chl-a), atmospheric CO_2 mole fraction (xCO_2), and geographical coordinates (longitudes and latitudes). This data product is accessible at: https://data.ipsl.fr/catalog/srv/eng/catalog.search#/metadata/a2f0891b-763a-49e9-af1b-78ed78b16982.

(b) **CMEMS-LSCEv2:** CMEMS-LSCEv2 corresponds to the latest version of the CMEMS-LSCE FFNN. It uses the same ensemble-based reconstruction method for pCO_2 maps as CMEMS-LSCEv1. Improvements include downscaling the spatial resolution to 0.25° × 0.25° and reproducing additional surface ocean carbonate system variables on a global grid from 1985 onwards (Chau et al., 2024a). The additional surface ocean carbonate system variables are: pCO_2, DIC, TA, pH, and saturation states with respect to aragonite (Ω_{ar}) and calcite (Ω_{ca}). Surface ocean pCO_2 is reconstructed based on an ensemble of neural network models mapping gridded observation-based data provided by SOCATv2022 (Bakker et al., 2016). Surface ocean TA is estimated with a multiple linear regression approach (Carter et al., 2016, 2017). The remaining carbonate variables are calculated from pCO_2 and TA using a MATLAB version of CO2SYS (Lewis and Wallace, 1998; Van Heuven et al., 2011). The CMEMS-LSCE product is updated yearly for surface ocean pCO_2, air-sea fluxes, and the carbonate system variables. Updates are phased with release of the SOCAT database. For surface ocean pCO_2 and air-sea fluxes the temporal coverage is extended to the present date with a latency of 1 month (Chau et al., 2024b). Both the multi-year reconstruction and the near-real time prediction can be accessed through the CMEMS portal: https://doi.org/10.48670/moi-00047.

31) CarboScope (Jena-MLS): The Jena Mixed-Layer Scheme (within the CarboScope family of data-based estimates of carbon-cycle variability) is based on observed sea surface pCO_2 from the Surface Ocean CO_2 Atlas (SOCAT; see above No. 1) (Bakker et al., 2014). It provides daily global fields of pCO_2 and sea-air CO_2 fluxes from 1957 to the year before present, on a resolution of 2.5×2 degrees. In the original method (Rödenbeck et al, 2013), a diagnostic model of the carbon balance in the ocean mixed layer is being fitted to the pCO_2 data, by adjusting the ocean-interior sources and sinks of carbon of the mixed layer. The multi-decadal trend is derived from the data-based Ocean Circulation Inverse Model (OCIM) estimate provided by DeVries et al. (2022). Since a later extension described in Rödenbeck et al. (2022), the variability in the ocean-interior sources and sinks is first regressed against variability in SST and wind speed. The regression step is followed by a correction step with explicit temporal variability, to also represent data variability not yet represented by the predictors of the regression. The CarboScope product is updated yearly. The results from current and previous releases can be downloaded from https://www.bgc-jena.mpg.de/CarboScope/.

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

32) **UOEx-Watson:** This product is an estimate of the atmosphere-ocean flux of CO_2 that takes into account near-surface temperature deviations (Watson et al., 2020). Most estimates use data on surface ocean pCO_2 without considering corrections due to temperature gradients within the uppermost few millimeters of the sea surface ("Skin temperature effects") or small effects due to changes in temperature that occur during sampling and measurement, especially when the measurement is from a commercial vessel rather than a research ship. This product takes these effects into account by recalculating pCO_2 from the SOCAT data base (v2019) using co-located satellite observations of skin temperature. The result is a substantial increase in the calculated net global uptake of CO_2. In other respects, the methodology for this data product follows the two-step neural network approach described by Landschützer et al. (2013, 2014). The gridded data set of sea surface fCO_2 adjusted to satellite-derived subskin surface temperature, is available at https://doi.org/10.1594/PANGAEA.905316. Ocean-atmosphere fluxes interpolated to monthly and 1° × 1° degree spatial resolution is available at OCADS (DOI: "10.25921/2dp5-xm29"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0301544.html.

33) **NIES-ML3:** The National Institute for Environmental Studies (NIES-ML3) product includes monthly global surface ocean fCO_2 in 1982-2023 on a 1° × 1° grid. Using a leave-one-year-out (LOYO) validation method and three machine learning models, Zeng et al. (2022) found that the time variant trends of ocean CO_2 could be estimated approximately by a harmonic function fitting of the annual atmospheric CO_2. They removed the estimated trends from the ocean CO_2 and applied the LOYO to the trend-removed data to obtain the trend that could not be approximated by the fitting for trend correction. The trend-removed data by the corrected trends were used to train the models. The gap-filled CO_2 maps were constructed by adding the trends to model predictions. The product is available at NIES: https://doi.org/10.17595/20220311.001 (Zeng 2022).

34) **CSIR-ML6:** Provides monthly 1° × 1° estimates of surface pCO_2 (Gregor et al., 2019a). The approach uses the conceptual two-step approach of clustering and performing regressions for each cluster as Landschützer et al. (2016). CSIR-ML6 investigates the efficacy of various machine learning (ML) methods in estimating surface pCO_2, namely, feed-forward neural networks (FFNN), extremely randomized trees (ERT), gradient boosting machines (GBM), and support vector regression (SVR). It is found that the ensemble of all but the ERT method resulted in the best estimate, highlighting the fact that various ML methods do not produce the same outcome, particularly when data is sparse. Further, the variance between ensemble members can inform us about regions where uncertainty may be large due to methodological differences. Despite this, all methods achieve roughly the same uncertainty – a barrier, or wall beyond which the community has yet to overcome. The data are available at OCADS (DOI: "10.25921/z682-mn47"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0206205.html. The product is one of the six ensemble members of the SeaFlux dataset.

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

35) **AOML-ET:** Wanninkhof et al. (2024, 2025) developed a monthly global ocean data product of seawater pCO_2 and sea-air CO_2 fluxes, referred to as AOML-ET, using an extremely randomized trees (ET) machine learning technique. These maps are created on 1° × 1° spatial grids, providing global surface ocean coverages from 1998 to 2023. AOML-ET incorporates several predictor variables, including time, location, SST, SSS, MLD, and chlorophyll-a. The model was trained using the v2020 and v2023 releases of the SOCAT data product (No. 1). Sea-air CO_2 fluxes were calculated using the air-sea CO_2 partial pressure difference (ΔpCO_2) and a bulk gas transfer formulation incorporating windspeed. The dataset contains monthly 1° × 1° NetCDF files of the AOML-ET outputs, along with the predictor variables. The data are available at OCADS (DOI: "10.25921/0s8y-q287"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0298989.html.

36) **ULB-SOM-FFN-coastalv2.1:** Roobaert et al. (2024) present high-resolution (0.25° × 0.25° grid) monthly maps showing the distribution of sea surface pCO_2 across the global coastal oceans, spanning from 1982 to 2020. This product (ULB-SOM-FFN-coastalv2.1) builds upon the work by Laruelle et al. (2017), incorporating a two-step methodology that utilizes Self Organizing Maps (SOM) and Feed Forward Networks (FFN). This updated product now captures temporal variability, enabling the assessment of interannual variability and long-term trends in coastal air-sea CO_2 exchange, unlike the product by Laruelle et al. (2017), which only offers a climatology for a short period (1998-2015). The enhancements include additional environmental predictors and an expanded dataset for training and validation, featuring approximately 18 million direct coastal observations from the Surface Ocean CO_2 Atlas (SOCAT) database, specifically the SOCATv2022 release (Bakker et al., 2016). The product is available at OCADS (DOI: "10.25921/4sde-p068"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0279118.html (Roobaert et al., 2023).

37) **RFR-LME:** Sharp et al. (2024b) developed a data product delineating the temporal trends of OA indicators mapped on a 0.25 °× 0.25° spatial grid, across eleven U.S. Large Marine Ecosystems (LMEs), with monthly coverage from 1998–2023. These indicators, which include the pCO_2, pH, Ω_{arag}, DIC, TA, Revelle Factors, among others, were derived from SOCATv2023, along with other oceanographic properties, e.g., SST, SSS, SSH, and MLD. The methodology combined Gaussian Mixture Models to categorize the data into environmentally similar subregions, Random Forest Regressions for the spatial and temporal extrapolation of observational fCO_2 data, and regressions to estimate TA (Carter et al. 2021) to provide a second carbonate system constraint. The resulting maps are available at OCADS (DOI: "10.25921/h8vw-e872"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0287551.html (Sharp et al., 2024a), while an online portal at https://ecowatch.noaa.gov/thematic/ocean-acidification presents regionally averaged time series for three key indicators: the partial pressure of carbon dioxide, calcium carbonate saturation state with respect to aragonite, and seawater pH.

