Beyond FAIR:

Manifesting marine data synthesis products within the ocean observing system

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A biogeochemical essential ocean variables perspective

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Summary

In times of increasing anthropogenic impacts jeopardizing the environmental status of the ocean and the associated services for society, sustained and globally well-coordinated observations of biogeochemistry (BGC) essential ocean variables (EOV) are vital. Efficient usage of the highly heterogeneous, high-volume BGC EOV data determines the success of BGC observations in supporting the development of evidence-based strategies for climate change mitigation, and adaptation, ecosystem health conservation, and sustainable resource management. Recognizing the limiting factor of the fragmented BGC data landscape in this context, and addressing the key data challenges, community-driven BGC EOV data synthesis products constitute key outputs from the Global Ocean Observing System. These products connect BGC EOV observations with societal services by applying customized techniques to combine datasets from multiple sources to provide comparable, Findable, Accessible, Interoperable, Reusable (FAIR), and fit-for-purpose data. However, BGC EOV synthesis products are far from a sustained status, and insufficient BGC data still represent a weak spot in the ocean observing system, resulting in large uncertainties and unresolved issues in marine BGC research. Acknowledging the positive impacts of BGC EOV data synthesis products on the BGC data landscape, the overarching goal of this thesis was to further manifest BGC EOV synthesis products as an integral part in the ocean observing system.

For this purpose, first, a novel evaluation scheme was developed that enables an objective assessment of the readiness of BGC EOV data synthesis products following the system-engineering approach of the Framework of Ocean Observing. Its application to four community-driven BGC EOV data synthesis products, in descending readiness level order: The Surface Ocean CO_2 Atlas (SOCAT), the Global Ocean Data Analysis Project (GLODAP), the MarinE MethanE and NiTrous Oxide (MEMENTO) data product, and the Global Ocean Oxygen Database and ATlas (GO_2DAT) enabled the identification of critical features of BGC synthesis data products. Eventually, the identified features, e.g. traceable and customized Quality Control (QC), and the developed readiness evaluation scheme at large are envisioned to guide new and existing BGC data synthesis products in eliminating their weaknesses and realizing their full potential.

In parallel, the goal of annual GLODAP product updates was realized, and over the course of this thesis GLODAPv2.2019, GLODAPv2.2020, GLODAPv2.2021, and GLODAPv2.2022 were released. Combined, a total of 361 new cruises with 381,800 water samples were harmonized, QC'ed, archived, and added. Building upon GLODAPv2, the consistency of the original data could be significantly enhanced. Therefore, the generated GLODAPv2.2022 represents the largest and most consistent dataset for carbon-relevant hydrographic cruise data, including data from 1,085 hydrographic cruises with 1,381,248 water samples, and covering a time period from 1972 until 2021. Several implemented software developments further improved GLODAP's provenance, and data handling, including the developed Make Ocean merging routine and the applied AtlantOS QC software. Further, in pursue of a higher readiness for GLODAP, the vision of a uniform, semi-automatic, and standards-compliant data ingestion system in combination with a modern and versatile data extraction system were developed and outlined.

Furthermore, benefitting from the gained knowledge, and leading the community effort on the Synthesis Product for Ocean Time Series (SPOTS), a pilot was successfully produced during this thesis. Thereby, a template for a sustained living SPOTS was created and the BGC data landscape was expanded by the previously overlooked ship-based time-series programs. For the pilot, a total of 108,332 water samples from 12 ship-based time-series programs, each representative for a different marine environment, and a different program structure, were synthesized. Besides increasing the level of FAIR, implemented i) "Best-Practice" flags, ii) comparisons to GLODAP, and iii) measurement quality continuity estimations, further resulted in an increased utility of the data. Moreover, the pilot helped to position ship-based time-series programs for expansion under the United Nations Decade of Ocean Science umbrella as evidenced by the Marine Ecological Time Series network recently obtaining the status of an “Ocean Coordination Group potential new emerging network”.

All achievements of this thesis emphasized the value of BGC EOV data synthesis products for the ocean observing system. Particularly, their unique contributions regarding more FAIR, efficient, and utile data were exposed and implemented, guided by Aristotle’s slightly adapted notion “the whole is greater than the sum of its parts”. Thereby, their key aspects for continuous and sustainable success were revealed. Altogether, through the work in this thesis, important steps towards the overarching goal of improving the BGC data landscape through the manifestation of BGC EOV data synthesis products as an integral part in the ocean observing system were realized. However, the thesis also highlighted that more work needs to be done to fully reach this vital goal.

Zusammenfassung

In Zeiten zunehmender anthropogener Einflüsse, die den Zustand des Ozeans und die damit verbundenen Leistungen für die Gesellschaft gefährden, sind nachhaltige und global koordinierte Beobachtungen der biogeochemischen (BGC) Essential Ocean Variables (EOV) von entscheidender Bedeutung. Insbesondere bestimmt eine effiziente Nutzung der heterogenen, und großen BGC EOV Datenmengen den Erfolg von marinen BGC Beobachtungen bei der Entwicklung evidenzbasierter Strategien zur Minderung und Anpassung an den Klimawandel, zum Schutz des Ökosystemzustandes und zum nachhaltigem Ressourcenmanagement. In diesem Zusammenhang stellen Community-basierte BGC EOV Datensynthese Produkte wichtige Outputs des Global Ocean Observing System dar, welche die Herausforderungen einer stark fragmentierten BGC Datenlandschaft erkannt haben und angehen. Diese Produkte verwenden maßgeschneiderte Methoden und Software, um Daten aus verschiedenen Quellen zu kombinieren, um letztendlich vergleichbare, Findable, Accessible, Interoperable, Resuable (FAIR) Daten mit einem hohen Nutz-Faktor zu generieren. Sie stellen so eine direkte Verbindung zwischen BGC EOV Beobachtungen und gesellschaftlichen Dienstleistungen dar. Allerdings haben BGC EOV Datensynthese Produkte noch keinen „sustained“ Zustand im Sinne des Frameworks for Ocean Observing erreicht. Dies ist auch daran zu erkennen, dass unzureichende BGC Daten und Informationsprodukte weiterhin eine Schwachstelle im Ozeanbeobachtungssystem sind, welche folglich zu großen Unsicherheiten und ungelösten Fragen in der marinen BGC Forschung führen. Den Wert von BGC EOV Datensynthese Produkten für die BGC Datenlandschaft anerkennend und darauf aufbauend, war das übergeordnete Ziel dieser Arbeit zu der Manifestierung und Etablierung von BGC EOV Datensynthese Produkte als integralen Bestandteil des Ozeanbeobachtungssystems beizutragen.

Für diesen Zweck wurde zunächst ein neuartiges Bewertungsschema entwickelt, das basierend auf dem systemtechnischen Ansatz des Frameworks for Ocean Observing eine objektive Bewertung der „Readiness“ von BGC EOV Datensynthese Produkten ermöglicht. Dessen Anwendung auf vier Community-basierten BGC EOV Datensynthese Produkten; in absteigender Readiness, der Surface Ocean CO_2 Atlas (SOCAT), das Global Ocean Data Analysis Project (GLODAP), das MarinE MethanE and NiTrous Oxide (MEMENTO) Datenprodukt und die Global Ocean Oxygen Database and ATlas (GO_2DAT) ermöglichte die Identifizierung entscheidender Merkmale von BGC Synthese Datenprodukten. Das entwickelte Bewertungsschema selbst, sowie die identifizierten Merkmale, wie zum Beispiel rückverfolgbare und maßgeschneiderte Qualitätskontrolle, stellen so eine Orientierungshilfe für neue und bestehende BGC Datensynthese Produkte dar. Insbesondere werden so die Erörterung und Beseitigung einzelner Schwächen unterstützt, sodass Produkte ihr volles Potenzial erreichen können.

Parallel dazu wurde das Ziel der jährlichen Aktualisierung von GLODAP erreicht, entsprechend wurden im Rahmen dieser Doktorarbeit GLODAPv2.2019, GLODAPv2.2020, GLODAPv2.2021 und GLODAPv2.2022 veröffentlicht. Insgesamt wurden 361 neue Forschungsfahrten mit 381,800 Wasserproben harmonisiert, einer Qualitätskontrolle unterzogen, archiviert und hinzugefügt. Basierend auf GLODAPv2 konnte die Konsistenz der Originaldaten signifikant verbessert werden. So ist das generierte GLODAPv2.2022, mit Daten von 1,085 hydrographischen Forschungsfahrten und 1,381,248 Wasserproben (1972 bis 2021), der größte und konsistenteste Datensatz für kohlenstoffrelevante hydrographische Forschungsfahrtdaten. Mehrere implementierte Softwareentwicklungen haben die Daten Provenance- und Prozesse von GLODAP weiter verbessert. Darunter fallen die entwickelte Make Ocean Merging Routine und die eingesetzte AtlantOS QC Software. Darüber hinaus wurden im Streben nach einer höheren Readiness von GLODAP das Zukunftskonzept eines einheitlichen, halbautomatischen und standardkonformen Daten-

Aufnahmesystems in Kombination mit einem modernen und flexiblem Datenextraktionssystem entwickelt und skizziert.

Des Weiteren, profitierend von dem gewonnenen Wissen und Erfahrungen, wurde im Zuge dieser Doktorarbeit das Synthesis Product for Ocean Time Series (SPOTS) Projekt geführt und dessen Pilotprojekt erfolgreich fertigstellt. Der erstellte Pilot bietet eine Vorlage für einen „sustained“ SPOTS und hat die BGC Datenlandschaft mit den bisher vernachlässigten schiffsbasierten Zeitreihenprogrammen erweitert. Insgesamt wurden hierfür 108,332 Wasserproben aus 12 schiffsbasierten Programmen, die jeweils für eine andere Meeresumgebung und eine andere Programmstruktur repräsentativ sind, synthetisiert. Neben der Verbesserung der Daten-FAIRness, führten implementierte i) „Best-Practice Flags“, ii) Vergleiche mit GLODAP und iii) Berechnungen der Messqualitätskontinuität zu einer erhöhten Nützlichkeit der Zeitreihendaten. Darüber hinaus trug der Pilot dazu bei, die Bedeutung schiffsbasierter Zeitreihenprogramme im Rahmen des Übereinkommens der United Nations Decade of Ocean Science zu verdeutlichen. Der kürzlich erworbene Status des Marine Ecological Time Series Netzwerks als "Ocean Coordination Group potential new emerging network" untermauert dies.

Alle Errungenschaften dieser Doktorarbeit haben den Wert von BGC EOV Datensynthese Produkten für das Ozeanbeobachtungssystem hervorgehoben und vertieft. Insbesondere wurden ihre einzigartigen Beiträge zu mehr FAIRness, Effizienz und Nutzbarkeit von BGC Daten ganz im Sinne von Aristoteles These "das Ganze ist mehr als die Summe seiner Teile" herausgestellt und implementiert. Dabei wurden die wichtigsten Elemente für einen kontinuierlichen und nachhaltigen Erfolg von BGC EOV Datensynthese Produkten aufgezeigt. Insgesamt wurden im Rahmen dieser Doktorarbeit wichtige Schritte in Richtung des übergeordneten Ziels, die BGC Datenlandschaft durch die Manifestierung und Etablierung von BGC EOV Datensynthese Produkte als integralen Bestandteil des Ozeanbeobachtungssystems zu verbessern, realisiert. Allerdings hat diese Doktorarbeit auch verdeutlicht, dass weitere Anstrengungen erforderlich sind, um dieses wichtige Ziel vollständig zu erreichen.

Manuscript overview

This thesis contains the following manuscripts which have been prepared in collaboration with other authors:

Publication 1

Citation	Lange, N., Tanhua, T., Pfeil, B., Bange, H.W., Lauvset, S.K., Grégoire, M., Bakker, D.C.E., Jones, S.D., Fiedler, B., O'Brien, K.M., Körtzinger, A., 2023. A status assessment of selected data synthesis products for ocean biogeochemistry. Front. Mar. Sci. 10, 1078908. https://doi.org/10.3389/fmars.2023.1078908
Status	Published
Nico Lange's contribution	Conceptualization of study, Coordination of co-author contributions, Development of readiness evaluation scheme, Evaluation of synthesis products, Writing and editing manuscript, Creation of tables and figures

Publication 2

Citation	Lauvset, S.K., Lange, N., Tanhua, T., Bittig, H.C., Olsen, A., Kozyr, A., Alin, S., Álvarez, M., Azetsu-Scott, K., Barbero, L., Becker, S., Brown, P.J., Carter, B.R., da Cunha, L.C., Feely, R.A., Hoppema, M., Humphreys, M.P., Ishii, M., Jeansson, E., Jiang, L.-Q., Jones, S.D., Lo Monaco, C., Murata, A., Müller, J.D., Pérez, F.F., Pfeil, B., Schirnick, C., Steinfeldt, R., Suzuki, T., Tilbrook, B., Ulfsbo, A., Velo, A., Woosley, R.J., Key, R.M., 2022. GLODAPv2.2022: the latest version of the global interior ocean biogeochemical data product. Earth Syst. Sci. Data 14, 5543–5572. https://doi.org/10.5194/essd-14-5543-2022
Status	Published
Nico Lange's contribution	Retrieval, formatting, and harmonization of data, QC preparations for reference group meetings, Compilation of product, Discussing QC results, Contributing to the manuscript, Co-Creation of tables and figures

Publication 3

Citation	Tanhua, T., Lauvset, S.K., Lange, N., Olsen, A., Álvarez, M., Diggs, S., Bittig, H.C., Brown, P.J., Carter, B.R., da Cunha, L.C., Feely, R.A., Hoppema, M., Ishii, M., Jeansson, E., Kozyr, A., Murata, A., Pérez, F.F., Pfeil, B., Schirnick, C., Steinfeldt, R., Telszewski, M., Tilbrook, B., Velo, A., Wanninkhof, R., Burger, E., O'Brien, K., Key, R.M., 2021. A vision for FAIR ocean data products. Commun Earth Environ 2, 136. https://doi.org/10.1038/s43247-021-00209-4
Status	Published
Nico Lange's contribution	CO-development of (parts of) vision, Co-Creation of figures, Contributing to project and manuscript

Publication 4

Citation	Lange, N., Fiedler, B., Álvarez, M., Benoit-Cattin, A., Benway, H., Buttigieg, P.L., Coppola, L., Currie, K., Flecha, S., Honda, M., Huertas, I.E., Lauvset, S.K., Muller-Karger, F., Körtzinger, A., O'Brien, K.M., Ólafsdóttir, S.R., Pacheco, F.C., Rueda-Roa, D., Skjelvan I., Wakita, M., White, A., Tanhua, T., submitted. Synthesis Product for Ocean Time-Series (SPOTS) – A ship-based biogeochemical pilot.
Status	Submitted to Earth System Science Data
Nico Lange's contribution	Conceptualization of time series product, Development of the BGC EOV metadata template and recommended QC Guidelines for BGC EOV time-series programs, Application of additional QC analysis on several original datasets, Execution of the assessments (method evaluation, minimum variability, GLODAP offset), Compilation of the SPOTS pilot and application of the TOATS notebook to the data, Generation of machine-readable metadata (ODIS), Writing and editing publication, Coordination of coauthor contributions, Creation of tables and figures

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Introduction

1 Introduction

Introducing this thesis, this Section first provides the motivation and sets it in context with the present research. The overarching goal, corresponding objectives, and research questions are expressed, and the structure of the thesis is given. Lastly, relevant existing frameworks and Concepts are explained.