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

38) **ReCAD-NAACOM-pCO$_2$:** Wu et al. (2025) developed a reconstructed pCO$_2$ product for the North American Atlantic Coastal Ocean Margins (NAACOM), spanning from the Gulf of Mexico/Gulf of America to the Grand Banks, called the Reconstructed Coastal Acidification Database-pCO$_2$ (ReCAD-NAACOM-pCO$_2$). This product employed a two-step approach combining random forest regression and linear regression to generate monthly pCO$_2$ data at 0.25° spatial resolution from 1993–2021. The model was trained using SOCAT v2023 observations as ground-truth values, incorporating various satellite-derived and reanalysis environmental variables known to influence sea surface pCO$_2$. The ReCAD-NAACOM-pCO$_2$ product demonstrates robust performance, with a coefficient of determination of 0.83, a root-mean-square error of 18.64 µatm, and an accumulative uncertainty of 23.83 µatm when compared against all SOCAT observation samples. This high accuracy was maintained across model training and validation phases. The model exhibits robust performance when validated against independent test data from a period excluded from both training and validation, underscoring the product's capability to reliably reconstruct pCO$_2$ in periods lacking direct observational data within the NAACOM. Significantly, the product enables detailed investigation of regional spatial differences, seasonal cycles, and decadal changes in pCO$_2$ across the NAACOM. The ReCAD-NAACOM-pCO$_2$ dataset is publicly accessible (https://doi.org/10.5281/zenodo.11500974) and will be updated regularly.

39) **Gridded surface OA indicators, and air–sea CO$_2$ fluxes in the northern Caribbean Sea:** This dataset contains a high-quality dataset of derived products from over a million observations of surface water partial pressure/fugacity of carbon dioxide (pCO$_2$w/fCO$_2$w), for the Caribbean Sea, Gulf of Mexico/Gulf of America and North-West Atlantic Ocean covering the timespan from 2002-01-01 to 2019-12-30. The derived quantities include total alkalinity (TA), acidity (pH), aragonite saturation state (Ω_{Ar}) and air-sea CO$_2$ flux (Wanninkhof et al., 2020). This data product is available at OCADS (DOI: "10.25921/2swk-9w56"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0207749.html (Wanninkhof et al., 2019)

40) **Ocean acidification data in the Gulf of Mexico/Gulf of America and wider Caribbean from 2014 to 2020**: The Acidification, Climate, and Coral Reef Ecosystems Team (ACCRETE) Lab within AOML's Ocean Chemistry and Ecosystems Division (OCED) developed a data product for tracking ocean acidification in the Caribbean and Gulf of Mexico/Gulf of America (van Hooidonk, 2022). Utilizing satellite imagery and a data-assimilative hybrid model, the tool maps key indicators of the water's carbonate system, including pCO$_2$, TA, pH, Ω_{arag}, and Ω_{calc}. This innovation builds upon an update to the experimental Ocean Acidification Product Suite (OAPS) developed by NOAA's Coral Reef Watch. The data product is available at OCADS (DOI: "10.25921/tt1c-dx53"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0245950.html. (van Hooidonk, 2022)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

41) **Regional pCO_2 climatology of the Baltic Sea:** Bittig et al. (2024) used biogeochemical model output to inform the mapping of sea surface pCO_2 observations in the Baltic Sea and to build a mean monthly climatology for the period 2003 to 2021 with 3 nautical mile resolution. In a first step, spatial patterns of variability were extracted from 20 years of model surface pCO_2 data by an EOF analysis. These spatial patterns were then used to map surface pCO_2 observations from the Surface Ocean CO_2 Atlas (SOCAT; see above No. 1) (Bakker et al., 2014) onto the Baltic Sea domain. By using an ensemble approach with varying number of EOF patterns, the spatial scales of the mapping were locally adjusted based on the observation's data density. Mapped monthly fields of pCO_2 from 2003-2021 were combined for the product into a mean monthly climatology and a spatially-resolved linear trend. The climatology product is available at PANGAEA (DOI: "10.1594/PANGAEA.961119"): https://doi.org/10.1594/PANGAEA.961119 (Bittig et al., 2023).

Table 3. Gridded and derived ocean carbonate chemistry data synthesis products in the surface ocean.

No.	Name	Open or coastal ocean	Spatial resolution	Temporal resolution	Methodology	Highlights	Reference
22	Updated Takahashi delta fCO_2 and flux climatology	Open ocean	1° × 1°	12-month climatology for a base year of 2010	Advection Scheme	Does not use proxy variables for extrapolation. Only produced as monthly climatology.	Fay et al. (2024)
23	MPI-ULB-SOM-FFN	Open + Coastal	0.25° × 0.25°	Monthly climatology (January through December) without reference year	2-step machine learning: Merged product of the SOM-FFN approach applied to the open ocean (Landschützer et al 2016) and the coastal ocean (Laruelle et al 2017)	Monthly gridded pCO_2 without adjusting for a specific reference year, high-resolution coastal ocean coverage	Landschützer et al. (2020a)
24	VLIZ SOM-FFN	Open ocean	1° × 1°	Monthly from January 1982 onwards	2-step machine learning: Self organizing map clustering followed by a feed forward network (SOM-FFN)	Monthly gridded pCO_2 from 1982 through near present	Landschützer et al. (2016)
25	JMA-MLR	Open ocean	1° × 1°	Monthly from January 1990 onwards	Multiple linear regressions	Temporal trends of DIC, TA, pCO_2, air-sea CO_2 flux, pH, and Ω_{arag}	Iida et al. (2021)
26(a)	OceanSODA -ETHZv1	Open ocean	1° × 1°	Monthly from 1982 to 2023	Ensemble of 2-step members: K-means clustering with gradient boosting and SVR regression	Temporal trends of DIC, TA, pCO_2, pH, Ω_{arag}, and Ω_{calc}	Gregor and Gruber (2021)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

26(b)	OceanSODA -ETHZv2	Open + Coastal ocean	0.25° × 0.25°	8-day from 1982 to 2022	FFNN	Highlighting fine-scale and short-term variability of the ocean carbon sink	Gregor, Shutler, and Gruber (2024)
27	LDEO-HPD fCO_2 product	Open ocean	1° × 1°	Monthly from 1982	XGBoost algorithm	Temporal evolution of surface ocean fCO_2 and air-sea CO_2 exchange	Gloege et al. (2022)
28	LDEO HPD with extended temporal coverage	Open ocean	1° × 1°	Monthly from 1959	XGBoost algorithm	uses model-data misfit climatology to extend estimate back in time to 1959	Bennington et al (2022a)
29	LDEO fCO_2 - Residual Method	Open ocean	1° × 1°	Monthly from 1982	XGBoost algorithm	Removes the temperature component before ML	Bennington et al (2022b)
30(a)	CMEMS -LSCEv1	Open + Coastal	1° × 1°	Monthly from 1985 to 2019	FFNN	seamless reconstruction from coastal to open ocean	Chau et al. (2022)
30(b)	CMEMS -LSCEv2	Open + Coastal	0.25° × 0.25°	Monthly from 1985 to 2021	FFNN	yearly extension of time series & monthly reconstruction at low latency	Chau et al. (2024)a,b
31	CarboScope (Jena-MLS)	Open ocean	2.5° × 2°	Daily from 1957	Multi-linear regression against long-term predictors, plus auto-regressive correction	Variability of pCO2 and sea-air CO_2 fluxes since 1957, sensitivities to SST and wind speed variations	Rödenbeck et al. (2022)
32	UOEx-Watson	Open ocean	1° × 1°	Monthly from January 1992	Two-step neural network approach described by Landschützer et al.	air-sea fluxes of CO_2 with adjusted skin temperature effect	Watson et al., 2020
33	NIES-ML3	Open ocean	1° × 1°	Monthly from 1982 to 2023	FNN, GBM, RF	The prediction of a ML method was obtained from ten trainings with different seeds. The mean of the three methods was taken as the final prediction.	Zeng (2022), Zeng et al. (2022)
34	CSIR-ML6	Open ocean	1° × 1°	Monthly from 1982 to 2016	Ensemble: FFNN, SVR, ERT, Gradient Boosted Trees	Various ML methods produce different results when data is sparse, but all still achieving roughly the same uncertainty.	Gregor et al. (2019a)
35	AOML-ET	Open ocean	1° × 1°	Monthly from 1998 to 2023	Extremely randomized trees (ET) machine learning technique	Monthly global sea-air CO_2 flux maps in modern era	Wanninkhof et al. (2015)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

36	ULB-SOM-FFN -coastalv2.1	Coastal ocean	0.25° × 0.25°	Monthly from 1982 to 2020	2-step machine learning: Self organizing map clustering followed by a feed forward network (SOM-FFN)	Global temporal trends of coastal pCO_2 and air-sea CO_2 fluxes based on SOCATv2022 with data collected from 1982–2020	Roobaert et al. (2024)
37	RFR-LME	Coastal	0.25° × 0.25°	Monthly from 1998 to 2023	Gaussian mixture models and random forest regressions	Temporal trends of OA indicators and estimated uncertainties across 11 U.S. Large Marine Ecosystems (LMEs), with monthly coverage from 1998–2023.	Sharp et al. (2024b)
38	ReCAD -NAACOM -pCO_2	Coastal	0.25° × 0.25°	Monthly from 1993 to 2021	2-step machine learning: random forest regression followed by linear regression	Sea surface pCO_2 in the North American Atlantic Coastal Ocean Margins (NAACOM)	Wu et al. (2025)
39	Gridded surface OA indicators, and air–sea CO_2 fluxes in the northern Caribbean Sea	Coastal	1° × 1°	Monthly from 2002 to 2019	Gridding of the observations of fCO_2, SST and SSS was performed by binning and averaging the data in (1° × 1° by month) cells	A 17-year record of fCO_2, TA, pH, Ω_{Ar}, and air-sea CO_2 flux in the Caribbean Sea	Wanninkhof et al. (2020)
40	OA data in the Gulf of Mexico/Gulf of America and wider Caribbean from 2014 to 2020	Regional	0.088° × 0.88°	Monthly from 2014 to 2020	Utilizing satellite imagery and a data-assimilative hybrid model, the tool maps key indicators of the water's carbonate system, including pCO_2, TA, pH, Ωarag, and Ωcalc.	A new tool to monitor ocean acidification over the wider Caribbean and Gulf of Mexico/Gulf of America.	van Hooidonk (2022)
41	Regional pCO_2 climatology of the Baltic Sea	Regional	0.1° × 0.05°	12-month climatology for a base year of 2013; linear trend 2003-2021	Extrapolation using model-based patterns of variability	Does not use proxy variables for extrapolation. Spatial scales adjust locally to data density	Bittig et al. (2024)

3.1.4 Gridded and derived data products – Interior ocean:

Although cruise data compilations are valuable for making data available in a uniform format, they often are constrained by their sampling strategies and can have significant gaps in space and time. Gridded and derived data products address this limitation by making some variables available at all grid points on a standardized spatial grid and at standardized depth levels through processes such as interpolation and gap filling.

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

42) **Global interior ocean mapped climatology from GLODAPv2 (referenced to 2002)**: Lauvset et al. (2016) generated a comprehensive set of global interior ocean climatologies, mapping key biogeochemical variables on a 1°×1° grid for 33 depth levels from surface to 5500 m. These climatologies cover temperature, salinity, oxygen, nitrate, phosphate, silicate, DIC, TA, pH, and the saturation states of aragonite and calcite (Ω_{arag} and Ω_{calc}). This data product was created based on the quality-controlled and internally consistent GLODAPv2.2016 (Olsen et al., 2016) using the Data-Interpolating Variational Analysis (DIVA) method (Barth et al., 2014). The conceivably confounding temporal trends in DIC, pH, Ω_{arag} and Ω_{calc} due to anthropogenic influence were removed prior to mapping by normalizing their values to a reference year of 2002 using first-order calculations of anthropogenic carbon accumulation rates. For all variables, all data from the full 1972–2013 period were used, including data that did not receive full secondary quality control. This data product is not updated each year along with the main GLODAPv2 data product. The mapped data product is available at OCADS (DOI: "10.3334/cdiac/otg.ndp093_glodapv2"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0286118.html (Lauvset et al., 2023b). It can also be accessed from the GLODAP website: https://glodap.info/.

43) **Global aragonite saturation state climatology (referenced to 2000)**: Jiang et al. (2015a) developed a climatology of the derived variable, aragonite saturation state (Ω_{arag}) across the global interior ocean, on a 1° x 1° grid at 9 standardized depth levels from the surface down to 4000m. This was accomplished by integrating data from the first version of GLODAP (Key et al., 2004), CARINA (Key et al., 2010), and PACIFICA (Suzuki et al., 2013), along with additional recent cruise datasets up to 2012. Calculations of Ω_{arag} utilized a MATLAB version of the CO2SYS program (Orr et al., 2015), with the dissociation constants for carbonic acid of Lueker et al. [2000], potassium bisulfate ($KHSO_4^-$) of Dickson [1990], hydrofluoric acid (HF) of Perez and Fraga (1987), and the total borate concentration equations of Lee et al. [2010]. Temporal adjustments were made to a reference year of 2000, accounting for an annual increase of fCO_2 of 1.6 µatm in the surface mixed layer (SML), with a rate that decreases linearly to zero µatm yr^{-1} from the bottom of the SML to a depth of 1000 m (Sabine et al., 2008). The data product is available at OCADS (DOI: "10.1002/2015GB005198"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0139360.html (Jiang et al., 2015b).

44) **MOBO-DIC (Version 2020):** Keppler et al. (2020) produced a global interior ocean DIC monthly climatology (average climatological values for January through December) on a 1° × 1° grid at 33 standardized depth levels from the surface to 2000 m. The Mapped Observation-Based Oceanic Dissolved Inorganic Carbon (MOBO-DIC) mapping method adapts and extends the SOM-FFN technique originally introduced by Landschützer et al. (2013). It starts by categorizing the ocean into clusters with comparable physical and biogeochemical characteristics using self-organizing maps (SOM). Subsequently, within each SOM-defined cluster, a feed-forward network (FFN) is employed to estimate and enforce the statistical correlation between the targeted dissolved inorganic carbon (DIC) data and the predictor data available in

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

globally mapped fields. The product uses data from January 2004 to December 2017, and is thus centered around the years 2010/2011. The data product is available at OCADS (DOI: "10.25921/yvzj-zx46"): https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/ndp_104/ndp104.html.

45) **Monthly global interior ocean TA climatology:** Broullón et al. (2019) developed a monthly global interior ocean TA climatology using a feed-forward neural network approach. This dataset offers a spatial resolution of 1° × 1° in the horizontal, spans 102 depth levels (ranging from 0–5500 m) in the vertical dimension, and features a temporal resolution that varies from monthly (0–1500 m) to annual (1550–5500 m). The development of this climatology was based on the analysis of TA in relation to several key predictor variables, including temperature, salinity, nutrients (phosphate, nitrate, and silicate), dissolved oxygen, and sampling position (coordinates and depth), as outlined in Velo et al. (2013). Both TA and these predictor variables were sourced from GLODAPv2 (version 2016) (Olsen et al., 2016). The global interior ocean TA climatology was constructed by leveraging the established relationships between TA and the predictor variables, as well as the monthly climatologies of temperature, salinity, and dissolved oxygen from the World Ocean Atlas 2013 (WOA13) (Locarnini et al., 2013; Zweng et al., 2013; Garcia et al., 2014), and nutrients data that were obtained through the CANYON-B neural network process, applied to the previously mentioned fields. The data product is available at OCADS (DOI: "10.25921/5p69-y471"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0222470.html.

46) **Monthly global interior ocean DIC climatology:** Broullón et al. (2020) employed a feed-forward neural network approach to create a monthly global interior ocean DIC climatology, centered around the year 1995. This dataset offers a 1° × 1° spatial resolution in the horizontal domain, encompassing 102 depth levels ranging from 0–5500 m vertically. The temporal resolution varies, ranging from monthly (0–1500 m) to annual (1550–5500 m). In contrast to their previous work on TA (Broullón et al., 2019), this analysis includes the variable "year" to account for anthropogenic DIC pool changes. It also incorporates data from the Lamont–Doherty Earth Observatory (LDEO) pCO_2 database (Takahashi et al., 2017) alongside GLODAPv2.2019 (Olsen et al., 2019) to establish relationships between DIC and its input variables: temperature, salinity, dissolved oxygen, as well as location, pressure, and time. The DIC climatology was derived using these relationships, along with monthly climatological data for temperature, salinity, and dissolved oxygen from the World Ocean Atlas 2013 (Locarnini et al., 2013; Zweng et al., 2013; Garcia et al., 2014), as well as phosphate, nitrate, and silicate values computed from the CANYON-B neural network fed with the aforementioned fields. The data product is available at OCADS (DOI: "10.25921/ndgj-jp24"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0222469.html.