1.1 Motivation and Scientific Background

Covering approximately 71% of the Earth's surface, the ocean plays a fundamental role in the Earth's system and for our society. Amongst others, the ocean takes part in storing, transporting, and exchanging large amounts of heat, freshwater, and multiple greenhouse gases with the atmosphere (Rhein et al., 2013). One of the key aspects that governs the ocean's functionality is ocean biogeochemistry (Buesseler et al., 2020; Séférian et al., 2020). Understanding its importance is essential, as ocean biogeochemistry is closely linked to climate regulation, ocean acidification, ecosystem health, and sustainable resource management (Doney et al., 2020; IPCC 2021; IPCC, 2022; Jiang et al., 2023). Even more so in times of anthropogenic climate change, as the environmental status of the ocean and the associated services for society are at risk (Cooley et al., 2023).

Most prominent, the ocean is the biggest reservoir of carbon in the earth system through both, the physical and biological carbon pump. It currently stores about 25% (Friedligstein et al., 2022) of the anthropogenic carbon emissions of carbon dioxide (CO_2) including land-use change, and thereby buffers and mitigates the impacts of climate change (Jiang et al., 2019). The ocean is also a very important component of the global cycles of other greenhouse gases, such as halocarbons, and nitrous oxide (N_2O) (Freing et al., 2012, Weber et al., 2019; Yang et al., 2020). In this context, observations of ocean biogeochemistry help to i) elucidate the factors controlling the uptake, storage, and changes of greenhouse gases in the ocean, and are thus essential to close their global budgets, ii) provide insights into the efficiency of the carbon pumps, iii) expand our knowledge regarding the potential feedbacks between oceanic cycling of greenhouse gases and climate change, and iv) enable estimates of ventilation and respiration rates of the ocean (Tanhua et al., 2013; Grégoire et al., 2021; Gruber et al., 2023). Hence, observations of ocean biogeochemistry are vital in supporting the development of informed strategies for climate change mitigation and adaptation.

Another reason for observations of ocean biogeochemistry being crucial for society lies in the importance of biogeochemical (BGC) processes for the health and productivity of marine ecosystems. It is the absorption of atmospheric CO_2 that leads to the most prominent effect related to ocean health: Ocean acidity increasing by about 30% since the preindustrial period, i.e. ocean acidification (Jiang et al., 2023). Ocean acidification poses large risks to marine organisms and ecosystems with significant effects on all levels of the trophic chain directly impacting future food security (Gattuso et al., 2013). Its importance is also reflected in the Sustainable Development Goal 14.3 “Minimize and address the impacts of ocean acidification, including through enhanced scientific cooperation at all levels”. Furthermore, ocean health is directly influenced by anthropogenic perturbations affecting the elemental cycles of nitrogen and phosphorus (fertilizer over-usage, runoff, atmospheric deposition) (Jickells et al., 2017; Yuan et al., 2018). These perturbations significantly impact ocean chemistry and increasingly lead to eutrophication and hypoxia, as well as harmful algal blooms. The cycles of the underlying essential elements (e.g. nitrogen) directly link to the productivity of phytoplankton, i.e. the growth of primary producers, and the intricate food web dynamics (Maúre et al., 2021). Hence, observations of ocean biogeochemistry are also crucial for gauging ocean health, specifically to better comprehend ecosystem resilience, predict shifts in species distributions, and develop evidence-based strategies to mitigate the impacts of human activities on marine ecosystems. All of which is needed for a sustainable marine resource management beneficial for society.

It is clear that planning and implementing all-encompassing BGC ocean observations are of paramount importance for society (Moltmann et al., 2019, Tanhua et al., 2019a). Regarding observations, it is very important to understand that ocean observations encompass far more than the act of sampling and measuring. In particular, ocean observation encompasses the management of resulting data (Lindstrom et al., 2012). Accordingly, BGC observations and BGC data are closely tight to each other, to the extent that marine BGC observations are only as impactful and useful, as the (resulting) data. This is also reflected in data being an integral part of the Ocean Decade Challenges, emphasizing that BGC data is just as important for society as the other parts of the BGC observation design. This recent shift of the ocean community to put a stronger focus on data also resulted from the observatory-based approach in marine science reaching a global scale following the examples set by the World Ocean Circulation Experiment and the Joint Global Ocean Flux Study (WOCE/JGOFS; JGOFS, 1990) during the 1990s (IOC, 1994), and from ongoing advancements in sensor technologies and autonomous platforms (Tanhua et al., 2019b). Hence, gaining an improved holistic understanding of the climate and the ocean's environmental status in this new “era of marine big data” (Abbott, 2013) strongly depends on the efficient usage of highly heterogeneous, high-volume data originating from a variety of complementing observing platforms.

Unfortunately, it is still common practice in academic studies to fail making underlying data publicity available and reusable by either only publishing them as “Supplementary Material”, or not publishing the dataset at all (Starr et al., 2015). The reasons for the lack of data sharing are numerous, ranging from a competitive mindset to having no capacity for data management (Snowden et al., 2019). Especially the latter is very common despite the beneficial cost-reward ratio of good data management significantly improving the return on investment for any ocean observation (Tanhua et al., 2019b). Additionally, ocean observing campaigns are usually funded as research projects and often have very specific research targets. Consequently, for the BGC data that is made publicly available, a multitude of data centers are managing those data with varying extents to which data is further processed (Shepherd 2018; Miguez et al., 2019). Even though, more recently a stronger focus is put into following the guidelines of Findable, Accessible, Interoperable, and Reusable (FAIR) data (Wilkinson et al., 2016), data processing routines of many data centers are restricted to the archival and provision of data by assigning a persistent identifier. In combination with the increasing amount of data, data mining has become increasingly difficult and time-consuming leading to large amounts of “dark data” that remains unused (Figure 1) (Ferguson et al., 2014). Moreover, data users are required to manage a plethora of data versions, file formats, cope with duplicates, and differing levels of documentation and quality. Thus, many parts of the fragmented BGC data landscape are a limiting factor for the value of observations, and scientific progress overall.

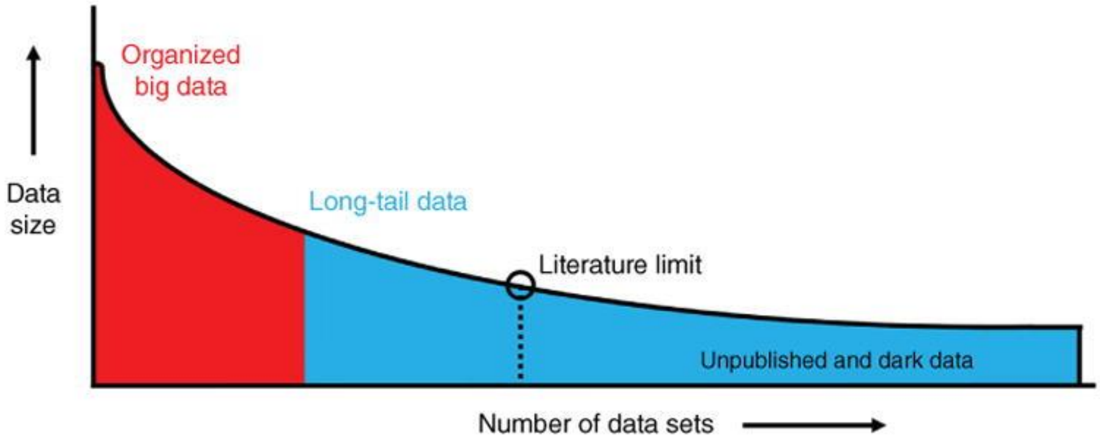

Figure 1: Schematic illustration of the capability of scientists to discover and use literature (data), from Ferguson et al. (2014).

Community-driven BGC synthesis efforts address these data challenges striving for stream-lined and user-orientated data access (e.g. Bakker et al., 2016; Kock and Bange, 2015; Bowie and Tagliabue, 2018; Lauvset et al., 2022). Focusing on specific societal issues related to marine BGC, BGC synthesis products apply customized techniques to combine datasets from multiple sources to form coherent and consistent data products, going far beyond simply merging individual data. Accordingly, the generation of a synthesis product covers the entire data value chain, from data acquisition to usage (Curry, 2016). More precisely, synthesis includes collection, harmonization, formatting, archival, and Quality Control (QC) of original (meta)data, as well as data integration, product generation, and provision. In particular, the development and application of advanced QC routines represents an incremental part of the synthesis data flow. This combination differentiates synthesis efforts from other data management efforts (Table 1). All data management efforts in turn are (ideally) linked to the International Oceanographic Data and Information Exchange (IODE), the program of the Intergovernmental Oceanographic Commission (IOC) "[...] responsible for enhancing marine research, exploitation and development, by facilitating the exchange of oceanographic data and information between participating Member States, and by meeting the needs of users for data and information products" (IODE, 2022).

Table 1: Simplified overview of existing (BGC) Data Landscape. Adapted from Table 1 in Pouliquen et al., 2010. The star (*) denotes the larger category to which synthesis products belong.

Who	**What**	**From**	**To**	**Example**
Data Providers	Collect, measure, and record the data	Platform	Media	Principal Investigator
(National) Data Centers	Archive, QC, and distribute the (FAIR) (meta)data	Media	Repository	Bundesamt für Seeschifffahrt und Hydrographie
Data Assembly Centers (DAC)	(Semantic) Harmonization of (FAIR) (meta)data and provision of “data portal”	Repository	Service Provider	Global Argo DAC
World Ocean Database	Harmonization, enhancement of (FAIR) (meta)data	Repository	Service Provider	Not applicable
Thematic Assembly Centers*	Harmonization, integration, and enhancement of (FAIR) (meta)data	Repository	Service Provider	Copernicus Marine Service in-Situ TAC
Service Providers	Providing customized services from data analysis and manipulation (e.g. assessments)	Service Provider	End-Users	Global Carbon Budget

Since the first synthesis product release of the Global Ocean Data Analysis Project (GLODAP) in 2004 (Key et al., 2004), BGC data synthesis products continue to gain increasing popularity and demand. While GLODAP was initiated to enable the quantification of the anthropogenic ocean carbon sink (e.g. Sabine et al., 2004), and focuses on carbon-relevant data from repeated hydrography, other prominent BGC synthesis products have different foci. For example, the Surface Ocean CO_2 Atlas (SOCAT; Pfeil et al., 2013, Sabine et al., 2013) focuses on relevant data for the oceanic CO_2 uptake and synthesizes in-situ surface ocean fCO_2 (CO_2 fugacity) measurements from multiple platforms. Another example is given by the MarinE MethanE and NiTtrous Oxide database (MEMENTO; Bange et al., 2009, Kock and Bange 2015) that focuses on hydrographic cruise data relevant for the oceanic distributions, and exchanges of N_20 and methane (CH_4).

Multiple synthesis efforts established to be important components within the ocean observing system, connecting BGC observations with societal services as exemplarily illustrated for measurements of the carbon chemistry in Figure 2. Their impact on research is further evidenced by large numbers of citations, in some cases reaching thousands, as well as their usage in higher-level scientific assessments, e.g. the global carbon budget (Friedligstein et al., 2022).

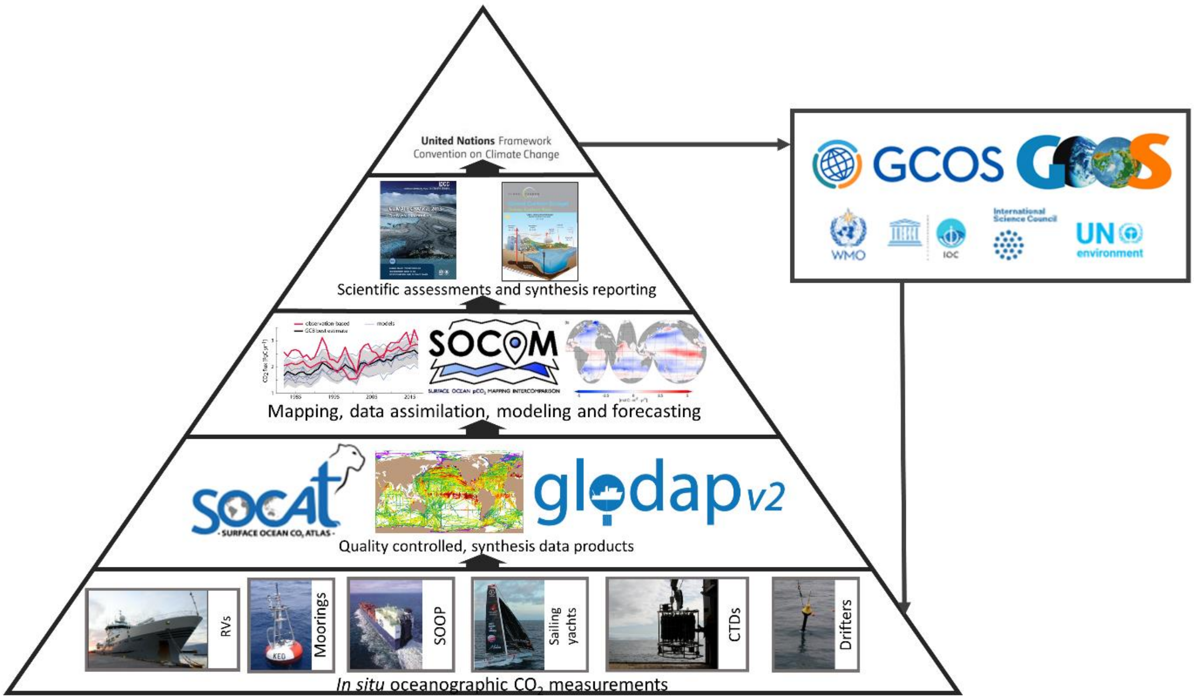

Figure 2: The value chain that connects in situ oceanographic measurements of carbon chemistry to climate negotiations. Adapted from Bakker et al. (2023) by Tanhua (2023).

Nevertheless, there are still large uncertainties and many unresolved issues due to insufficient availability of BGC observations, e.g. increasing dissimilarities of the ocean carbon sink estimates (up to 1.1 GtC yr^{-1} in 2020) between ensemble means of global BGC ocean models and observation-based data products (Friedlingstein et al., 2022); disagreement on the strength and spatial distribution of deoxygenation between models and observation-based products (IPCC, 2019); vastly varying estimated contributions of N_2O fluxes from oxygen minimum zones to the global ocean source (4% to 50%; IPCC, 2021). Hence, synthesis efforts are far from complete and the community still works towards having fully comparable, fully FAIR high-quality BGC data, supporting the ocean BGC observing system to reach its full potential and become truly fit-for-purpose. This goal entails:

1. Evaluating BGC Essential Ocean Variable (EOV) synthesis products in support of the elimination of any weaknesses
2. Continuously updating BGC EOV existing living synthesis products with new data
3. Developing and implementing improvements
4. Expanding the BGC EOV synthesis product landscape to previously overlooked observations

1.2 Thesis Objectives and Structure

The above-identified objectives, motivated by the identified research gap, all relate to the overarching goal of this thesis:

Improving the BGC data landscape through the manifestation of BGC EOV synthesis products as an integral part in the BGC ocean observing system.

To better grasp this objective, first, two fundamentally important frameworks and/or concepts are introduced in Section 1.3, (i) the Framework of Ocean Observing (FOO), elaborating on the thesis' focus on EOVs; and (ii) the concept of FAIR data. Subsequently, Section 2 describes the methodologies used to develop and generate the BGC data synthesis products GLODAP and the Synthesis Product for Ocean Time-Series (SPOTS). Eventually, the publications that relate to the individual goals are included as Sections 3 to 6. Thereby, the chronological order of the individual goals is followed:

O1. Evaluating BGC EOV synthesis products in support of the elimination of any weaknesses
The first included publication (Section 3), describes the current BGC synthesis product landscape by means of four complementing synthesis products that focus on different EOVs and/or observing platforms. To enable an objective assessment of the maturity of synthesis products, and to guide their further development, a scoring scheme that is based upon FOO is introduced. By exemplarily applying it to the four selected synthesis products, their strengths, weaknesses, and potential improvements are discussed, as is the scoring scheme itself.