47) **MOBO-DIC (Version 2023):** Keppler et al. (2023) extended the temporal resolution of MOBO-DIC to resolve monthly fields from January 2004 to December 2019, as opposed to the average climatological values in Keppler et al. (2020). This data product is on a 1° × 1° grid at 28 depth levels from the surface to 1500 m. The data product is available at OCADS (DOI: "10.25921/z31n-3m26"):

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0277099.html.

48) **Metrics of acidification in the ocean interior:** Fassbender et al. (2023) generated estimates of global interior ocean changes to pH, [H^+], Ω_{Ar}, pCO_2, and the Revelle sensitivity factor driven by the accumulation of anthropogenic carbon (C_{ant}) from the preindustrial period to the year 2002, and quantified the component of those changes caused by nonlinearities in the carbonate system. For each OA metric, the dataset includes year 2002 values and quasi-preindustrial values, which were estimated by subtracting C_{ant} from the year 2002 carbonate chemistry information and recomputing each OA metric without considering any warming, circulation, or biological changes that may have occurred since the preindustrial era. Data from the upper 2000 m of the GLODAPv2.2016b mapped data product (DOI: "10.3334/cdiac/otg.ndp093_glodapv2"), described in Lauvset et al., 2016, and from the preformed properties product of Carter et al., 2021 were used to make these estimates on the GLODAPv2.2016b 1° × 1° grid for 26 depth levels from surface to 2000 m. The provided uncertainties were estimated using a 1000-iteration Monte Carlo simulation. Calculation details are described in Fassbender et al. (2023). Year 2002 aragonite saturation state and pH values, and their uncertainties, are reproduced from the GLODAPv2.2016b mapped data product and are provided in this dataset for user convenience with the permission of the original data producer. This data product is available at OCADS (DOI: "10.25921/rdtr-9t74"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0290073.html.

49) **Anthropogenic CO_2 from 1994 to 2007**: Gruber et al. (2019a) estimated decadal changes in the oceanic content of anthropogenic CO_2 (ΔCant) for the years 1994, 2004, and 2014. The results have been derived from the GLODAPv2.2016 product (Olsen et al., 2016), utilizing the eMLR(C*) methodology pioneered by Clement and Gruber (2018). All estimates are geospatially distributed on a horizontal grid with a resolution of 1° × 1°. Two primary files are available: one providing the complete three-dimensional distribution of ΔC_{ant}, and the other containing vertically integrated values, i.e., the column inventories. This data product is available at OCADS (DOI: "10.25921/wdn2-pt10"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0186034.html (Gruber et al., 2019b) .

50) **Decadal trends in anthropogenic CO_2 from 1994 to 2014**: Müller et al. (2023) extended the analysis by Gruber et al. (2019a) to reconstruct decadal trends in the oceanic storage of anthropogenic CO_2 (ΔC_{ant}) in the global ocean interior from 1994 to 2014. They applied the extended multiple linear regression (eMLR) method (Clement and Gruber 2018) to ship-borne observations of DIC and other biogeochemical variables from GLODAPv2.2021 (Lauvset et al., 2021). All estimates are provided on a 1° × 1° horizontal grid. Two principal data files are provided: one featuring the comprehensive three-dimensional distribution of ΔC_{ant}, and the other presenting the vertically integrated quantities, i.e., the column inventories. The data product is available at OCADS (DOI: "10.25921/ppcf-w020"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0279447.html.

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

51) **Progression of Ocean Interior Acidification over the Industrial Era:** Building on the total anthropogenic carbon estimates for 1994 from Sabine et al. (2004) and the decadal changes between 1994 and 2014 reconstructed by Müller et al. (2023), Müller et al. (2024) quantified ocean interior acidification over the industrial era. To convert the increasing anthropogenic carbon concentrations into acidification estimates, their approach relied on time-invariant climatologies of ocean interior DIC, TA, temperature, salinity, and other relevant variables to determine the background state of the marine carbonate system. Hence, their estimates resolve exclusively the acidification driven by the anthropogenic carbon accumulation. In contrast to direct observations of acidification parameters—such as those collected at time series stations—this approach does not account for changes in the natural carbon cycle or the displacement of water masses. The approach by Müller et al. (2024) is conceptually similar to that of Fassbender et al. (2023), but provides temporally resolved estimates, enabling the tracking of both the spatial distribution and temporal evolution of ocean interior acidification. The data product is available at OCADS (DOI: "10.25921/tefm-x802"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0298993.html

52) **CODAP-NA climatology:** Jiang et al. (2024) developed a coastal OA indicators climatology on a 1°×1° grid, covering North American ocean margins from surface to 500 m at 14 standardized depth levels: 0, 10, 20, 30, 50, 75, 100, 125, 150, 200, 250, 300, 400, and 500 m. This product includes 10 key oceanographic parameters: fugacity of carbon dioxide (fCO_2), pH, total hydrogen ion content, free hydrogen ion content, carbonate ion content ($[CO_3^{2-}]$), Ω_{arag}, Ω_{calc}, DIC, TA, and Revelle Factor (RF), as well as temperature and salinity. The climatology was produced with the World Ocean Atlas (WOA) gridding technologies of the NOAA National Centers for Environmental Information (NCEI), based on the recently released Coastal Ocean Data Analysis Product in North America (CODAP-NA) (Jiang et al., 2021), along with GLODAPv2.2022 (Lauvset et al., 2022). The relevant variables were adjusted to the year of 2010 before the gridding. The first-guess fields for this analysis were calculated using ESPERs (Carter et al., 2021), based on the WOA (Version 2018) climatologies for salinity (Zweng et al., 2019), temperature (Locarnini et al., 2019) and dissolved oxygen (Garcia et al., 2018b). The data product is available in NetCDF at OCADS (DOI: "10.25921/g8pb-zy76"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0270962.html. Additionally, maps of these indicators are available in jpeg at: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/synthesis/nacoastal.html (Jiang et al., 2022b).

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

902 **Table 4. Gridded and derived ocean carbonate chemistry data synthesis products in the subsurface ocean.**

No.	Name	Open or coastal ocean	Reso-lution	Temporal resolution	Methodology	Highlights	Reference
42	Global interior ocean mapped climatology from GLODAPv2	Open ocean	1° × 1°	adjusted to 2002	Data Interpolating Variational Analysis (DIVA)	Ocean interior climatology for multiple variables from surface to the bottom of the ocean (referenced to year 2002)	Lauvset et al. (2016)
43	Global aragonite saturation state climatology	Open ocean	1° × 1°	adjusted to 2000	Data Interpolating Variational Analysis (DIVA)	Ocean interior climatology for aragonite saturation state from surface to 4000 m (referenced to year 2000)	Jiang et al. (2015a)
44	MOBO-DIC (Version 2020)	Open ocean	1° × 1°	monthly climatology, centered around 2010/2011	Machine learning	Seasonal variability of DIC in the interior ocean from surface to 2000 m	Keppler et al. (2020)
45	Monthly global interior ocean TA climatology	Open ocean	1° × 1°	monthly climatology	Machine learning	Ocean interior climatology for TA from surface to bottom	Broullón et al. (2019)
46	Monthly global interior ocean DIC climatology	Open ocean	1° × 1°	monthly from 1957 to 2018	Machine learning	Ocean interior climatology for DIC from surface to bottom (referenced to year 1995)	Broullón et al. (2020)
47	MOBO-DIC (Version 2023)	Open ocean	1° × 1°	monthly from Jan 2004 to Dec 2019	Machine learning	Temporal trends and interannual variability of DIC in the interior ocean from surface to 1500 m	Keppler et al. (2023)
48	Metrics of acidification in the ocean interior	Open ocean	1° × 1°	2002 and preindustrial	Reproduced from GLODAPv2.2016b (Lauvset et al., 2016) and the preformed properties of Carter et al., (2021)	Metrics of acidification in the ocean interior (to 2000 m) and the component of those changes caused by carbonate system nonlinearities	Fassbender et al. (2023)
49	Anthropogenic CO_2 from 1994 to 2007	Open ocean	1° × 1°	1994 and 2007	Extended multiple linear regression (eMLR)	The oceanic sink for anthropogenic CO_2 over the period 1994 to 2007	Gruber et al. (2019a)
50	Decadal trends in anthropogenic CO_2 From 1994 to 2014	Open ocean	1° × 1°	Decadal from 1994 to 2014	eMLR(C*) extended Multiple Linear Regression applied to the tracer C*	Temporal trends in the accumulation of anthropogenic CO_2 in the interior ocean are resolved	Müller et al. (2023)
51	Progression of Ocean Interior Acidification over the Industrial Era	Open ocean	1° × 1°	1800 – 1994 – 2004 - 2014	Conversion of anthropogenic carbon accumulation into acidification rates	Temporal trends in the progression of acidification in the interior ocean are resolved	Müller et al. (2024)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

52	CODAP-NA climatology	Coastal	1° × 1°	adjusted to 2010	Objective analysis approach of the World Ocean Atlas	The first discrete bottle based climatology in the North American ocean margins	Jiang et al. (2024)

3.1.5 Multi-product analyses:

This section includes data products that have been generated by community synthesis efforts designed to inform global carbon budgets.