O2. Continuously updating existing living BGC EOV synthesis products with new data
To deepen the understanding of all processes involved in generating and updating a living BGC data synthesis product, the second publication (Section 4) describes GLODAPv2.2022 in detail. This publication is representative for all the work involved in synthesizing global BGC observations from repeated hydrography that mounted in the fourth consecutive annual update of GLODAPv2.

O3. Developing and implementing improvements
The third publication (Section 5) further emphasizes the importance of GLODAP for climate research. It outlines the vision for FAIR ocean data products and in particular GLODAP. For GLODAP, envisioned improvements for its data handling are depicted accordingly.

O4. Expanding the BGC EOV synthesis product landscape to previously overlooked observations
The last publication (Section 6) included in this thesis describes the pilot of a new BGC synthesis data product: SPOTS. The generation of this pilot leveraged the knowledge gained from existing synthesis efforts and the results given in the three previous publications. Targeting the gap in temporal resolution of the current BGC data synthesis product landscape, SPOTS complements the existing synthesis products by synthesizing BGC data from fixed location time-series.

Section 7 synthesis the contribution of the thesis towards these objectives and discusses their limitation. Eventually, the overall conclusion and outlook of the thesis (Section 8) are guided by two research questions that embody the essence of the overarching goal and the related objectives:

- Why are BGC EOV data synthesis products so important for the BGC data landscape, more specifically if all data would be FAIR, will synthesis products become redundant?
- What are the key aspects for the sustainable success of BGC EOV data synthesis products?

Figure 3 illustrates the thesis structure, setting the thesis, its overarching goals, the related objectives and the guiding research questions in context with the BGC data landscape and ocean observing system at large.

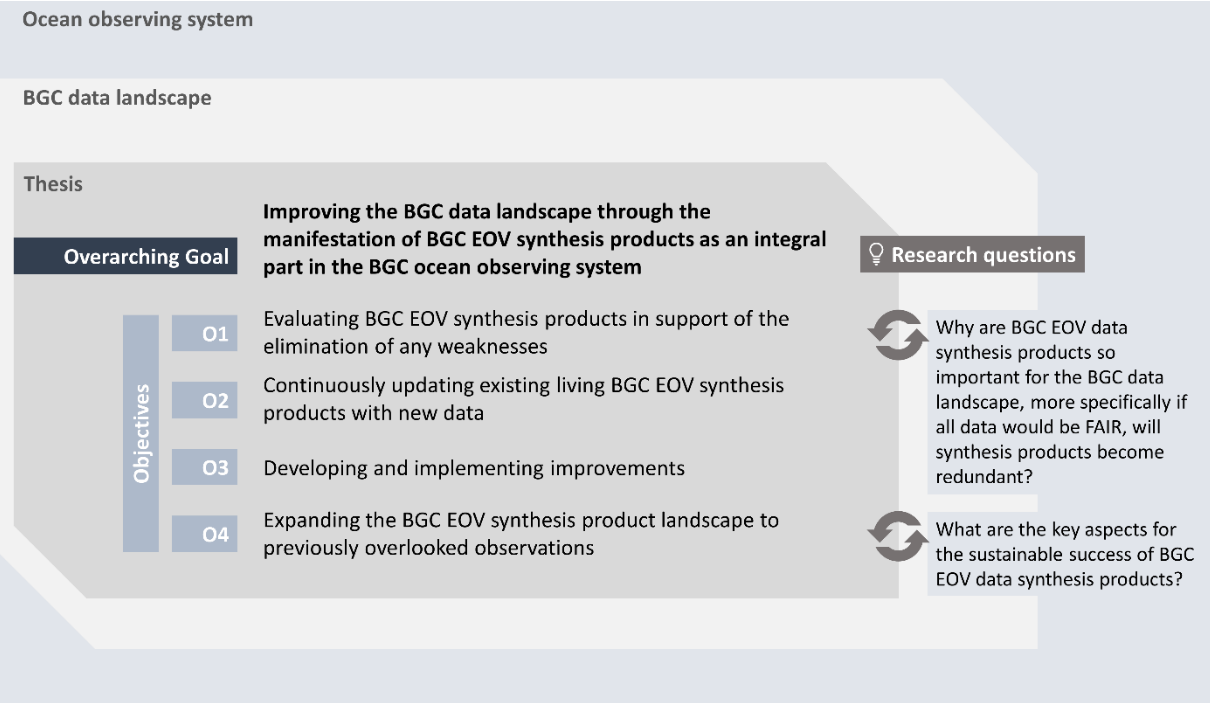

Figure 3: Schematic illustration of thesis structure and its position within the larger BGC data landscape and the ocean observing system at large.

1.3 Frameworks and Concepts

1.3.1 Framework of Ocean Observing (FOO)

The Global Ocean Observing System (GOOS, Moltmann et al., 2019), led by IOC of UNESCO, leads and supports the ocean observing community to build an integrated and sustained ocean observing system aiming to deliver maximum impact for society. The GOOS strategy follows the Framework for Ocean Observing (FOO) systems engineering concept (Lindstrom et al., 2012) that encompasses the entire ocean observation value chain[1] , "[…] a chain of processes addressing "why to observe?" (requirement setting process), "what to observe?" (scoping of observational foci), "how to observe?" (coordination of observing elements), and "how to integrate, use and disseminate observational outcomes and understand their impacts?" (Pearlman et al., 2019, p. 2). FOO divides this ocean observing value chain, i.e. the system's inputs, processes, and outputs, into: "Requirements", "Observations", and "Data and Information". The "Requirements" are the oceanographic information needed to address specific societal issues, the "Observations" the technology and ocean observing networks (platforms) used to collect the required data, and the "Data and Information products[2]" the resultant data and services (Figure 4). To facilitate the concept, FOO makes use of EOVs, inspired by the success of the Essential Climate Variables. The focus of FOO on EOVs enables to set "essential" requirements for sustained ocean observations. Amongst others, this system approach promotes data standards, broad accessibility, as well as free and open exchange of data and products, following the leading principle of "measure once - use many times" (Lindstrom et al., 2012, p. 5).

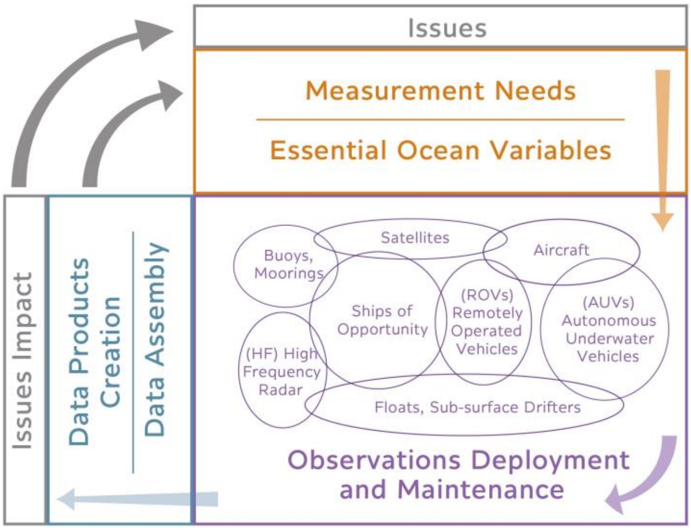

Figure 4: Framework of Ocean Observing (FOO) Ocean Observing Process Diagram (Tanhua et al., 2019a).

The guiding societal issues/drivers for marine biogeochemistry are (Telszewski et al., 2018):

1. The role of ocean biogeochemistry in climate
2. Human impacts on ocean biogeochemistry
3. Ocean ecosystem health

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[1] a term broadly defined as a set of value-adding activities that one or more communities perform in creating and distributing goods and services (Longhorn and Blakemore, 2008)

[2] with its sub-categories: "Oversight and Coordination", "Data Quality Control", "Near Real-Time Data Stream delivery", "Data Repository", and "Data Products"

The related scientific research questions and applications are:

1.1. How is the ocean carbon content changing?

1.2. How does the ocean influence cycles of non-CO_2 greenhouse gases?

2.1. How large are the ocean's dead zones and how fast are they growing?

2.2. What are the rates and impacts of ocean acidification?

3.1. Is the biomass (production) of the ocean changing?

3.2. How does eutrophication and pollution impact the ocean productivity and water quality?

To evaluate the ocean observing system regarding particular societal issues and oceanographic phenomena[3], e.g. ocean acidification, the FOO concept adopted the technical readiness level, a scheme developed by NASA (National Aeronautics and Space Administration) (Sadin et al., 1989). This holistic approach enables the classification (concept, pilot, mature) of an ocean observing system activity in terms of feasibility, capacity, and impact (Figure 5). Key characteristics of a fit-for-purpose ocean observing system are that i) the resultant "data and information" address the societal issues that determined the requirements, and ii) a feedback loop that links the system's outcomes to its inputs is established (Figure 4). Hence, for observational networks to become a sustained part of GOOS, networks must first "[…] mature the associated requirements for acceptance, mature their measurement technology for inclusion, and mature their data and information products for appropriate accessibility and application to a range of scientific and societal issues" (Lindstrom et al., 2012).

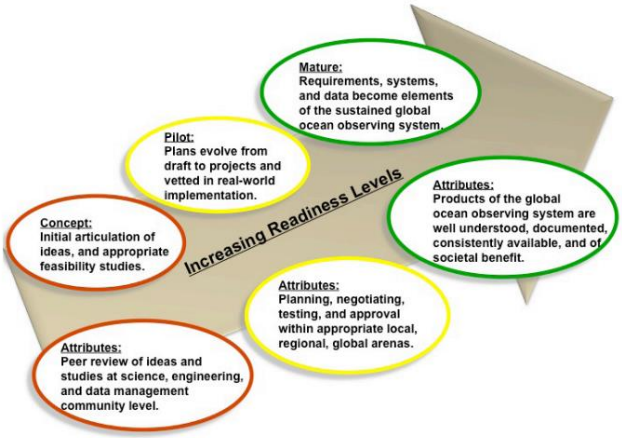

Figure 5: FOO's three main "phases" of an observing system: "Concept", "Pilot", "Mature" their attributes, and readiness (Lindstrom et al., 2012).

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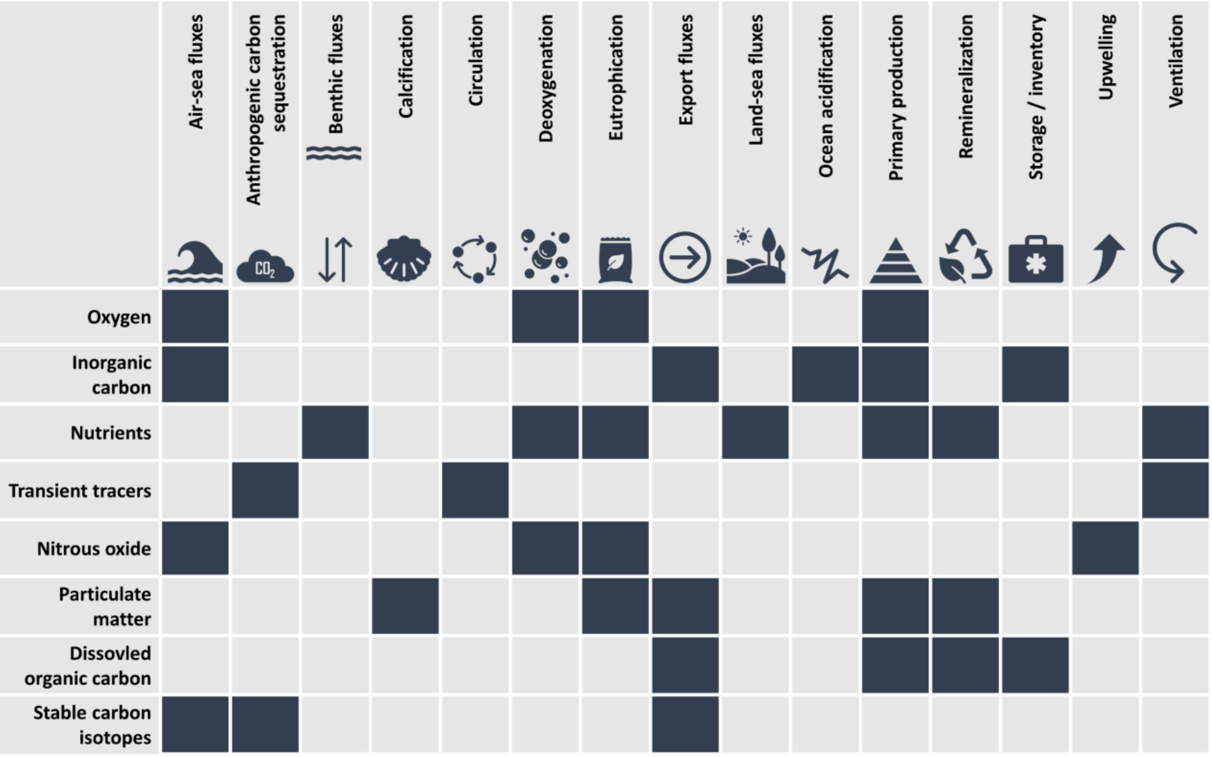
[3] Defined as: "A phenomenon is an observed process, event, or property, with characteristic spatial and timescale(s), measured or derived from one or a combination of EOVs, and needed to answer at least one of the scientific questions asked in order to address relevant societal need" (Telszewski et al., 2018, p. 138).

Essential Ocean Variables (EOV)

The GOOS Expert Panels identify EOVs according to a scoring system based upon the three criteria “Relevance”, “Feasibility”, and “Cost-effectiveness” (Telszewski et al., 2018).

- The relevance indicates how effectively a variable addresses the overall GOOS Themes – Climate, Operational Services, and Ocean Health.
- Feasibility corresponds to whether deriving the variable, i.e. the actual act of observing and analyzing, has proven to be technically feasible on a global scale.
- Cost-effectiveness is defined as the data generation and archiving being affordable (Sloyan et al., 2019).

By implementing a scoring system that addresses the above-described criteria and utilizes the outlined marine biogeochemistry research questions, eight BGC EOVs have been defined. The eight BGC EOVs and related phenomena are displayed in Figure 6.



	Air-sea fluxes	Anthropogenic carbon sequestration	Benthic fluxes	Calcification	Circulation	Deoxygenation	Eutrophication	Export fluxes	Land-sea fluxes	Ocean acidification	Primary production	Remineralization	Storage / inventory	Upwelling	Ventilation
Oxygen	■					■	■				■				
Inorganic carbon	■							■		■	■		■		
Nutrients			■			■	■		■		■	■			■
Transient tracers		■			■										■
Nitrous oxide	■					■	■							■	
Particulate matter				■			■	■			■	■			
Dissovled organic carbon								■			■	■	■		
Stable carbon isotopes	■	■						■							

Figure 6: Captured phenomena by the eight BGC EOVs following the biogeochemical expert panel of GOOS (International Ocean Carbon Coordination Project). Dark squares indicate that a particular phenomenon is captured by the related EOV.

A brief introduction into each BGC EOV following Telszewski et al. (2018) is given in the following.

Oxygen

Dissolved oxygen (O_2) in the ocean is the result of a balance between oxygen supply and consumption. Oxygen supply can be attributed to ocean circulation and ventilation, whereas consumption relates to the process of respiration. Changes in either process strongly influence the absolute amount of oxygen at a given location. The observation of O_2 plays a critical role in understanding the, for the most part, strong decline in O_2 in the ocean in recent decades. As recent oxygen trends influence our understanding of anthropogenic climate change, O_2 should further be regarded as a crucial indicator of climate change. Additionally, O_2 observations are vital to interpret water mass ventilation rates; (ii) for calculations of export production and (iii) to interpret repeat hydrographic data, which are of great relevance to document the anthropogenic CO_2 inventory in the ocean.