53) **SeaFlux:** Harmonization of air–sea CO_2 fluxes from surface pCO_2 data products using a standardized approach (Gregor and Fay, 2021). This resource provides an ensemble of six pCO_2 products with air-sea CO_2 fluxes computed consistently. The six included products are: CMEMS-FFNN, CSIR-ML6, JENA-MLS, JMA-MLR, MPI-SOMFFN, and NIES-FNN. First, missing areas of pCO_2 estimates (mostly high-latitude and marginal seas) are filled using a linear-regression approach, thus addressing differences in spatial coverage between the mapping products. Further, also accounts for methodological inconsistencies in flux calculations. Fluxes are calculated using three wind products (CCMPv2, ERA5, and JRA55) along with the application of a scaled gas exchange coefficient for each of the wind products. Through these steps, SeaFlux presents an product ensemble of interpolated global surface ocean pCO_2 and air–sea carbon flux estimates for the years 1990–2019. For more details, refer to Fay et al. (2021).

54) **RECCAP2:** In the context of the second iteration of the project REgional Carbon Cycle Assessment and Processes (RECCAP2), the ocean carbon community compiled, quality controlled and harmonized (in the sense of providing output on the same regular grid at the same spatial and temporal resolution) 12 global ocean biogeochemical model simulations, 11 pCO_2 products, one ocean interior DIC products, and three data assimilation models to constrain the ocean carbon sink between 1985 and 2018. The RECCAP2 synthesis effort stands as a distinct but complementary resource to the Global Carbon Budget (GCB) project (Friedlingstein et al., 2025), which primarily focuses on anthropogenically perturbed surface CO_2 fluxes from a global budgeting perspective. The individual chapters of RECCAP2 were published in this special issue of Global Biogeochemical Cycles: https://agupubs.onlinelibrary.wiley.com/doi/toc/10.1002/(ISSN)2169-8961.RECCAP2. The data products of this assessment are available on a 1° × 1° horizontal grid, with monthly resolution for surface ocean variables such as air-sea CO_2 fluxes, and annual resolution for interior ocean variables, such as DIC content. The data compilation, which is described in detail in DeVries et al. (2023), is available at: https://zenodo.org/records/7990823 (Müller, 2023).

55) **Global Carbon Budget:** The GCB collects annually updated estimates of the ocean carbon sink from currently nine fCO_2-products and ten Global Ocean Biogeochemical Models for the period 1959 to the past calendar year (Friedlingstein et al., 2025, https://globalcarbonbudget.org/gcb-2024). In contrast to Earth System Models, the GOBMs are here forced with atmospheric reanalysis that ingested atmosphere and

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

ocean observations and are thus thought to be closer to the observed climate. Gridded fields are provided on a 1° × 1° horizontal grid and monthly resolution. In addition, globally and regionally integrated air-sea CO_2 fluxes from the native model grids are provided. Globally integrated time-series are adjusted for full ocean coverage and model bias and drift and are available for each individual fCO_2-product and GOBM (https://globalcarbonbudget.org/download/1442/?tmstv=1731323337). The model data goes well beyond surface fluxes and includes data to analyze drivers of carbon fluxes, including several 3D variables. The model data request has been updated since RECCAP2 and also provides, for example, monthly interior ocean data of DIC, alkalinity, nutrients and oxygen. The GOBM data request was also updated to have all variables available that are needed to serve as a testbed for fCO_2-products (e.g., sea surface height). Gridded surface data of sea surface fugacity and air-sea CO_2 flux of all fCO_2-products and GOBMs as used in the latest release of GCB (2024) are published on Zenodo (https://zenodo.org/records/14639761, Hauck et al., 2025). All other GOBM output is available via https://globalcarbonbudgetdata.org/closed-access-requests.html.

Table 5. Ocean carbonate chemistry data product synthesis and harmonizations.

No.	Name	Open or coastal ocean	Surface or water column	Spatial resolution	Temporal resolution	Methodology	Highlights	Reference
53	SeaFlux	Open ocean + coastal	Surface only	1° × 1°	Monthly	Consistent flux calculations for 6 pCO_2 products to produce an ensemble estimate	Careful consideration of flux calculation provides a resource and code to the community for independent flux calculations	Gregor and Fay (2021)
54	RECCAP2	Open ocean + coastal	Surface + Water column	1° × 1° (open) 0.25° x 0.25° (coastal)	Monthly	Harmonized compilation of surface fCO_2 products, model simulations and ocean interior products	Quality controlled data compilation with a harmonised horizontal grid and temporal resolution	Müller (2023); DeVries et al. (2023) Resplandy et al (2024)
55	Global Carbon Budget	Open ocean + coastal	Surface + Water column	1° × 1°	Monthly	Harmonized compilation of surface fCO_2 products, and global ocean biogeochemical model simulations	Annually updated and quality controlled data sets. Availability of monthly 4D ocean model output.	Friedlingstein et al., 2025

3.1.6 Model based and hybrid data products and analyses:

Model-based projections of biogeochemical variables are often available from global and regional models, such as those in the Sixth Coupled Model Intercomparison Project (Dunne et al., 2024; Durack et al., 2025). This section further includes hybrid data products, which adjust model estimates towards observation-based constraints.

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

56) **Decadal trends in the ocean carbon sink:** The DeVries et al. (2019) analysis examines decadal trends in global and regional air-sea CO_2 fluxes from a variety of ocean biogeochemical models that contributed to the Global Carbon Budget (see No. 55). Three sets of model simulations were performed. Simulation A uses variable climate forcing (e.g., variable wind stress, heat and freshwater fluxes) and observed atmospheric CO_2 forcing, Simulation B uses constant (repeated) climate forcing and observed atmospheric CO_2, and simulation C uses both constant climate forcing and constant atmospheric CO_2 concentrations. With these simulations, the authors partitioned decadal trends in ocean CO_2 uptake into those driven by climate variability and those driven by atmospheric CO_2. They found that climate variability drove a weakening trend of the ocean carbon sink during the 1990s, and a strengthening trend during the first decade of the 2000s. The magnitude of these trends agreed with those of an OCIM that was trained to replicate tracer data from the 1990s and 2000s (DeVries et al., 2017), indicating that the decadal trends may be driven by variability in ocean circulation. This data from this analysis is accessible through figshare at https://doi.org/10.6084/m9.figshare.8091161.v1.

57) **ECCO-Darwin:** Carroll et al. (2022) used the Estimating the Circulation and Climate of the Ocean-Darwin (ECCO-Darwin) global-ocean biogeochemistry state estimate to generate a data-constrained DIC budget and investigate how spatiotemporal variability in advection and mixing, air-sea CO_2 flux, and the biological pump have modulated the ocean sink for 1995–2018. ECCO-Darwin assimilates ocean circulation and physical tracers, including temperature, salinity, and sea ice, derived from the Estimating the Circulation and Climate of the Ocean (ECCO) LLC270 global-ocean and sea-ice data synthesis (Zhang et al., 2018). Additionally, it assimilates biogeochemical observations encompassing the cycling of carbon, nitrogen, phosphorus (PO_4), iron (Fe), silica (SiO_2), oxygen, and alkalinity. This inclusive approach enhances the model's fidelity by aligning it with a diverse array of observations. All ECCO-Darwin model output is available on the ECCO Data Portal: https://data.nas.nasa.gov/ecco/. The model code and platform-independent instructions for running ECCO-Darwin simulations can be found at: https://github.com/MITgcm-contrib/ecco_darwin.

58) **Global surface ocean pH, acidity, and Revelle factor from 1770 to 2100:** Jiang et al. (2019a) produced a high-resolution (1°×1°) data product delineating regionally varying view of global surface ocean pH, acidity, and Revelle Factor (RF) from the beginning of the Industrial Revolution to the end of this century by amalgamating recent observational seawater CO_2 data from the SOCAT database (Version 6, 1991–2018, ~23 million observations) (Bakker et al., 2016), and temporal trends at individual locations of the global surface ocean from an Earth System Model, i.e., GFDL-ESM2M (Dunne et al., 2013). The calculations were conducted under historical atmospheric CO_2 levels (pre-2005) and four Representative Concentrations Pathways (post-2005) corresponding to the Intergovernmental Panel on Climate Change (IPCC)'s 5th Assessment Report, specifically RCP2.6, RCP4.5, RCP6.0, and RCP8.5. Surface ocean TA was calculated from SSS, SST using the updated locally interpolated alkalinity regression (LIARv2)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

method (Carter et al., 2017). Surface ocean pH, acidity, and RF were then calculated using a MATLAB version of the CO2SYS program (Orr et al., 2015). The data product is available at OCADS (DOI: "10.25921/kgqr-9h49"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0206289.html (Jiang et al., 2019b).

59) **Global surface ocean acidification indicators from 1750 to 2100:** Jiang et al. (2023) developed a comprehensive model-data fusion product that delineates the trajectory of 10 OA indicators: $f CO_2$, pH, total hydrogen ion content, free hydrogen ion content, $[CO_3^{2-}]$, Ω_{arag}, Ω_{calc}, DIC, TA, and RF, as well as temperature and salinity at all locations of the global surface ocean from 1750 to 2100. This product marks a significant breakthrough in OA forecasting by refining temporal trends with data from 14 Earth System Models (ESMs) within the Coupled Model Intercomparison Project Phase 6 (CMIP6), and by applying bias and drift corrections from three updated observational ocean carbon data products: SOCAT (Version 2022) (Bakker et al., 2016), GLODAPv2.2022 (Lauvset et al., 2022), and CODAP-NA (Jiang et al., 2021). This dataset offers 10-year averages on a 1° × 1° global surface ocean grid, capturing trends from preindustrial times (1750), through historical conditions (1850–2010), and projects future conditions to 2100 across five Shared Socioeconomic Pathways: SSP1-1.9, SSP1-2.6, SSP2-4.5, SSP3-7.0, and SSP5-8.5. The gridded data product is available in NetCDF at OCADS (DOI: "10.25921/9ker-bc48"): https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0259391.html, and global maps of these indicators are available in jpeg at: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/synthesis/surface-oa-indicators.html (Jiang et al., 2022c).

60) **Simulated and constrained ocean carbon sink from 1850 to 2100 for the global ocean and the Southern Ocean:** These two datasets include spatially-integrated and annually averaged values for the ocean carbon sink from 1850 to 2100 for different scenarios over the 21st century for the global ocean (Terhaar et al., 2022a, 2022b) and the Southern Ocean (Terhaar et al., 2021b, 2021c). All results are based on CMIP5 and CMIP6 models. For the global ocean carbon sink, values are available for SSP1-2.6, SSP2-4.5, and SSP5-8.5. For the Southern Ocean, values are also available for SSP1-2.6, SSP2-4.5, and SSP5-8.5 and additionally also for RCP2.6, RCP4.5, and RCP8.5. In addition, to the raw simulated values, constrained estimates of the annually averaged ocean carbon sink estimates are available. These constrained estimates adjusted the simulated carbon sink estimates for biases on the ocean's circulation and surface carbonate chemistry (see Terhaar et al., 2021b, 2022a for details). It is recommended to use the constrained estimates. The datasets are available at https://doi.org/10.17882/103934 and https://doi.org/10.17882/103938.

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

Open Access Earth System Science Data Discussions

Table 6. Model based data synthesis products and analyses for ocean carbonate chemistry.

No.	Name	Open or coastal ocean	Surface or water column	Spatial resolution	Temporal resolution	Highlights	Reference
56	Decadal trends in the ocean carbon sink	Open ocean	Surface	Variable	Decadal	Climate variability drove weakened ocean CO_2 uptake in the 1990s, and strengthened CO_2 uptake in the 2000s	DeVries et al. (2019)
57	ECCO-Darwin	Open + Coastal	Water column	⅓° × ⅓°	3-hourly, daily, and month fields available	Model-data synthesis product based on the Estimating the Circulation and Climate of the Ocean (ECCO) ocean state estimate. Fully-closed, physically-consistent 3-D biogeochemical budgets.	Carroll et al. (2020, 2022, 2024)
58	Global surface ocean pH, acidity, and buffer capacity from 1770 to 2100	Open ocean	Surface	1° × 1°	Decadal	A model-observation fusion product for pH, acidity and Revelle Factor, leveraging GFDL-ESM2M and SOCATv6	Jiang et al. (2019)
59	Global surface ocean acidification indicators from 1750 to 2100	Open ocean	Surface	1° × 1°	Decadal	A model-observation fusion product for all major OA indicators, leveraging a consortium of 14 Earth System Models and 3 observational data products	Jiang et al. (2023)
60	Simulated and constrained ocean carbon sink from 1850 to 2100 for the global ocean and the Southern Ocean	Open ocean	Surface	Spatially integrated	Annual (1850-2100)	A constrained estimate of the ocean carbon sink based on the simulated carbon sink from CMIP5 and CMIP6 models and constrained with observations of the ocean physics and carbonate chemistry	Terhaar et al. (2021b, 2022a)

3.2 Overlaps and history

Many of the data products described above exhibit significant overlap in various forms. In some cases, one or more products are used to generate new ones, while in others, the same collection-level cruise datasets underpin multiple products. There are a few foundational data products, such as GLODAPv2 and SOCAT, which are widely utilized to develop other data products, including their respective gridded products (e.g., Lauvset et al., 2016). For instance, SOCAT forms the backbone of nearly all derived products listed in Table 3, serving as a key resource for product development or validation. Some derived products, such as the JMA-MLR (No. 25) and OceanSODA-ETHZv1 (No. 26), incorporate both SOCAT and GLODAPv2 during development. Having overlaps in data and derived products has provided opportunities for data quality control and intercomparison of different approaches to gap filling that would not have been available otherwise. Additional overlaps between these data products are provided below:

3.2.1 SOCAT and LDEO:

The quality control and synthesis of global surface ocean CO_2 data began in 1997 with Dr. Taro Takahashi and his colleagues at the Lamont-Doherty Earth Observatory (LDEO) in Palisades, New York. His pioneering work led to the creation of the LDEO Surface pCO_2 Database (No. 2), which focused on high-quality data collected by his team and from various U.S. and international expeditions. Over time, this data set expanded to include contributions from other laboratories, resulting in a highly influential collection of pCO_2 data and several seminal papers on global surface ocean CO_2 variations and air-sea CO_2 fluxes (Takahashi et al., 1997; 2002; 2009). The last update to the LDEO database was in 2019, following Dr. Takahashi's passing, and no further updates are anticipated (Takahashi et al., 2021).

The Surface CO_2 Atlas (SOCAT) project was developed to address questions around the current and future drivers of CO_2 fluxes raised at the 2007 Surface Ocean CO_2 Variability and Vulnerability (SOCOVV) workshop in Paris, France (Metzl et al., 2007). SOCAT was developed to synthesize all of the publicly available, discoverable, and citable surface CO_2 data. Following the GLODAP model, there was a strong emphasis on an open and transparent secondary quality control process to ensure the highest data quality. The first data release came in 2011 (Pfeil et al., 2013; Sabine et al, 2013) and included contributions from numerous laboratories, as well as the freely available CO_2 data from the LDEO database. As of 2024, SOCAT contains ~40 million data points, with new observations added annually. All data are rigorously standardized, and recalculated as fCO_2. SOCAT represents an ongoing global community effort, with participants from all continents contributing data and to the quality control process. Initially new versions were released every other year, but automation allowed annual public releases since version 4.