Inorganic Carbon

The ocean exchanges vast amounts of carbon naturally through its circulation and biogeochemistry. Due to the high capacity of seawater to absorb carbon, the ocean influences the rate of carbon accumulation in the atmosphere. The ocean's net uptake of carbon, which is around 25% of the yearly anthropogenic emissions, causes the pH value of the seawater to decrease. This process, referred to as ocean acidification, has severe ecological consequences which are being investigated in numerous recent studies. Integral knowledge of the ocean's current carbon uptake and ocean acidification rates is crucial for understanding the evolution of the climate and the carbon cycle influenced by anthropogenic activities. In particular, the underlying mechanisms are of relevance for enhancing predictions of the state of the climate system. To describe the inorganic carbon system, next to temperature and salinity, at least two of the following observations are required; Dissolved Inorganic Carbon (DIC), Total Alkalinity (TA), partial pressure of carbon dioxide (pCO_2), and pH.

Nutrients

The level of organic carbon sequestered by phytoplankton in the upper ocean is frequently constrained and, thus, regulated by the availability of inorganic macronutrients (nitrate (NO_3), nitrite (NO_2), phosphate (PO_4), silicic acid ($SiOH_4$), ammonium (NH_4)). Hence, the concentration of inorganic macronutrients needs to be considered as a primary factor controlling carbon and BGC cycling. Different marine biogeographical regions can be identified, which are characterized by distinctive macronutrient regimes that permanently or seasonally limit phytoplankton growth. Besides identifying shifts in these biogeographic regions, through measuring the macronutrient concentrations net biological production and export fluxes can be determined and eutrophication can be detected and monitored accordingly.

Transient Tracers

Transient tracers are either fully conservative in seawater or have well-defined decay and source functions at the ocean surface. Their observations can be used "[…] to quantify ocean ventilation, transit time distribution, and transport time-scales" (GOOS EOV: Transient tracers). Based on this, e.g. anthropogenic carbon concentrations can be estimated. The most commonly measured transient tracers are chlorofluorocarbons (CFCs (11, 12, 113)), compound sulfur hexafluoride (SF_6), radiocarbon (^{14}C), and tritium (^3He). Due to their different origin, pathways, and decay times, they enable conclusions about different aspects of the global ocean ventilation.

Nitrous Oxide (N_2O)

Nitrous oxide (N_2O) is a crucial climate-relevant trace gas, being a strong greenhouse gas in the troposphere and an ozone-depleting substance in the stratosphere. The ocean is a major source and contributes approximately 30% to the atmospheric N_2O budget. The production processes, nitrification, and denitrification, being enhanced under low O_2 conditions, leads to elevated N_2O concentrations at the oxic/suboxic and oxic/anoxic boundaries.

Particulate Matter (POM)

The term encompasses the organic and inorganic fractions of suspended particulates (total suspended matter; TSM) as well as particulate matter transport within the seawater. Here, biological processes including primary production, formation of calcite or aragonite, and sinking of particles play a crucial role. Particulate organic matter (POM) concentrations in the surface ocean provide a proxy for spatial and temporal variations in biomass. Below the euphotic zone, POM measurements give insight into the export of organic matter and the microbial respiration rate. Further, observations of Particulate Inorganic Carbon (PIC), mainly from calcareous shells of calcifying organisms, and biogenic silica, give insight into the effects of ocean acidification on calcifying organisms.

Dissolved Organic Carbon (DOC)

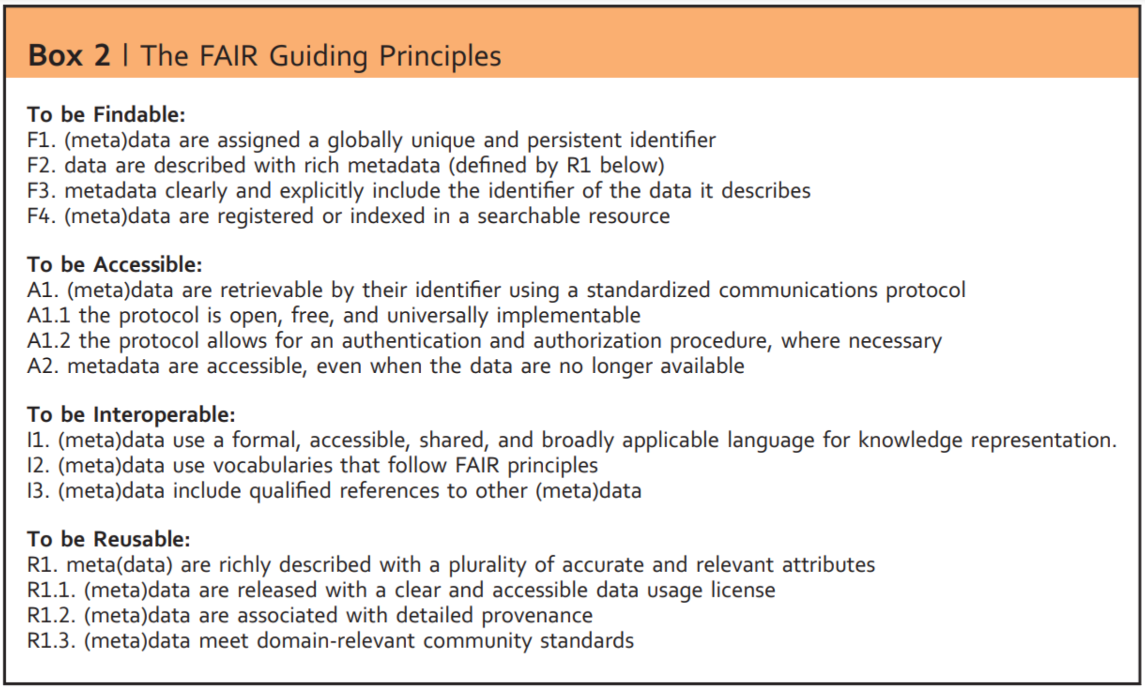
In the ocean, dissolved organic carbon (DOC) has been identified as the second largest bioreactive carbon pool, right after DIC. Next to the size of the pool, the following aspects emphasize its relevance in the ocean's carbon as well as nitrogen cycle; its role as (i) a sink for autotrophically fixed carbon, (ii) a substrate to heterotrophic microbes, and (iii) a sink/source of carbon involved in large scale climate variations. The export of DOC from the epipelagic zone contributes around 20% to the biological pump.

Stable carbon Isotopes

Burning of fossil fuels shifts the atmospheric CO_2 ratio of carbon isotopes ($^{13}C/^{14}C$, Suess effect) towards the lighter carbon-13. Hence, measuring δ13C ($^{13}C/^{12}C$) in the ocean, as a tracer of the ocean's carbon cycle, enables the estimation of the anthropogenic carbon fraction of DIC. In particular, δ13C can be used to separate changes in anthropogenic CO_2 concentrations into changes related to air-sea fluxes and changes related to ocean circulation. Further, δ13C measurements are used in the context of organic matter export rate estimations.

1.3.2 Findable Accessible Interoperable Reusable – FAIR Data

The FAIR Guiding Principles provide guidance for good data management aiming at "machine-actionability[4]" and data provision with longevity in mind (Figure 7) (Wilkinson et al., 2016). Ultimately, the goal of FAIR is effective data provision that optimizes data discovery and data re-usage. To this end, four leading principles have been established (go-fair.org).



Box 2 | The FAIR Guiding Principles

To be Findable:
F1. (meta)data are assigned a globally unique and persistent identifier
F2. data are described with rich metadata (defined by R1 below)
F3. metadata clearly and explicitly include the identifier of the data it describes
F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:
A1. (meta)data are retrievable by their identifier using a standardized communications protocol
A1.1 the protocol is open, free, and universally implementable
A1.2 the protocol allows for an authentication and authorization procedure, where necessary
A2. metadata are accessible, even when the data are no longer available

To be Interoperable:
I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
I2. (meta)data use vocabularies that follow FAIR principles
I3. (meta)data include qualified references to other (meta)data

To be Reusable:
R1. meta(data) are richly described with a plurality of accurate and relevant attributes
R1.1. (meta)data are released with a clear and accessible data usage license
R1.2. (meta)data are associated with detailed provenance
R1.3. (meta)data meet domain-relevant community standards

Figure 7: The FAIR Guiding Principles from Wilkinson et al. (2016).

Findability

The principle of Findability stipulates that data should be easy to find and identify, for both humans and machines. The latter, i.e. machine-readability, is essential for the automatic discovery of data. To be "findable" four criteria must be met:

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[4] The ability for machines to i) identify the type of object (structure and intent), ii) understand/scan the content, iii) comply with the assigned license, and iv) take appropriate action.

F1 (Meta)data are assigned a globally unique and persistent identifier
Usually, all datasets submitted to repositories will automatically receive a globally unique and persistent identifier that removes any ambiguity in the meaning of the published data. The identifier must be i) globally unique, and assigned by a registry service, e.g. Digital Object Identifiers (DOIs), ii) persistent, and iii) ideally point to a landing page, which persists even if the data are no longer available.

F2 Data are described with rich metadata
Humans and machines should be able to find the data purely based on their metadata, even without the data's identifier. Accordingly, the metadata should be as extensive as possible, including higher-level information such as the dataset identifier, the title of the dataset, a brief dataset description, creator/publisher information, publication date, and licensing information provided, and information on the data characteristics itself, e.g. units and information on data quality.

F3 Metadata clearly and explicitly include the identifier of the data they describe
Linking the metadata file to the associated dataset should be explicit through the inclusion of the globally unique and persistent identifier of the dataset in the metadata. This is crucial given that metadata and dataset are usually two separate files.

F4 (Meta)data are registered or indexed in a searchable resource
In addition to the assigned identifiers and rich metadata, the data is ideally indexed by major search engines, e.g. Google Search. A process of search engines to "organize" information eventually enabling fast responses to (data) search queries. In the analog world (small scale) indexing could be compared to the "organization" of literature in libraries. If datasets are not indexed, the data might potentially not be discovered at all. The indexing process strongly relies upon structured metadata, a standardized format for providing information about digital resources, guaranteeing the readability of the content. In this context, schema.org (Section 2.4.2) and the Ocean Data and Information System (ODIS) services are of great importance for ocean data.

Accessibility

The principle of Accessibility stipulates that (machine) access to the data and metadata is ensured through the implementation of standardized communication protocols, supporting machine-to-machine interaction using web services (Haas and Brown, 2004). Ideally, the access is fully automated, including any authentication and authorization procedures.

A1 (Meta)data are retrievable by their identifier using a standardized communication protocol
Standard communication protocols, such as the File Transfer Protocol (FTP, as implemented by the Ocean Carbon Acidification Data System (OCADS[5])) or the Hypertext Transfer Protocol (HTTP, as implemented by ERDDAP[6]) should be used for retrieving the data. To guarantee (at least) metadata access for anyone with internet access, and to guarantee (legal) data protection, the protocol should:

- be open, free, and universally implementable (A1.1)
- allow for an (automatic) authentication and authorization procedure where necessary (A1.2)

Thus, accessible (meta)data should not be confused with open and free data.

A2 Metadata should be accessible even when the data is no longer available
Datasets might get outdated and potentially become unavailable over time. For such instances, it is important that metadata remains accessible, to enable e.g. retrieving contact information of related data.

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[5] https://www.ncei.noaa.gov/products/ocean-carbon-acidification-data-system
[6] https://coastwatch.pfeg.noaa.gov/erddap/index.html

Interoperability

The principle of Interoperability stipulates that (meta)data are provided in common, and published standards. These standards relate to the structures and formats used, as well as implemented semantics and ontologies, which in turn should be FAIR themselves.

I1 (Meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation

The implemented language or ontology should adequately represent the content, be clearly defined, and accessible to enable machine-readable (meta)data. Further, the language should be designed to serve multiple (scientific) applications reducing the need for customized parsers. A typical example in oceanography would be the climate and forecasting variable definitions (Climate and Forecast Standard Names (Eaton et al., 2022), NERC P07[7]), which are extended regularly to meet the community needs.

I2 (Meta)data use vocabularies that follow the FAIR principles

The implemented ontology should also be FAIR itself. Above all, the ontology must be documented, and that documentation should meet at least the FAIR criteria outlined in F1, A1, and I1.

I3 (Meta)data include qualified references to other (meta)data

All connections to related (meta)data should be given, including a clear description of the relation(s). These cross-references can either be links to applied methodologies, and/or also link to other data resources used for the data generation. In either case, a proper citation is expected. In particular, for data synthesis products, the latter becomes very important, as it supports data recognition and provenance.

Reusability

The principle of Reusability stipulates that (meta)data is provided with enough information to enable data users (machine or human) to identify whether the data is useful for given societal issues/scientific applications. This additional information include, in particular, the scope and purpose of the data, the associated limitations, information about data quality, and provenance-related information. Above all, this principle embraces the core of the other principles and the core of FAIR.

R1 (Meta)data are richly described with a plurality of accurate and relevant attributes

The metadata should be as complete as possible and should not be restricted to a targeted group of end-users, as indicated by the term “plurality”, and go beyond data discovery. The (meta)data should:

- be released with a clear and accessible data usage license (R1.1)
- be associated with detailed provenance (R1.2)
- meet domain-relevant community standards (R1.3)

Such metadata are characterized by i) providing sufficient information to describe the context in which the data were created, ii) clearly describing the conditions of usage, i.e. legal interoperability, iii) defining warranted acknowledgments, and iv) providing a clear provenance track recognizing all contributors. In addition, the metadata should follow Best-Practices (BP), and use community-agreed standards and structures. All of which aim at the overarching goal of increasing the usability of the data.

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[7] https://vocab.nerc.ac.uk/collection/P07/current/

2

Methods

2 Methods

In this Section, the methods applied in this thesis are briefly presented. A particular focus is given to the applied QC methods. Several methods already existed and are well-established within the BGC community and applied accordingly. Table 2 provides an overview.

Table 2: A list of methods that have been used during the course of the thesis, including their main application. Whether the method has been developed as part of this thesis is indicated (Novel), as well.

Method	**Application in Thesis**	**Novel / Pre-existing**
Engagement with Community	Participation in GLODAP Reference Group Establishing SPOTS Core Group	Not applicable
FOO Readiness Evaluation Scheme	Evaluation of: GLODAP, SOCAT, MEMENTO, GO_2DAT	Novel
Data Retrieval and Pre-Processing	Harmonization of Original Data	Pre-existing
(Structured) Metadata Templates	Collection of Metadata Schema.org compliant SPOTS Metadata	Novel
AtlantOS QC	QC of Oxygen, Inorganic Carbon, Nutrients, Transient Tracer	Novel (Consulted)
Saturation Plots	QC of transient tracer	Pre-existing
Tracer Ratios	QC of transient tracer	Pre-existing
Crossover Analysis	QC of GLODAP's "core variables" (except tracer) Comparison of SPOTS and GLODAP	Pre-existing (Adapted)
Comparison to Neural Networks	QC of Oxygen, Inorganic Carbon, Nutrients, Transient Tracer	Pre-existing
Multi-Linear Regressions	QC of GLODAP's "core variables" (except tracer)	Pre-existing
Statistical Outlier Test(s)	QC of ship-based BGC time-series	Novel
Minimum Variability	QC of ship-based BGC time-series	Novel
Make Ocean Routine	Merging of GLODAP	Novel

2.1 Engaging with the Community

Synthesis products are community-driven efforts. Accordingly, the process of updating existing products, as well as developing new ones, relies heavily on engagement and consensus building with and within the community (e.g. Lauvset et al., 2022).

2.1.1 GLODAP – Reference Group

The regular (reference group) meetings of GLODAP represent a well-established mechanism for the annual updates of its product. These meetings are mainly related to the organization of a new update, as well as the evaluation of QC results and the determination of adjustment. However, the meetings are also very valuable in terms of:

- sharing updates in data handling (e.g. new persistent cruise identifier from OceanOPS[8])
- obtaining feedback for newly implemented technologies (e.g. data visualization using the Digital Earth Viewer, Python-based crossover tool)
- discussing known issues of applied methodologies (e.g. using inorganic carbon interconsistency in the QC)
- planning and improving outreach (e.g. defining submission requirements)
- identifying and prioritizing problems (e.g. uncertainty calculations)
- planning GLODAPv3

Above all, these regular meetings ensure maintaining a strong core group of scientists with complementing expertise (specific region, variable, basin) around GLODAP and ensure that connections to other relevant and closely related communities are established. Examples of the latter include the above-mentioned collaboration with Digital Earth that resulted in the Python-based “Make Ocean” routine (Section 2.6) and the visualization of GLODAP data in the Digital Earth Viewer but also include ongoing communication and data sharing with other data synthesis products (Coastal Ocean Data Analysis Product in North America, CODAP-NA, Jiang et al., 2021; CARbon IN the MEDiterranean Sea, CARIMED, Sanleón-Bartolomé, 2017; GEOTRACES, Schlitzer et al., 2017, Bowie and Tagliabue, 2018) as well as maintaining a strong connection to the International Ocean Carbon Coordination Project (IOCCP). Importantly, the reference group members are routinely exchanged so that new perspectives and insights are continuously incorporated into GLDOAP’s development. In addition to regular reference group meetings, it is also very important to mention the regular contact with data providers, during all stages of the GLODAP workflow (data retrieval, formatting, QC, archival).

2.1.2 SPOTS – Core Group

Using the approach of GLODAP for community engagement as a role model, establishing a strong community around SPOTS is vital. To this date, the generation of SPOTS included in total four IOCCP-endorsed workshops; the Earth Cube Workshop (Benway et al., 2020), the Marine Ecological Time Series Research Coordination Network (METS-RCN[9]) informatics meeting, and two SPOTS workshops. The latter two exclusively focused on the development of SPOTS itself. The first SPOTS workshop that was held virtually in November 2020 resulted in the establishment of a general consensus towards SPOTS, including the onset of a concept note that clearly outlines the purpose, benefits, methods, timeline, and participants of its pilot. Moreover, four working groups (Concept/Head; Commonality of methods; Data handling; Data policy) were formed, which, during the course of the following two years, developed the underlying structure and methods of SPOTS (Section 6). During the second SPOTS workshop (virtual, November 2022), the results of the working groups were discussed. Besides, the workshop established consensus on applied “Best-Practice” requirements (Section 6) and led to an

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[8] https://www.ocean-ops.org/board

[9] https://www2.whoi.edu/site/mets-rcn/

accompanying manuscript. The two SPOTS-focused workshops, brought together BGC time-series experts from 15 time-series programs around the globe, as well as numerous experts from other synthesis activities (International Group for Marine Ecological Time Series – IGMETS; O'Brien et al., 2017, GLODAP, SOCAT), and related efforts (Global Ocean Acidification Observing Network - GOA-ON; Newton et al., 2019, Integrated Carbon Observation System – ICOS; Steinhoff et al., 2019). In particular, a strong collaboration with the Ocean Carbon and Biogeochemistry[10] program-led METS-RCN network was established. Through this community engagement synergies were created, and collaborations were fostered (Section 2.1.2). Therefore, at this stage, the SPOTS pilot incarnates one of METS-RCN use-cases i) increasing the outreach of SPOTS (e.g. Ocean Science Townhall), ii) establishing a close cooperation with IODE-led ODIS, resulting in the development of structured metadata (Section 2.4.3), and iii) resulting in the selection of the Biological & Chemical Oceanography Data Management Office[11] as datacenter for SPOTS.

2.2 FOO Readiness Evaluation Scheme for BGC Data Synthesis Products

The maturity assessment of BGC EOV data synthesis is carried out using the FOO readiness level scheme for "Data Management and Information Products", which has adopted the technical readiness level concept developed by NASA (National Aeronautics and Space Administration) (Sadin et al., 1989). Following FOO, the readiness levels are categorized into "Concept," "Pilot," and "Mature" (Lindstrom et al., 2012). Since the corresponding nine FOO readiness levels are quite broad, a customized criteria catalog was developed that refines the existing FOO criteria for each level. This catalog serves as a basis for assessing typical characteristics of data products using a level-by-level ("equal-weighted") scoring system, with full compliance to the criteria resulting in a 100% score for a given readiness level. A score of 80% or higher is considered a "pass". Although the readiness levels follow a hierarchical structure, a data product can meet some requirements of higher levels before fully complying with all lower levels. To align with the FAIR guidelines, which strongly influence the maturity of a BGC EOV synthesis data product, these guidelines were incorporated into the criteria at multiple readiness levels to varying degrees. Additionally, the criteria catalog considers the degree of being "fit-for-purpose", which is an important requirement within the ocean observing value chain, and the degree of the data flow's automation, at multiple levels. Given the diverse nature of BGC EOV data, the criteria are intentionally kept as generic as possible. Section 3 provides further insights into the details of this evaluation scheme by exemplarily depicting the criteria and scoring system for readiness level five in detail, and by its application to four selected BGC EOV data synthesis products.

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[10] https://www.us-ocb.org/

[11] https://www.bco-dmo.org/

2.3 Data Retrieval and Pre-Processing

Before data can be retrieved, first awareness about (new) data must be gained. Therefore, GLODAP annually calls for submission of new cruise data. These calls are disseminated through multiple channels (e.g. IOCCP). Besides, through closely collaborating with OCADS and the CLIVAR and Carbon Hydrographic Data Office[12], the GLODAP team is made aware of new (relevant) additions to their data holdings constantly. Accordingly, for the retrieval of "original data" GLODAP directly works with the data generators (i.e. principal investigators), which provide the "bottle data" directly (via email), or the "bottle data" are retrieved from national data centers or larger repositories (e.g. CCHDO). For the SPOTS pilot on the other hand, data retrieval exclusively works through direct communication with principal investigators of the time-series programs. Given the number of data generators, this is not sustainable nor possible for GLODAP.

Once the data is retrieved, each original dataset of GLODAP and SPOTS is formatted into exchange format (Barna et al., 2023). This "harmonization" mainly entails:

- Mapping to WOCE ontology, i.e. WOCE variable names (not always trivial, e.g. P(O)M)
- Mapping to WOCE flagging scheme (Table 3 exemplarily shows a mapping between three frequently used flagging schemes)
- Time, date, and unit conversions (Section 4)
- Creating missing required variables (e.g. missing cast number or bottle numbers)
- Assigning a cruise-identifier, i.e. an expocode for GLODAP (4-character ship code followed by the date given in yyyymmdd format)
- Applying sanity check, i.e. realistic value check (e.g. -100° C water temperature)
- Inspecting (linear regression) CTD- and bottle fit for salinity and oxygen (Section 4)
- Creating a comma separated value file with defined numbers of digits for each variable

Eventually, the harmonized original dataset included in GLODAP is archived at OCADS. Further changes resulting from the additional 1st QC (Section 2.5) are forwarded to both, OCADS, and the corresponding national data center. For SPOTS, additionally individual (harmonized) datasets belonging to the same time-series program, but covering different time spans, are merged into one dataset.

Table 3: Meaning of primary quality flags in three different often used semantics. Note that other semantics with different flagging schemes exist, see Schlitzer 2023.

Flag	Ocean Data Viewer (ODV; Schlitzer, 2023)	WOCE (Barna et al., 2023)	SeaDataNet (L20[13])
0	Acceptable	Interpolated	No quality control
1	Not evaluated / Not calibrated (CTD)	Not evaluated / Not calibrated (CTD)	Good value
2	Not used	Acceptable	Probably good value
3	Not used	Questionable	Probably bad value
4	Questionable	Known bad	Bad value
5	Not used	Not reported	Changed value
6	Not used	Median of replicates	Value below detection
7	Not used	Manual chromatographic peak measurement	Value in excess
8	Known bad	Irregular digital chromatographic peak integration	Interpolated value
9	Not used	Not measured	Missing value

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[12] https://cchdo.ucsd.edu/

[13] http://seadatanet.maris2.nl/v_bodc_vocab_v2/browse.asp?order=conceptid&formname=search&screen=0&lib=l20

2.4 (Structured) Metadata

Metadata is a highly important aspect of datasets regarding FAIR data. However, often an insufficient amount of metadata are provided to data managers and synthesis efforts alike. To enable easier metadata provision, templates to collect rich metadata have been designed and used.

Furthermore, not all metadata are machine-readable to the same degree. Consequently, even very rich metadata, when provided in an inferior format, can limit the FAIRness of the data that is described. Using structured metadata, leveraging from existing and well-established structured metadata practices and web standards solves this issue. Structured metadata can be understood as a standardized concept that implements a well-defined metadata scheme and a common vocabulary. Specifically, structured metadata enable efforts like Google's Data Set Search[14] and GeoCODES[15] to crawl and index the corresponding data into a knowledge graph, enabling the discovery of related datasets, i.e. enabling the discovery and identification of datasets that are merged into synthesis products.

2.4.1 Metadata Collection

The collection of metadata is carried out by collaborating with data providers. During the submission process of the synthesis products, data providers are asked to provide additional metadata, ideally by filling out customized metadata templates. Two excel-templates were employed for this thesis:

- GLODAP: The Ocean Carbon and Acidification Data System (OCADS) ocean carbon data submission form[16]
- SPOTS: SPOTS' customized metadata template for BGC EOV ship-based time-series programs

Both of these templates are developed with ship-based data in mind. If filled out correctly, the templates provide general information about the observation program (e.g. principal investigator, location, and time), and measured variables (e.g. sampling method, and units), as well as about more detailed information (e.g. analytical methods, associated instrumentation, calibration, and QC procedures, and standards). While the OCADS template focuses on the variables of the inorganic carbon system (pH, TA, DIC, pCO_2), the SPOTS template additionally focuses on O_2, nutrients, DOC, and POM. The focused SPOTS working group "Commonality of methods" (Section 2.1.2) developed the latter template. Using the OCADS template as basis, it implements additional information from the Bermuda Time-Series Workshop report (Lorenzoni and Benway, 2013), GO-SHIP manuals (Langdon et al., 2010; Becker et al., 2019), and results from the Scientific Committee on Research Working Group 147 "Towards comparability of global oceanic nutrient data" (Bakker et al., 2016a; Bakker et al., 2016b; Aoyama et al., 2015).

However, note that for GLODAP, many datasets were not directly submitted to its data management team, but rather retrieved from other data centers (e.g. through CCHDO, Section 2.4.1). Accordingly, often submitted metadata do not meet the rich level of the OCADS template. Moreover, presently, only the responsible principal investigator, chief scientist, vessel name and, cruise-date are required metadata for GLODAP. These information are usually attached as header-lines to the data file itself.

2.4.2 Schema.org

To derive structured metadata from the above described user-friendly templates, through the collaboration with "Science on Schema" (Shepard et al., 2022) and ODIS, in the course of this thesis, structured metadata (templates) for BGC EOV ship-based time-series datasets were developed for

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[14] https://datasetsearch.research.google.com/

[15] https://geocodes.earthcube.org/

[16] https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/support/SubmissionForm_carbon_v1.xlsx

SPOTS. For the structure metadata, one of the most common vocabularies in structured metadata, Schema.org, “[…] a collaborative, community activity with a mission to create, maintain, and promote schemas for structured data on the Internet, on web pages, in email messages, and beyond” (Schema.org, 2023), has been applied. Following the recommendations of Google-Search (Google Search Central, 2023), the encoding format used is json-ld. Note that OCADS uses MD Metadata ISO 19115 (ISO, 2014) for GLODAP’s original datasets.

Explaining Schema.org entirely is beyond the thesis, however, a few important aspects of the type “Dataset” are explained here to demonstrate the vocabulary and its structure. In Schema.org the type “Dataset” has a fixed list of “Properties” that can be used to describe the dataset, e.g. “Keywords”. These properties in turn are expected to be given as a certain type, e.g. “Text”. Often sub-properties are implemented as well to enable a more sophisticated attribute description, e.g. “DefinedTerm”. For illustration purposes, a non-exhaustive set of example properties is shown in Table 4 and the corresponding structures/connection are displayed in Figure 8.

Table 4: Selected properties, their description, and recommended (expected) type for “Datasets” in Schema.org.

Property	Description	Recommended type
Name	A descriptive name of a dataset	text
Description	A short summary describing a dataset	text
Url	Location of a page describing the dataset	url
SameAs	Other URLs that can be used to access the dataset page	url
License	A license document that applies to this content	url
isAccessibleForFree	Specifying if the dataset is accessible for free	Boolean
Keywords	Keywords summarizing the dataset	Defined Term
Identifier	An identifier for the dataset, such as a DOI	PropertyValue
VariableMeasured	What does the dataset measure?	PropertyValue

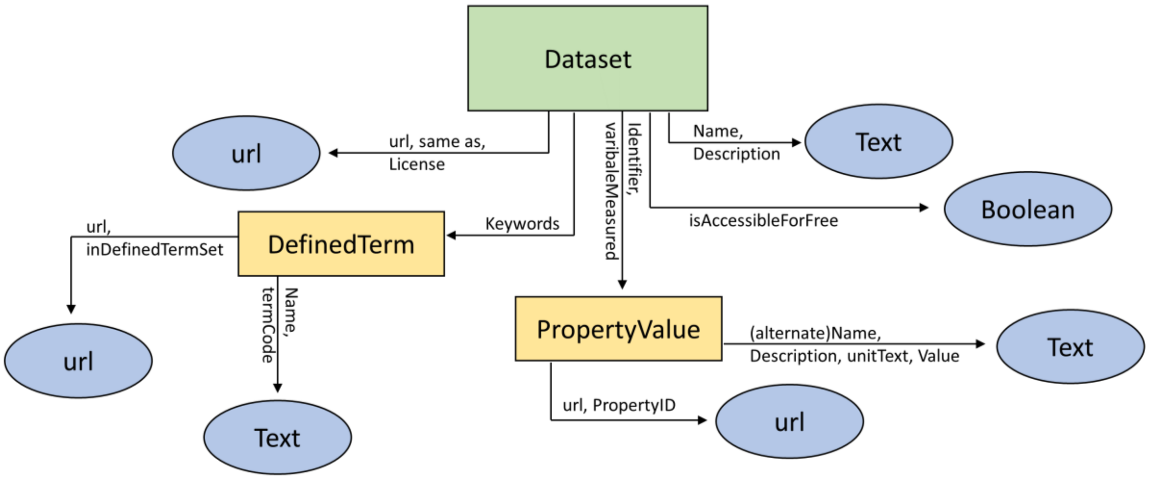

Figure 8: Schematic illustration displaying the Schema.org structure of the selected properties listed in Table 4.

Note that to describe the metadata of other schema.org types, e.g. “Events”, another fixed list of expected properties must be used to describe its attributes. The principle remains the same.