3.2.2 GLODAPv2 and Java OceanAtlas (JOA) Suite:

Starting in the late 1980s, the World Ocean Circulation Experiment (WOCE), Joint Global Ocean Flux Study (JGOFS), and the NOAA Ocean-Atmosphere Exchange Study (OACES) collaborated in a multinational effort to conduct a decadal global hydrographic survey of unparalleled quality and quantity. At the conclusion of the survey at the end of the 1990s, the Global Ocean Data Analysis Project (GLODAP) combined and publicly released all of the available hydrographic data with high-quality carbon measurements as a single database (Key et al., 2004; Sabine et al., 2005). The data were subjected to extensive secondary quality control checks where cruise tracks intersected one another, making it the most comprehensive and highest-quality ocean inorganic carbon dataset ever generated. A gridded, full-depth global ocean carbon climatology was also created and released as part of the project. These data and associated climatology have been extensively used to evaluate carbon distributions as well as the accumulation of anthropogenic CO_2 in the ocean. Other regional datasets, like CARINA (CARbon dioxide IN the Atlantic Ocean) data synthesis project, an international collaborative effort of the European Union CARBOOCEAN program (Key et al., 2010; Tanhua et al., 2010) and PACIFICA (PACIFic ocean Interior CArbon), an international synthesis of Pacific Ocean data organized through the North Pacific Marine Science Organization (PICES) (Ishii et al., 2011b; Suzuki et al., 2013), were combined with GLODAP after its initial release. The

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

GLODAP database is continuing to grow with new data collected as part of the Global Ocean Ship-Based Hydrographic Investigations Program (GO-SHIP).

For discrete bottle measurements spanning the entire oceanic water column, GLODAPv2 (No. 3) and the Java Ocean Atlas (JOA, No. 4) are the primary data products. Most cruise datasets contributing to these two data products overlap, but the key difference lies in their approach to data adjustment. The former applies crossover and inversion analysis for bias correction, while the latter presents the data without such adjustments. GLODAPv2 achieves consistency by applying adjustments based on deep-ocean offsets, whereas JOA provides the data in its original form. While there is substantial overlap between the two, data from a specific expedition might differ slightly due to GLODAPv2's secondary quality control adjustments. Both GLODAPv2 and JOA offer global coverage, but several independent regional data products are also available, such as SNAPO-CO_2 (No. 6), CODAP-NA (No. 8), AZMP Carbon (No. 9), MOCHA (No. 10), and ARIOS (No. 11). Data from these regional products often partially or fully overlap with GLODAPv2 and JOA.

a) GLODAPv2 and CODAP-NA:

All cruise datasets contributing to CODAP-NA were forwarded to the GLODAPv2 quality control team in 2022. Data from select cruises with deep-water sampling (>1500 m), enabling crossover analysis, were subsequently incorporated into the GLODAPv2.2022 data product update (Lauvset et al., 2022).

b) GLODAPv2 and SPOTS:

Some time-series data are included in both GLODAPv2 and the Synthesis Product for Ocean Time-Series (SPOTS). Usually, data present in both products have not been measured on dedicated time-series cruises but rather collected as part of a larger cruise passing by a time series location. As the quality control of SPOTS is restricted to assigning method flags, adjustments that are applied as a result of the QC of GLODAP are not present in SPOTS. Additional crossover analyses between SPOTS and GLODAP have revealed a good consistency (Lange et al., 2024).

3.2.3 RECCAP2 and GCB:

RECCAP2 and GCB are not data products themselves, but analyses and syntheses of data-based and model-based products. Users should be aware that there is a large degree of overlap between the fCO_2 - products and GOBMs that contributed to both RECCAP2 and GCB. However, RECCAP2 and GCB serve different purposes. GCB is updated annually to the latest complete calendar year and its main purpose is to present and estimate of the magnitude (and uncertainty) of the ocean CO_2 sink for that year, while RECCAP2 is presents a deeper analysis of the magnitude, trends, and variability of the ocean CO_2 sink over the period 1985-2018.

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

3.2.4 Jiang et al. (2019) and Jiang et al. (2023):

Both products contain the projection of surface ocean pH, total hydrogen ion content, and buffer capacity from 1750 to 2100. However, the former is based on one GFDL model ESM2M, while the latter is based on a consortium of 14 Earth system models, and additional observational data. The latter also contains the projection of seven other OA variables, including carbonate ions, aragonite saturation state, calcite saturation state, fCO_2, DIC, and TA.

4 Data availability

Access links for all data products mentioned in this paper are provided in their respective paragraphs. Additionally, their access links are available in Table 7 below.

Table 7. Access links for the compiled ocean carbonate chemistry data products. N/A is short for not applicable.

No.	Name	Data access link	DOI	Reference
1	SOCAT	https://socat.info/	https://doi.org/10.25921/9wpn-th28	Bakker et al. (2016, 2024)
2	LDEO Surface pCO_2 Database	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0160492.html	https://doi.org/10.3334/cdiac/otg.ndp088(v2015)	Takahashi et al. (2017)
3	GLODAPv2	https://glodap.info/	https://doi.org/10.25921/zyrq-ht66	Lauvset et al. (2023a, 2024)
4	JOA Suite	https://joa.ucsd.edu/	N/A	Swift and Osborne (2022)
5	WOD	https://www.ncei.noaa.gov/products/world-ocean-database	https://doi.org/10.25923/z885-h264	Mishonov et al. (2024)
6	SNAPO-CO_2	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0285681.html	https://doi.org/10.17882/95414	Metzl et al (2023, 2024)
7	Arctic Ocean anthropogenic carbon estimates	https://www.seanoe.org/data/00927/103920/	https://doi.org/10.17882/103920	Terhaar et al. (2024)
8	CODAP-NA	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0219960.html	https://doi.org/10.25921/531n-c230	Jiang et al. (2020, 2021)
9	AZMP Carbon	N/A	https://doi.org/10.20383/102.0673	Cyr et al. (2022)
10	MOCHA	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0277984.html	https://doi.org/10.25921/2vve-fh39	Kennedy et al., (2024)
11	ARIOS	https://digital.csic.es/handle/10261/205135	https://doi.org/10.20350/digitalCSIC/12498	Pérez et al. (2020)
12	Marine inorganic carbon chemistry observations in the northern Gulf of Alaska	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0277034.html	https://doi.org/10.25921/x9sg-9b08	Monacci et al. (2023, 2024)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

13	Coral Reef Carbonate Chemistry Off the Florida Keys	https://www.ncei.noaa.gov/access/metadata/landing-page/bin/iso?id=gov.noaa.nodc:NCRMP-CO3-Atlantic	https://doi.org/10.25921/vfz0-dg77	Manzello et al. (2018)
14	Salish cruise data package and multi-stressor data product	https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/SalishCruise_DataPackage.html, https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/SalishCruises_DataProduct.html	https://doi.org/10.25921/zgk5-ep63, https://doi.org/10.25921/5g29-q841	Alin et al. (2021, 2023, 2024a, 2024b)
15	BATS	https://demo.bco-dmo.org/project/2124	https://doi.org/10.26008/1912/bco-dmo.894099.4, https://doi.org/10.26008/1912/bco-dmo.893182.4, https://doi.org/10.26008/1912/bco-dmo.926534.4, https://doi.org/10.26008/1912/bco-dmo.893521.6, https://doi.org/10.26008/1912/bco-dmo.917255.5, https://doi.org/10.26008/1912/bco-dmo.939210.7, https://doi.org/10.26008/1912/bco-dmo.3782.6, https://doi.org/10.26008/1912/bco-dmo.3918.8, https://doi.org/10.26008/1912/bco-dmo.881861.5	Bates et al., 2024a,b,c,d,e; Johnson et al., 2024a,b,c; Steinberg and Cope, 2024
16	HOT	https://www.bco-dmo.org/project/2101, https://dhoi.org/10.5281/zenodo.15060930	https://doi.org/10.1575/1912/bco-dmo.3773.1, https://doi.org/10.5281/zenodo.15060931	Winn et al. (1994, 1998); Dore et al. (2003, 2009, 2014, 2025); Knor et al. (2023)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