2.4.3 SPOTS metadata

Regarding SPOTS, two different schema.org metadata types are relevant: Datasets and Events. The implementation of both types is beneficial as it allows one to differentiate between methodologies applied to create the dataset and multiple methodologies applied during the actual sample analyzes. This is of particular relevance as the latter commonly vary within one dataset. Hence, the "Dataset" metadata are purely linked to the generated datasets of a time-series or SPOTS itself, while the Event" metadata describe the time-series program with related (sub-)events that describe station visits (e.g. a particular year). Here, information on specific types of measurements (e.g. nutrient sample analysis) that result in the data of datasets are given. Accordingly, clear connections between all related files, as schematically illustrated in Figure 9, are provided. Note that one can focus on any particular event or dataset, i.e. multiple point-of-views are possible.

This setup and structure also enable the application of the scheme to all types of time-series measurements, e.g. net measurements, and the degree of granularity is very flexible, enabling a customized approach for each time-series program. However, in some instances, the rather rigid Schema.org construct was extended when necessary (e.g. accepting "DefinedTerm" for the property "variableMeasured"). In addition to the attributes listed in Table 4, the generated metadata files for each time-series program and SPOTS itself provide information on (following the FAIR principle, Section 1.3.2):

- Data providers- and generators
- Funding
- Date
- Location
- Measurement techniques
- Cruise reports

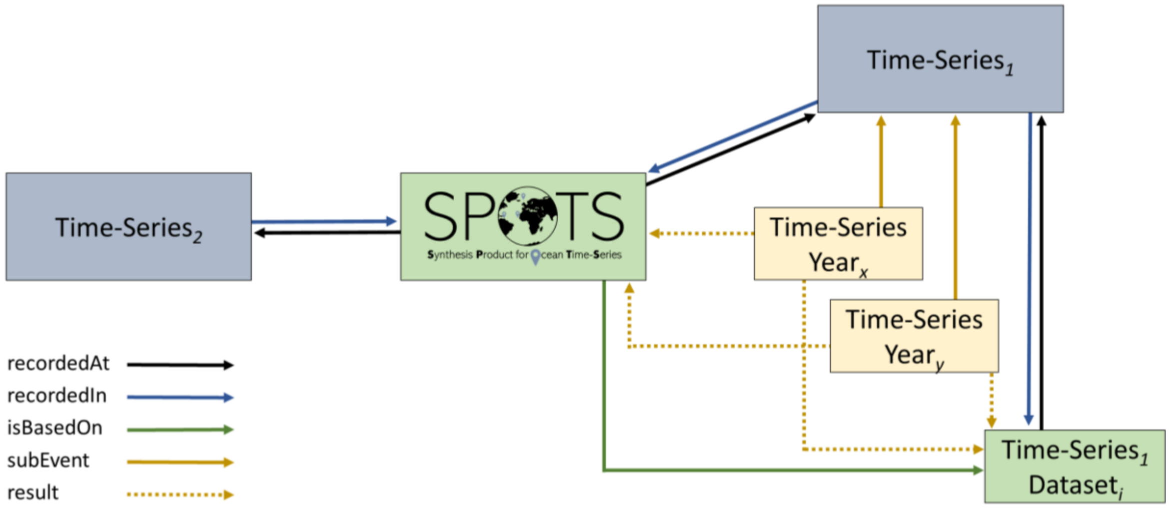

Figure 9: Schematic illustration of connections between the SPOTS Dataset and related time-series Events using the Schema.org vocabulary. Green rectangles indicate metadata of the type Datasets, Grey rectangles indicate metadata of the type Events, and yellow rectangles metadata of the type subEvents. The arrows indicate the relation (schmea.org vocabulary) between the different types of metadata. Clear provenance, as well as differentiation between methods applied during different years, and differentiation between product generation (Dataset) and data generation (Event) is enabled through this structure. Note that the illustration is kept non-specific and non-exhausting.

All structured metadata files are hosted by the METS-RCN GitHub repository[17], which has been specifically set up for this purpose. From the repository, ODIS obtains access to the metadata and is presently working on a dedicated “Time-Series” source type in its catalog[18] which is based upon these files.

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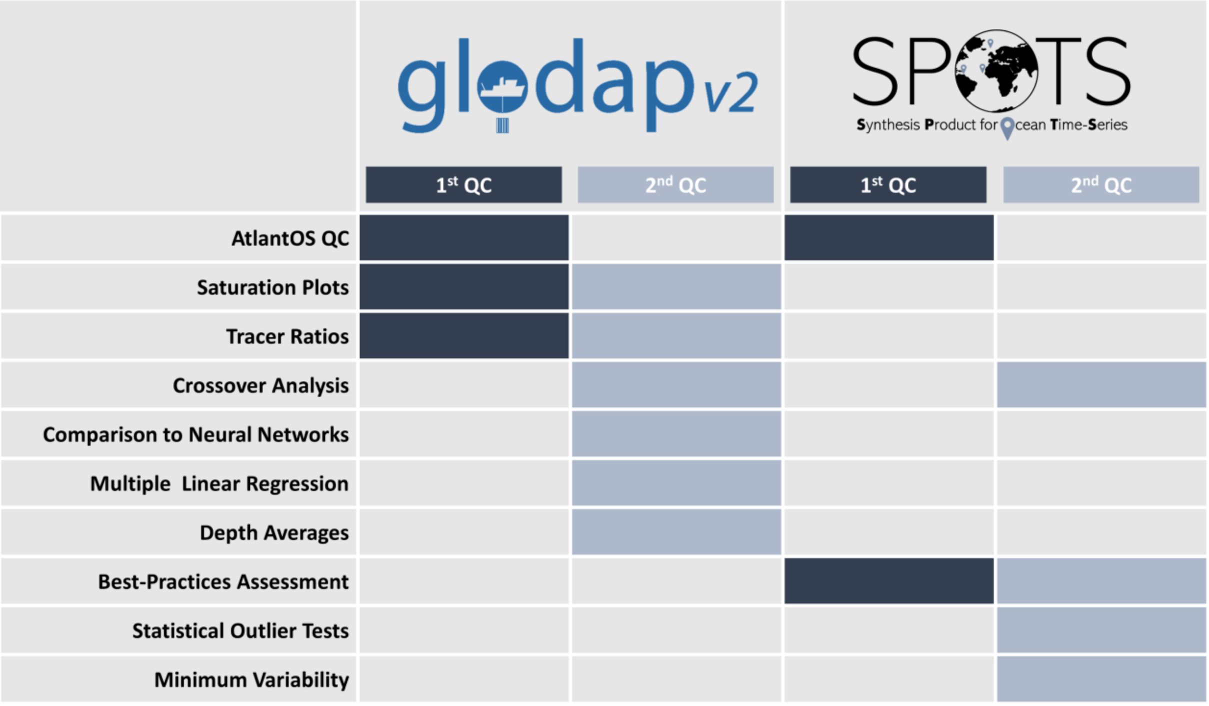
[17] https://github.com/earthcube/METS-RCN

[18] https://catalogue.odis.org/

2.5 Data Quality Control (QC)

Striving towards fully comparable data is a key mission for synthesis products. However, data from multiple heterogenic sources often show large artificial inconsistencies, especially historical data. To combat this and to provide comparable data, a fundamental part of the generation of a synthesis product is the underlying, external QC of the included data. In the following, the concept of QC is introduced and subsequently, the applied QC routines are briefly presented. Methods that are already explained in great detail in one of the included manuscripts are only briefly described, these are: “Neural network comparisons for GLODAP” (Section 4), the “Best-Practice Assessment for SPOTS” (Section 6), and “Minimum variability determination for SPOTS” (Section 6). Figure 10 summarizes which QC methods were applied for which synthesis product.



	glodapv2		SPOTS Synthesis Product for Ocean Time-Series	
	1st QC	2nd QC	1st QC	2nd QC
AtlantOS QC	■		■	
Saturation Plots	■	▨		
Tracer Ratios	■	▨		
Crossover Analysis		▨		▨
Comparison to Neural Networks		▨		
Multiple Linear Regression		▨		
Depth Averages		▨		
Best-Practices Assessment			■	▨
Statistical Outlier Tests				▨
Minimum Variability				▨

Figure 10: The applied QC methods related to GLODAP or SPOTS (or both). The color further indicates whether a QC method was used to increase the precision (dark blue) or accuracy (light blue) of the data. For GLODAP flagging (precision) and adjustments (accuracy) were applied, while for SPOTS only flagging was applied.

2.5.1 Quality Control (QC), Quality Assurance (QA), and Best-Practices (BP)

QC, Quality Assurance (QA), and BPs are often used synonymously. Even though these checks and guides are closely related and all aim at increasing the data quality, it is important to separate them. QA relates to processes that are employed to support the generation of high-quality data during the sampling and analyzing procedures (Bushnell et al., 2019). QC in turn relates to all checks of data quality applied post data generation. BPs are “guides” describing community-accepted methodologies in detail (e.g. Dickson et al., 2007) that have proven to produce the most precise and accurate results relative to other methodologies with the same objective (Pearlman et al., 2019). This distinction is particularly important given that some types of QC rely upon QA “results”, such as comparisons to reference materials, precision estimates from duplicate measurements, or outcomes from inter-laboratory calibration exercises (e.g. QUASIMEME, Wells et al., 1997). Further, some types of QC rely upon known BPs to evaluate applied methodologies. During the synthesis of data, the data generation process of the original data is already finished. Moreover, often an internal, i.e. by the data generator, QC of the data has already been applied before data is acquired by synthesis efforts. Hence, the applied checks for synthesis products are restricted to the external QC of the data, but, if necessary, make use of available QA results, and provided BP information.

2.5.2 1st QC vs. 2nd QC

To appreciate the effect of the different QCs on the QC'ed datasets, it is necessary to comprehend the difference between precision and accuracy. The precision of data is a measure of the statistical variability of the data, i.e. the closer samples from repeated measurements (e.g. duplicates) are to each other, the more precise the data is. It is important to understand that precise data do not need to be accurate, i.e. precise data can deviate from a so-called "true value" (Figure 11). Eventually, it is the aim of 1st QC techniques to improve the precision of the dataset by identifying single bad outliers of a particular cruise/cast. 1st QC quality flag schemes (e.g. WOCE, Table 3) assigned to the data indicate the result of related precision checks. Typical causes for individual outliers are contaminated samples or leaking sample bottles, which have not been detected during the QA. The 2nd QC in turn depends upon precise data (i.e. the 1st QC) and checks against historical data as a proxy for the true value. It aims at increasing the accuracy by identifying systematic biases. In some cases, the 2nd QC results in the application of correction factors to the data. Potential sources for systematic biases include errors during unit conversion, applying a method that itself introduces a bias (e.g. coulometry vs. potentiometric DIC analysis; using different silicate standards), or not correcting against certified reference materials (CRMs).

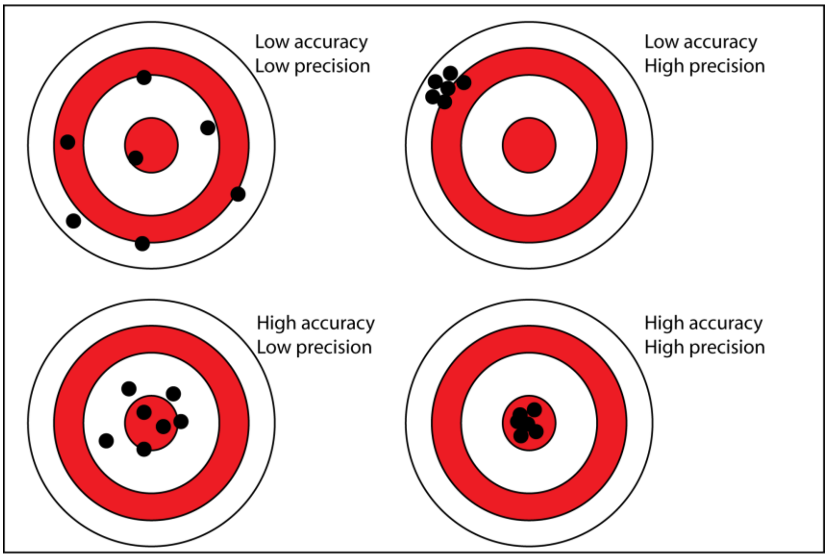


Figure 11: Schematic illustration of the differences between precision and accuracy (Portable Spectral Services, 2023).

2.5.3 AtlantOS QC: Visual inspection of property-property plots

To support scientists, the AtlantOS QC software (Velo et al., 2021) was developed for the 1st QC of repeated hydrography, however, it is also used for the QC of fixed station time-series data. The software enables to graphically illustrate, analyze, and manage data by providing an interactive interface. Note that for its application the entire dataset must be on the same scale/unit and be reported using the WOCE ontology (Barna et al., 2023).

By employing AtlantOS QC, surface-to-bottom measurement profiles are inspected using multiple property-property plots, that enable easy identification of outliers within a profile and against all other profiles. Commonly used property-property plots are based upon properties that strongly correlate with each other, ideally in a linear relation. Examples of often scrutinized relations are the well-known Redfield ratio describing expected ratios between nitrate and phosphate, silicate against apparent oxygen utilization, or TA against salinity. Further, samples are compared against "calculated" variables, variables such as N* (a quasi-conservative tracer of nitrogen, Gruber and Sarmiento, 1997), but also against variables calculated from a range of "models". Some of these models use multiple predictor variables to compute expected concentrations and exploit machine-learning techniques. The used models, implemented in AtlantOS QC, are the (equation-based) carbon system calculation program CO2SYS (van Heuven et al., 2011), as well as the neural networks NNG2 (Velo et al., 2013), NNGv2 (Broullon et al., 2019), CArbonate system and Nutrients concentration from hYdrological properties and Oxygen using a Neural-network (CANYON-B, Bittig et al., 2018), and Empirical Seawater Property Estimation Routines (ESPER, Carter et al., 2021). ESPER also makes use of locally interpolated regressions. The applied rule of thumb is to report a sample to the corresponding principal investigator (awaiting confirmation) and to flag it (WOCE flag 3, Table 3) if the sample is identified as an outlier in at least three different property-property plots. The application of the AtlantOS QC software also enables a transparent QC process as evidence and version control to the resultant flag changes are automatically stored. Note that the development of AtlantOS QC was supported through consultation.

2.5.4 Saturation Plots

The QC of transient tracers is an important part of the annual GLODAP routine. One of the applied methods is the analysis of the CFC saturation near the surface ($p < 20$ dbar) that enables the detection of single (surface) outliers and potential systematic biases. To obtain the saturation ratios, the CFC concentrations (pmol kg^{-1}) are converted to an atmospheric mixing ratio (ppt) using solubility functions. These are functions of salinity and temperature following Warner and Weiss (1985) for CFC-11 and CFC-12, Bu and Warner (1995) for CFC-113, and Bullister et al. (2002) for SF_6. Subsequently, the resultant atmospheric mixing ratios are divided by the actual atmospheric ratios of the year of sampling (Walker et al., 2000; Bullister 2017) yielding the saturation (given in %).

The detection of single outliers is executed visually and is rather self-explanatory (even though natural phenomena can also cause them), but especially to detect biases it is important to understand the expected saturation. Generally, these should be in the range of 90% - 110%. Strong(er) under-saturation may occur due to strong surface cooling, water mass formation (Rhein et al., 2002), and/or intrusion of older water masses due to intense deep convection events (Yashayaev, 2017). Over-saturation in turn is usually linked to strong heating events or can – in the case of SF_6 – be linked to tracer release experiments. Hence, saturations are always analyzed together with temperature and salinity data. Further, regressions (residuals) between the different tracers are also used during the QC process. For "good" data, the saturations of CFC-11 and CFC-12 should be very similar, while CFC-113 (SF_6) might show larger (smaller) under-saturations due to smaller (higher) gas transfer velocities and CFC-113 can have suspicious saturations in warmer waters as it is unstable under such conditions (e.g. Roether et al., 2001; Wanninkhof, 2014).

2.5.5 Tracer Ratios

A further applied method to QC CFCs is the analysis of the tracer ratios throughout the whole water column. Tracer surface saturations and tracer ratios are applied complementary in the QC (Jeansson et al., 2010). For the latter, the tracer atmospheric mixing ratios of CFC-12 and CFC-113 are compared against the mixing ratios of CFC-11. Assuming that the tracers are stable in seawater, all interior ratios are expected to follow the historical atmospheric mixing ratios over time from zero concentrations (oldest waters at larger depths) to the measured atmospheric concentrations of the sampling year (surface). Note that the decrease of the atmospheric CFC concentrations for relatively recent data (1994 onwards for CFC-11 and CFC-113; 2004 onwards for CFC-12) is visible in the atmospheric curves as is the loss of CFC-113 in warm waters. If the samples deviate greatly from the atmospheric curve, one of the two CFC components is likely biased. Individual outliers are detected and scrutinized accordingly. The procedure for SF_6 slightly deviates as SF_6 does not follow a distinct curve and is compared against CFC-12. The exact procedure, including figures, is outlined in Section 4.

2.5.6 Crossover-Analysis

The underlying “running-cluster” routine (Tanhua et al., 2010) in the crossover analysis applied, compares data from two “crossing” or nearby cruises on a station-by-station basis. For each analyzed variable the routine calculates a depth-independent offset (inverse variance weighted) between the two cruises, defined as “crossover-pair offset”. Note that the higher the precision of the cruise data is, the better (easier and more robust) the crossover-pair offset can be determined. In the regular running-cluster method, the offset calculation is restricted to layers assumed to be stable, i.e. to layers with the least temporal variability. This ensures that the influence of natural signals on the calculated offsets is limited, which becomes especially important if the time period between crossing cruises is large. Ideally, this layer is determined by the identification of layers with the highest resident time and mean age (oldest) using measurements of transient tracers (Stöven and Tanhua, 2014). In the open ocean, usually, the bottom layers (below 1500 dbar) are chosen. In an adapted version of the running-cluster routine, developed explicitly for the QC of fixed ship-based time-series data, also data from shallower water layers with higher variability are used for the offset calculation.

For each analyzed cruise and variable, the running-cluster routine is repeated over all available crossing or nearby cruises. The calculated crossover-pair offsets are then weight-averaged to obtain the total cruise offset. Eventually, this cruise offset can be used to detect and correct for systematic biases, especially if the underlying crossover-pair offsets are similar. However, to correlate a cruise offset to a systematic bias, the crossing and nearby cruises must be known (or assumed) to be accurate. Since this is not the case for GLODAPv2 (Olsen et al., 2016), an additional inversion procedure step is necessary that used the calculated crossover-pair offsets. This additional weighted (damped) least-squares (Johnson et al., 2001) inversion determines the set of corrections required to simultaneously minimize all crossover-pair offsets for all included 724 cruises in GLODAPv2. Consequently, by applying these corrections, GLODAPv2 represents empirical true values for the variables that were 2nd QC’ed. This justifies using the previous GLODAP version as an “accurate” reference dataset for the QC of the annual GLODAP updates. During these updates, the crossover routine is applied to QC new cruises being adjusted towards the already included GLODAP cruises. By further assuming that any systematic bias should be constant for the entire duration of a cruise, one constant correction, i.e. adjustment, is applied per cruise, if applicable. More details on the individual steps involved in the regular crossover routine (Figure 12), as well as more details on the altered routine for time-series data, are given in Section 4 and Section 6, respectively. All crossover analyses applied are based on the MATLAB toolbox prepared by Lauvset and Tanhua (2015).

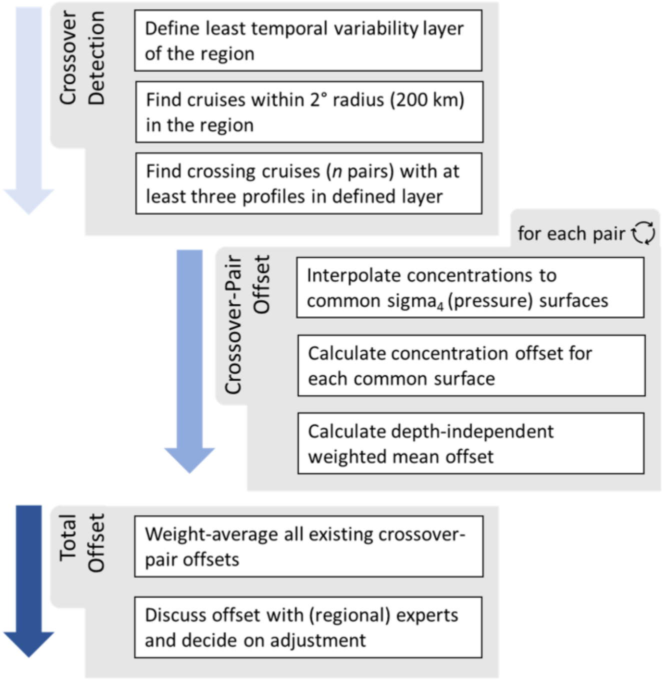


Figure 12: Schematic workflow of regular crossover QC. Note that the crossover radius and depth surface are dependent on user input. The most common ones are shown here: 2° and sigma$_4$, respectively.

2.5.7 Comparisons to CANYON-B and CONTENT

Being trained with GLODAPv2, the neural networks CANYON-B (Bittig et al., 2018), and CONsisTency EstimatioN and amounT (CONTENT, Bittig et al., 2018) represent dynamical climatologies, and estimate nutrients and seawater CO_2 chemistry variables based on the input parameters: Pressure, salinity, temperature, O_2, latitude, longitude, and time. For these estimations, the neural network of CONTENT additionally facilitates maximizing the consistency of the estimated inorganic carbon system.

Employing these dynamical climatologies in the QC of GLODAP offers the advantage of accounting for nonlinear relationships between ocean properties and changes in water masses within. Accordingly, these estimations are used to support the crossover analyses (Section 2.5.6) in detecting offsets to the reference dataset. For each estimated variable, differences between measured and estimated values are inspected for the entire cruise data (depth space). Moreover, the corresponding absolute differences divided by the CANYON-B and CONTENT uncertainty estimate, are inspected to set the model uncertainty in relation to the differences. The visual inspection of these comparisons, in combination with the overall mean difference (calculated using all differences below 500 m) eventually indicates the offset against GLODAPv2. Note that this method must be applied with extra caution, e.g. by disregarding comparisons for which the crossover analysis indicates biases in salinity and/or O_2 data. More details, including an example, are given in Lauvset et al. (2022; Section 4).

2.5.8 Multi-Linear Regressions (MLR)

To support the detection of systematic biases of new GLOPAP cruises with limited crossover analysis results (sparsely covered regions), multi-linear regression analyses (MLR) following Jutterström et al. (2010) are applied. The main steps of the MLR QC, for each QC'ed variable, are the following:

1. "GLODAP-MLRs": Apply MLRs to deep GLODAP data ($\geq$ 1,500m) that are nearby the stations of the new cruise (2° radius) using multiple combinations of predictor variables
2. Evaluate the robustness of the MLRs using R^2 and the root mean squared error
3. "Cruise-MLRs": Apply the same MLRs to the cruise that is QC'ed using the calculated coefficients from the "GLODAP-MLRs"
4. Compare the values calculated from the Cruise-MLRs to the measured samples
5. Calculate the median offset (+/- interquartile range) of all differences (ratios) for each Cruise-MLR

For any MLR a minimum of 10 samples is required, and only predictor variables known to be accurate are used. Here one example of a frequently used MLR for TA is presented:

- $TA=\alpha_1 +\alpha_2 Salinity+\alpha_3 Theta+\alpha_4 PO_4 +\alpha_5 SiOH_4$

Eventually, all calculated median offsets are used as a proxy for the accuracy of a variable. The application of potential corrections for systematic biases is additionally guided by the robustness of the MLRs, the comparability of all median offsets, as well as comparisons of deep-water averages.

2.5.9 Statistical Outlier Test: (Seasonal) Sigma-Tests

For a few time-series programs, statistical (automatic) QC routines are designed and applied to flag (WOCE flag 3) the BGC EOVs of the original datasets (Section 6). Taking advantage of the time-series measurements usually being measured at identical depth levels (pressure), these tests are designed to identify outliers in time on a constant depth surface. For the test to be applied a minimum of five samples on the analyzed layer are required.

The first test aims at detecting suspicious samples by applying a three-sigma criterion to each depth layer using z-scores. Samples outside of three standard deviations of the historical mean value, i.e. samples smaller or larger than 99% of the data (symmetrically), are flagged. Subsequently, a second two-sigma test (95%) that only compares seasonal data with each other, i.e. only winter samples with winter samples, spring samples with spring samples, etc., is applied to identify and flag remaining outliers. If oxygen is also measured, comparisons to CANYON_B (Bittig et al., 2018) estimates are used to support flagging decisions. Therefore, the following steps are applied:

1. Calculate CANYON_B values (nutrients and inorganic carbon) using oxygen, salinity, and temperature
2. Calculate the difference between the measured value and the calculated value for each depth surface
3. Normalize the difference to be centered around 0 (minimizing effects of seasonal biases)
4. Check for outliers using two-sigma criterion (z-score)

Given the irregular measurements, more advanced routines that were developed in the course of this thesis (Section 6) are not applied. Also note, that all applied flags are further examined and confirmed by the respective time-series PI. Figure 13 exemplarily shows the result of the statistical outlier QC for the Cape Verde Ocean Observatory (CVOO) time-series for oxygen measurements during autumn.

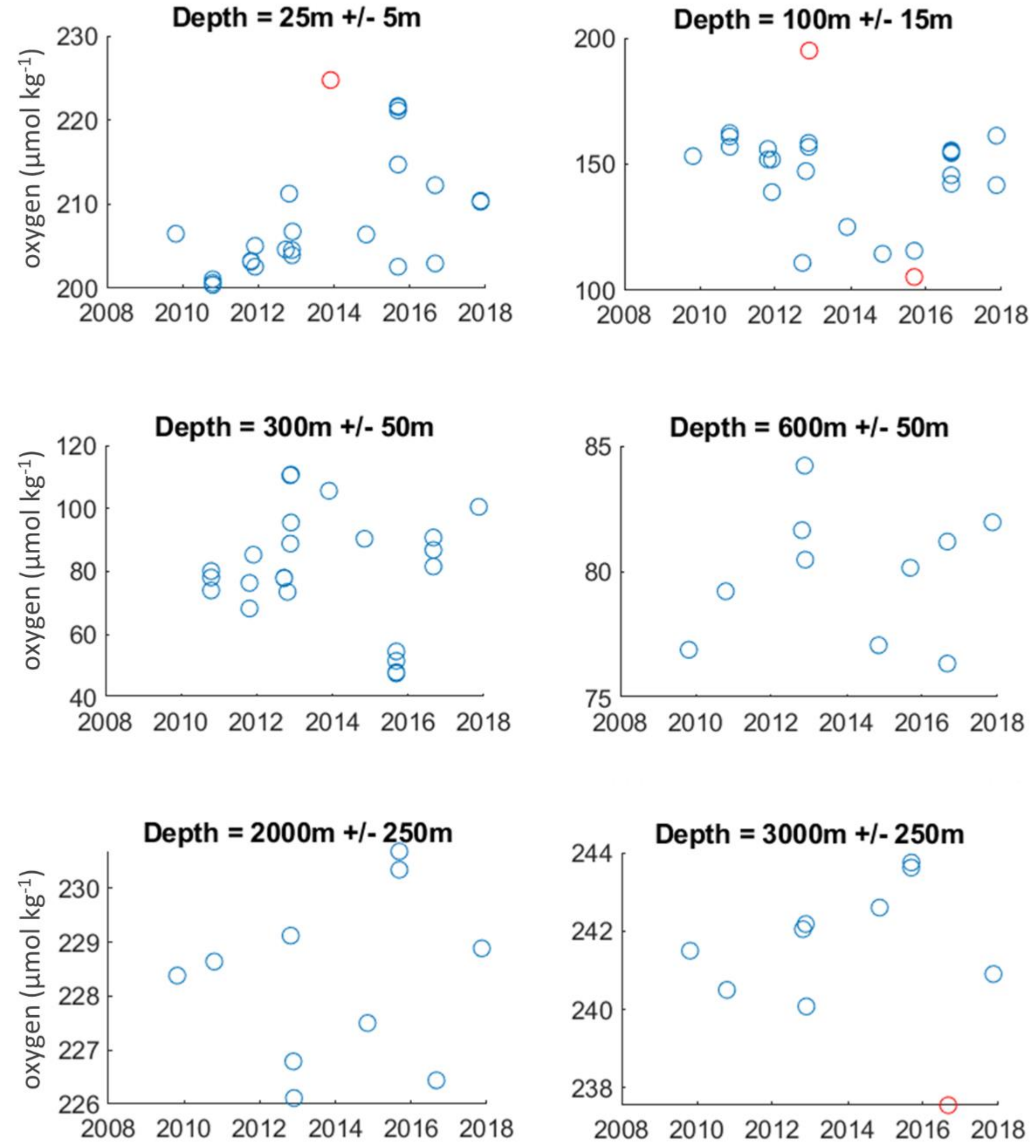


Figure 13: Results of statistical outlier QC for oxygen measurements at CVOO during autumn. Each subplot displays one layer/ slab, and red circles indicate outliers (two-sigma). For illustration purposes only 5 of the 17 "standard CVOO layers" are shown. Concentrations are given in µmol kg^{-1}.

2.5.10 Minimum Variability

To assess the consistency of measurement quality within a time-series program, the minimum variability estimation routine was developed. First, for each standard depth layer (+/- 100 dbar) of the time-series program, the coefficient of variation[19] for O_2 is calculated. Subsequently, the layer with the least oxygen variability, i.e. the layer with the lowest coefficient of variation in time for O_2, is determined. Eventually, for all other BGC EOVs, the minimum variability is calculated on the detected layer with the least oxygen variability (+/- 100 dbar) by means of the coefficient of variation. The choice of using the layer that is closest to an oxygen equilibrium for all calculations relates to oxygen concentrations being linked to (amongst others) variation in ventilation, water mass changes, or changes in consumption and production by biological activity (Sarmiento and Gruber, 2006; Keeling et al., 2010; Stramma and Schmidtko, 2019). This layer thus correlates to (relatively) stable conditions, and the natural variability of other BGC variables is expected to be rather low. For locations that are not characterized by large natural variability (as indicated by high coefficients of variation for oxygen and salinity), a low minimum variability indicates a consistent level of data quality throughout the measurement period for the analyzed variable. However, for locations with high natural variability, high minimum variability estimates do not necessarily relate to inconsistencies in measurement quality. Section 6 gives further insights into this method.

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[19] Coefficient of Variation = (Standard Deviation / Mean) * 100

2.6 Data Merging Routine: GLODAP's "Make Ocean"

To enable the reproducibility of GLODAP, a Python-based Juypter Notebook that generates the final global and regional GLODAP synthesis products was developed and applied. The notebook also generates consistent unadjusted and adjusted individual cruise files of newly added cruise data. The implemented merging routine follows a strict order of clearly defined steps (based upon Key et al., 2004 and Olsen et al., 2016) and uses the Python libraries numpy, pandas, scipy, shapely, seawater, oct2py, and netCDF4. It is designed for cruise bottle data in exchange format (WOCE semantics, Barna et al., 2023), the officially required submission format of GLODAP. The program processes cruise by cruise and merges the individual consistent cruise datasets in a final step. More details on the specifics of the Python script can be found at https://git.geomar.de/patrick-michaelis/python-for-glodap.