17	ESTOC	N/A	https://doi.org/10.1594/PANGAEA.959856, https://doi.pangaea.de/10.1594/PANGAEA.856590, https://doi.pangaea.de/10.1594/PANGAEA.856615, https://doi.pangaea.de/10.1594/PANGAEA.856608, https://doi.pangaea.de/10.1594/PANGAEA.856616, https://doi.pangaea.de/10.1594/PANGAEA.856593, https://doi.pangaea.de/10.1594/PANGAEA.856612, https://doi.pangaea.de/10.1594/PANGAEA.856614, https://doi.pangaea.de/10.1594/PANGAEA.856607, https://doi.pangaea.de/10.1594/PANGAEA.956272	González-Dávila and Santana-Casiano (2023)
18	Point B Time-series	N/A	https://doi.org/10.1594/PANGAEA.727120	Gattuso et al. (2021b)
19	Ny-Ålesund Time-series	N/A	https://doi.org//10.1594/PANGAEA.957028	Gattuso et al. (2023)
20	SPOTS	https://www.bco-dmo.org/dataset/896862	https://doi.org/10.26008/1912/bco-dmo.896862.2	Lange et al. (2024a, 2024b)
21	Autonomous *p*CO_2 and pH time series from 40 surface buoys	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0173932.html	https://doi.org/10.7289/v5db8043	Sutton et al. (2018)
22	Updated Takahashi delta *f*CO_2 and flux climatology	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0282251.html	https://doi.org/10.25921/295g-sn13	Fay et al. (2023)
23	MPI-ULB-SOM-FFN	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0209633.html	https://doi.org/10.25921/qb25-f418	Landschützer et al. (2020a, 2020b)
24	VLIZ SOM-FFN	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0160558.html	https://doi.org/10.7289/V5Z899N6	Landschützer et al. (2016), Jersild et al. (2017)
25	JMA-MLR	https://www.data.jma.go.jp/kaiyou/english/co2_flux/co2_flux_data_en.html	N/A	Iida et al. (2021)
26(a)	OceanSODA -ETHZv1	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/ metadata/0220059.html	https://doi.org/10.25921/m5wx-ja34	Gregor et al. (2020)
26(b)	OceanSODA -ETHZv2	N/A	https://doi.org/10.5281/zenodo.11206365	Gregor et al. (2024b)
27	LDEO-HPD fCO2 product	https://zenodo.org/records/4760205	https://doi.org/10.5281/zenodo.4760205	Gloege et al. (2022)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

28	LDEO HPD with extended temporal coverage	https://zenodo.org/records/13891722	https://doi.org/10.5281/zenodo.13891722	Bennington et al. (2022a)
29	LDEO fCO2 - Residual Method	https://zenodo.org/records/13941548	https://doi.org/10.5281/zenodo.13941548	Bennington et al. (2022b)
30(a)	CMEMS -LSCEv1	https://data.ipsl.fr/catalog/srv/eng/catalog.search#/metadata/a2f0891b-763a-49e9-af1b-78ed78b16982	https://doi.org/10.14768/a2f0891b-763a-49e9-af1b-78ed78b16982	Chau et al. (2022)
30(b)	CMEMS -LSCEv2	https://data.marine.copernicus.eu/product/MULTIOBS_GLO_BIO_CARBON_SURFACE_MYNRT_015_008/services	https://doi.org/10.48670/moi-00047	Chau et al. (2024a, 2024b)
31	CarboScope (Jena-MLS)	https://www.bgc-jena.mpg.de/CarboScope/?ID=oc	10.17871/CarboScope-oc_v2024E (or analogously for previous and upcoming releases)	Rödenbeck et al. (2022)
32	UOEx-Watson	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0301544.html	https://doi.org/10.25921/2dp5-xm29	Watson et al. (2025)
33	NIES-ML3	https://db.cger.nies.go.jp/DL/10.17595/20220311.001.html.en	https://doi.org/10.17595/20220311.001	Zeng (2022), Zeng et al. (2022)
34	CSIR-ML6	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0206205.html	https://doi.org/10.25921/z682-mn47	Gregor et al. (2019b)
35	AOML-ET	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0298989.html	https://doi.org/10.25921/0s8y-q287	Wanninkhof et al. (2024, 2025)
36	ULB-SOM-FFN -coastalv2.1	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0279118.html	https://doi.org/10.25921/4sde-p068	Roobaert et al. (2023, 2024)
37	RFR-LME	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0287551.html	https://doi.org/10.25921/h8vw-e872	Sharp et al. (2024a, 2024b)
38	ReCAD -NAACOM -pCO2	https://zenodo.org/records/14038561	https://doi.org/10.5281/zenodo.1150097.	Wu et al. (2025)
39	Gridded surface OA indicators, and air–sea CO2 fluxes in the northern Caribbean Sea	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0207749.html	https://doi.org/10.25921/2swk-9w56	Wanninkhof et al. (2019)
40	OA data in the Gulf of Mexico/Gulf of America and wider Caribbean from 2014 to 2020	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0245950.html	https://doi.org/10.25921/tt1c-dx53	van Hooidonk (2022)
41	Regional pCO_2 climatology of the Baltic Sea	N/A	https://doi.org/10.1594/PANGAEA.961119	Bittig et al. (2023)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

42	Global interior ocean mapped climatology from GLODAPv2	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0286118.html	https://doi.org/10.3334/cdiac/otg.ndp093_glodapv2	Lauvset et al. (2016, 2023b)
43	Global aragonite saturation state climatology	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0139360.html	https://doi.org/10.7289/v5q81b4p	Jiang et al. (2015a, 2015b)
44	MOBO-DIC (Version 2020)	https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/ndp_104/ndp104.html	https://doi.org/10.25921/yvzj-zx46	Keppler et al. (2020)
45	Monthly global interior ocean TA climatology	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0222470.html	http://doi.org/10.20350/DIGITALCSIC/8564	Broullon et al., (2019)
46	Monthly global interior ocean DIC climatology	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0222469.html	http://doi.org/10.20350/digitalCSIC/10551	Broullon et al., (2020)
47	MOBO-DIC (Version 2023)	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0277099.html	https://doi.org/10.25921/z31n-3m26	Keppler et al. (2023)
48	Metrics of acidification in the ocean interior	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0290073.html	https://doi.org/10.25921/rdtr-9t74	Fassbender et al. (2023), Fassbender (2024)
49	Anthropogenic CO_2 from 1994 to 2007	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0186034.html	https://doi.org/10.25921/wdn2-pt10	Gruber et al. (2019a, 2019b)
50	Decadal trends in anthropogenic CO2 From 1994 to 2014	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0279447.html	https://doi.org/10.25921/ppcf-w020	Müller et al. (2023)
51	Progression of Ocean Interior Acidification over the Industrial Era	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0298993.html	https://doi.org/10.25921/tefm-x802	Müller et al. (2024)
52	CODAP-NA climatology	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0270962.html	https://doi.org/10.25921/g8pb-zy76	Jiang et al. (2022b), Jiang et al. (2024)
53	SeaFlux	https://zenodo.org/records/8280457	https://doi.org/10.5281/zenodo.5482547	Gregor & Fay. (2021)
54	RECCAP2	https://zenodo.org/records/7990823	https://doi.org/10.5281/zenodo.7990823	Müller (2023)
55	Global Carbon Budget	https://zenodo.org/records/14639761	https://doi.org/10.5281/zenodo.14639761	Hauck et al. (2025)
56	Decadal trends in the ocean carbon sink	N/A	https://doi.org/10.6084/m9.figshare.8091161.v1	DeVries et al. (2019)
57	ECCO-Darwin	https://data.nas.nasa.gov/ecco/	N/A	Carroll et al. (2020)

https://doi.org/10.5194/essd-2025-255
Preprint. Discussion started: 15 May 2025

58	Global surface ocean pH, acidity, and buffer capacity from 1770 to 2100	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0206289.html	https://doi.org/10.25921/kgqr-9h49	Jiang et al. 2019(a), Jiang et al. (2019b)
59	Global surface ocean acidification indicators from 1750 to 2100	https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0259391.html	https://doi.org/10.25921/9ker-bc48	Jiang et al. (2022c), Jiang et al. (2023)
60	Simulated and constrained ocean carbon sink from 1850 to 2100 for the global ocean and the Southern Ocean	https://www.seanoe.org/data/00927/103934/, https://www.seanoe.org/data/00927/103938/	https://doi.org/10.17882/103934, https://doi.org/10.17882/103938	Terhaar et al. (2021c), Terhaar et al. (2022b)

5 Summary

The synthesis and gridded data products presented here reflect significant community-based efforts that have been made to advance understanding of the ocean's role in global carbon cycling. This synthesis provides a comprehensive overview of key data compilations and gridded data products essential for coastal and global ocean carbonate chemistry research. It highlights the key features of each product, serving as a resource for researchers seeking the necessary data for their work.

Author contributions

L-QJ prepared the initial draft. All authors contributed to the writing of the manuscript. The first 20 authors are listed based on their contributions, while the remaining authors are listed alphabetically by their last names.

Competing interests

One of the (co-)authors, Anton Velo (Instituto de Investigacions Mariñas, IIM - CSIC, Vigo, Spain), is a member of the editorial board of the Earth System Science Data.

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Preprint. Discussion started: 15 May 2025

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