The first processing functions import, select, and re-arrange the data and fix small issues of the cruise file. Amongst others, these functions exclude data with WOCE flags 3,4,5, and 8 (Table 3), as well as data without temperature or pressure data, by setting corresponding values to -999 and their WOCE flags to 9. Cruise numbers are also assigned that enable the differentiation between all GLODAPv2 updates. Non-trivial calculations are restricted to missing depths (bottom), and nitrate. Missing bottom depths are assigned by either the maximum sample depth or the extracted bottom depth from ETOPO1 (Amante and Eakins, 2009) – the larger value is used. Missing pressure or depth values are estimated following UNESCO (1981). Lastly, whenever possible, the division of nitrate plus nitrite values (NO_2+NO_3) into nitrate (NO_3) and nitrite (NO_2) is executed. If only nitrate plus nitrite values are given, these are renamed to nitrate.

The next set of functions start to alter the original data more drastically. Bottle salinity- and oxygen (SALNTY, OXYGEN) data is merged with their sensor counterparts (CTDSAL, CTDOXY), following the action (Section 4) implied in the GLODAP adjustment table[20]. Further, the merged salinity, and oxygen data, as well as nutrient data are vertically interpolated to fill data gaps using a quasi-Hermetian piecewise polynomial. Values are only interpolated if the maximum vertical data separation distances (Table 4 in Key et al., 2010) are met. The corresponding WOCE flags are set to 0.

The next functions incorporate aspects of GLODAP that result in its high consistency, and usability. Here, the first three functions must be executed first and in succession:

1. The adjustments resulting from the 2nd QC are implemented for the core variables of GLODAP except for pH. Note that all data that have passed the 2nd QC (no adjustment or adjusted) are indicated accordingly through additional 2nd QC flags (Section 4).

2. Whenever necessary, pH is converted to the total scale at 25°C and (pCO_2) fCO_2 to fCO_2 at 20°C and 0 dbar. For the conversion, CO2SYS is employed with TA used as the second inorganic carbon sub-parameter. Missing TA values are approximated as 67 times salinity. The carbonate dissociation constants of Lueker et al. (2000), the bisulfate dissociation constant of Dickson (1990), and the borate-to-salinity ratio of Uppström (1974) are used. Once pH is converted, adjustments to pH are applied as well.

3. If at least two sup-parameters of the inorganic carbon system are available, the missing inorganic carbon sub-parameters are calculated using CO2SYS. Here, some rules were established:
   - Adjustments and scale conversions have to be applied first
   - The same constants as for the conversions (pH, fCO_2) are used
   - DIC, TA is the preferred pair to calculate pH and fCO_2

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[20] https://glodap.geomar.de

- If either DIC or TA is missing and both pH and fCO_2 data existed, pH is preferred
- If less than a third of the total number of values is measured, then all values are replaced by calculated values (only for DIC, TA, and pH)

The so-calculated inorganic carbon sub-parameters are indicated by a WOCE flag 0

4. Values for potential temperature; potential densities referenced to 0; 1,000; 2,000; 3,000; and 4,000 dbar; neutral density; apparent oxygen utilization are calculated using Fofonoff (1977), Bryden (1973), Sérazin (2011), and Garcia and Gordon (1992)
5. Partial pressures for CFC-11, CFC-12, CFC-113, CCl_4, and SF_6 are calculated using the solubilities by Warner and Weiss (1985), Bu and Warner (1995), Bullister and Wisegarver (1998), and Bullister et al. (2002)
6. pH in-situ values are obtained following the same method as in 2

The last functions, processing the individual cruise dataset, create the columns DOI, and region, as well as sort the entire dataset according to (hierarchical) station number, pressure, and bottle number. Lastly, an adjusted cruise file that is consistent with the format and semantics of the existing GLODAP updates is saved as a comma-separated value file.

Eventually, all created individual consistent adjusted cruise files are appended to the previous GLODAP update to create the GLODAP master file. The regional files are split up using the region information stored in the online adjustment table.

3

A status assessment of selected data synthesis products for ocean biogeochemistry

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A status assessment of selected data synthesis products for ocean biogeochemistry

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Ocean data synthesis products for specific biogeochemical essential ocean variables have the potential to facilitate today's biogeochemical ocean data usage and comply with the Findable Accessible Interoperable and Reusable (FAIR) data principles. The products constitute key outputs from the Global Ocean Observation System, laying the observational foundation for information and services regarding climate and environmental status of the ocean. Using the Framework of Ocean Observing (FOO) readiness level concept, we present an evaluation framework for biogeochemical data synthesis products, which enables a systematic assessment of each product's maturity. A new criteria catalog provides the foundation for assigning scores to the nine FOO readiness levels. As an example, we apply the assessment to four existing biogeochemical essential ocean variables data products. In descending readiness level order these are: The Surface Ocean CO_2 Atlas (SOCAT); the Global Ocean Data Analysis Project (GLODAP); the MarinE MethanE and NiTrous Oxide (MEMENTO) data product and the Global Ocean Oxygen Database and ATlas (GO_2DAT). Recognizing that the importance of adequate and comprehensive data from the essential ocean variables will grow, we recommend using this assessment framework to guide the biogeochemical data synthesis activities in their development. Moreover, we envision an overarching cross-platform FAIR biogeochemical data management system that sustainably supports the products individually and creates an integrated biogeochemical essential ocean variables data synthesis product; in short a system that provides truly comparable and FAIR data of the entire biogeochemical essential ocean variables spectrum.

KEYWORDS

data synthesis product, essential ocean variable, FAIR, technical readiness level, GLODAP, SOCAT, MEMENTO, GO2DAT

1 Introduction

Covering approximately 71% of the Earth's surface, the ocean's importance for the earth system and our society is immense. In times of rising carbon dioxide (CO_2) and climate change, the environmental status of the ocean and the associated services for society are at risk (Cooley et al., 2022). Even more so as the ocean itself takes a crucial role in "[…] climate by storing and transporting large amounts of heat, freshwater, and carbon, and by exchanging these properties with the atmosphere." (Rhein et al., 2013). The Global Ocean Observing System (GOOS) has built a structure that coordinates and supports the entire range of ocean observations centered around Essential Ocean Variables (EOVs) (Moltmann et al., 2019; Snowden et al., 2019; Tanhua et al., 2019). Using the Framework of Ocean Observing (FOO) (Lindstrom et al., 2012), the International Ocean Carbon Coordination Project (IOCCP), as the GOOS expert panel for ocean biogeochemistry (BGC), defined the following eight BGC EOVs (IOCCP, 2017): Inorganic carbon, dissolved oxygen (O_2), nutrients, particulate matter, dissolved organic carbon, transient tracers and nitrous oxide (N_2O). A primary objective is to quantify their overall inventories, exchange fluxes and concentration trends. Generally, these quantifications advanced during the past decades, but there are still large uncertainties and many unresolved issues due to insufficient availability of BGC observations. To only mention a few examples, (i) ocean carbon sink estimates from ensemble means of global BGC ocean models and observation-based data products have become increasingly dissimilar with an offset of 1.1 GtC yr^{-1} in 2020 (Friedlingstein et al., 2022); (ii) models and observation-based products disagree on the strength and spatial distribution of deoxygenation (IPCC, 2019); and (iii) estimated contributions of N_2O fluxes from O_2 minimum zones to the global ocean source range from 4% to 50% (IPCC, 2021).

To gain an improved holistic understanding of the climate and the ocean's environmental status, large quantities of easily accessible BGC EOV data – that are spatially and temporally well-resolved, of high quality and from multiple and complementing observing platforms – are required. In particular, it is important to make available observational data FAIR (Findable Accessible Interoperable and Reusable), and enhance the value by proper quality control. Hence, the development of BGC data management systems complying with the FAIR guiding principles for scientific data management and stewardship has become more important (Wilkinson et al., 2016; Tanhua et al., 2019b). Continuous global efforts aim for more stream-lined and user-orientated data access systems such as the World Ocean Database (Boyer et al., 2018) and the European Marine Observation and Data Network (EMODnet, Miguez et al., 2019). Further user niches are filled in by community-driven synthesis data products that apply (advanced) merging techniques to combine datasets from multiple sources to form a coherent and consistent data product. These synthesis products are either tailored around specific BGC EOVs (e.g. Surface Ocean CO_2 Atlas (SOCAT), the Global Ocean Oxygen Database and Atlas (GO_2DAT), the MarinE MethanE and NiTrous Oxide (MEMENTO) database) or specific observing platforms [e.g. the Global Ocean Data Analysis Project (GLODAP)].

Generally, these synthesis data products try to solve many obstacles that the current landscape of BGC data has created. Observing campaigns are mostly funded as research projects and often have very specific research questions. Consequently, a multitude of data centers are managing ocean BGC EOV data. These range from local and national data centers (e.g. the Ocean Science Information System at GEOMAR Helmholtz Center for Ocean Research Kiel; the Information and Data Centre at CSIRO National Collections and Marine Infrastructure) to regional infrastructures (e.g. the Integrated Carbon Observing System (ICOS)) or international data centers (e.g. PANGAEA; CCHDO). Hence, data mining has become increasingly difficult and time-consuming, requiring downloading datasets from different entry points, searching for duplicates, and managing different metadata. Further, BGC EOV data have many users and stakeholders who have highly diverse needs from the data, especially in terms of quality-control (QC). Consequently, a plethora of data versions, file formats and levels of documentation exist (Shepherd, 2018; Miguez et al., 2019; Tanhua et al., 2019). Synthesis data products represent one solution to these data fragmentation issues by the provision of single access points to consistent data and metadata.

Nevertheless, some data are collected but not available: for example, many datasets submitted to SOCAT include atmospheric CO_2 measurements that could be useful for air-sea CO_2 flux calculations but are not published as part of the official SOCAT product. Similarly, some ship-based instruments have an O_2 sensor, but the measurements are not processed or archived anywhere. In addition, automated datastreams are uncommon for, in particular, reprocessed or delayed mode data. Such data has passed additional quality control, is characterized by high precision and accuracies and represents data with sufficient quality for climate studies. As a result of the lack of automation, the information exchange between multiple data systems, i.e. interoperability (ISO/IEC/IEEE, 2017), is also limited. These relatively low levels of interoperability hinder data reuse, preservation and integration, and increase associated data management costs (Snowden et al., 2019). The lack of automation also results in large elapsed times from the actual measurement to the provision of the data, i.e. in a high latency.

Thus, the many data synthesis efforts are far from complete and in "the era of big data comes to oceanography" (Abbott, 2013) there is a mandate for optimizing fit-for-purpose data synthesis products and their underlying workflows to enhance efficient and interoperable data usage (Tanhua et al., 2019b). The FOO readiness level concept (Lindstrom et al., 2012) becomes useful in this context. Applying it to existing BGC EOV products could guide both existing and new products in their development. Here we introduce such an evaluation framework for four existing BGC EOV data synthesis products: SOCAT, GLODAP, MEMENTO and GO_2DAT. We first describe the methodology for assessing the products before the four BGC data synthesis products are briefly presented and their maturity is assessed. Finally, we synthesize the findings and outline our vision of a larger-scale cross-platform BGC EOV data system.

2 Method

2.1 The FOO readiness level concept

To assess the maturity of an ocean observing system the Framework of Ocean Observing has adapted the technical readiness level, a scheme developed by NASA (National Aeronotics and Space Administration) (Sadin et al., 1989), and introduced the ocean observing "readiness level" (Lindstrom et al., 2012). Following this framework, ocean observing should be seen as "[…] a chain of processes addressing "why to observe?" (requirement setting process), "what to observe?" (scoping of observational foci), "how to observe?" (coordination of observing elements), and "how to integrate, use and disseminate observational outcomes and understand their impacts?" (data management, analyses and creation and assessment of information products)." (Pearlman et al., 2019). The three pillars of this ocean observing value chain [1] are: "Requirements", "Observations" and "Data and Information". For each of these pillars, FOO defined nine readiness levels and grouped these into the categories "Concept", "Pilot" and "Mature". A holistic approach enables the evaluation and classification of an entire ocean observing system in terms of feasibility, capacity, and impact. Here we only use the defined readiness levels for "Data Management and Information Products" (Figure 1). We restrict ourselves to climate quality data since these are strongly tied to high-quality BGC EOV synthesis data products, especially to their quality control procedures.

The nine readiness levels (Lindstrom et al., 2012) are quite general, so to suit the aim of this work, we have developed a criteria catalog (Appendix 1) which forms an objective basis for the evaluation of the individual data products. Applying the catalog assigns (weighted) scores to typical characteristics of data products on a level-by-level scheme. Full compliance with the criteria yields a 100% score for a given level, with 80% being defined as a "pass". For example, a product passes readiness level 5 if the data management practices are verified and validated through an existing data policy and archival plan. The criteria catalog (Appendix 1) assigns equally weighted scores to "Policy", "Archival" and "QC Verification". These, in turn, are linked to specific data product features, such as having a data usage statement for "Policy" (Figure 2). Note that even though the order of levels is structured hierarchically, a data product can meet some requirements of higher levels before fully complying with all lower levels. Since the maturity of a data product is strongly tied to the FAIR guidelines, we have incorporated the guidelines into the criteria. Following Tanhua et al. (2019), a data product is FAIR if it has a unique persistent identifier with enriched and standardized metadata (findable), enabling access to the machine-readable data and metadata (accessible and interoperable), and can be integrated into other data sources (reusable). The degree of the implementation of the FAIR principles is reflected in the order of the FOO readiness levels. The degree of being "fit-for-purpose", a requirement of the ocean observing value chain, is also incorporated into the criteria catalog.

Given the diverse nature of the data, the criteria have not been further specified and are kept generic on purpose. Workflows and tools used in different products might resemble one another but are tailored toward the specific requirements of the data products. In particular, the data upload (or ingestion) system and quality control methods differ as these are tailored towards the given observing platform, sampling method (continuous or discrete), analysis type, variable (e.g. Johnson et al., 2001; Dickson et al., 2007; Pierrot et al., 2009; Maurer et al., 2021) and stakeholder. Since many research groups and products implement different QC flagging schemes, we have applied a consistent set of quality levels (adapted from ICOS, https://www.icos-cp.eu/data-services/data-collection/data-levels-quality) to describe the data flow and QC of the different products (Table 1). Typical QC examples of the different levels are range tests (level 1), the identification of spikes in space or time (level 2) and the adjustment of known biases (level 3).

3 Synthesis data product assessment

In the following, we will briefly describe and evaluate four available BGC EOV data synthesis products for their maturity in terms of FOO readiness. The products were selected based on the goal of covering the entire BGC EOV data synthesis product spectrum. The products cover different BGC EOVs, observing platforms and approaches (cross-platform vs. cross-EOV) and range from products in the planning phase to well-established ones.

3.1 SOCAT

The Surface Ocean CO_2 Atlas (Pfeil et al., 2013; Sabine et al., 2013) is an international community-driven effort. It synthesizes *in-situ* surface ocean fCO_2 (fugacity of carbon dioxide) measurements from ships, moored stations, autonomous and drifting surface platforms and yachts with an estimated accuracy better than 10 µatm. SOCAT increases ocean surface fCO_2 data availability and forms the basis of several other data products, such as the SeaFlux data set (Gregor and Fay, 2021) and diverse scientific applications and assessments. The latter range from ocean and climate model and sensor evaluation, regional process studies of surface ocean fCO_2, the detection and estimation of surface ocean acidification trends (Freeman and Lovenduski, 2015; Lauvset et al., 2015), to the quantification of the ocean carbon sink and its variation (Bakker et al., 2016; Friedlingstein et al., 2022). Thus, SOCAT represents a "[…] key step in the value chain based on *in situ* inorganic carbon measurements of the oceans, which provides policymakers in climate negotiations with essential information on ocean CO_2 uptake" (Bakker et al., 2020; Guidi et al., 2020). SOCAT's first

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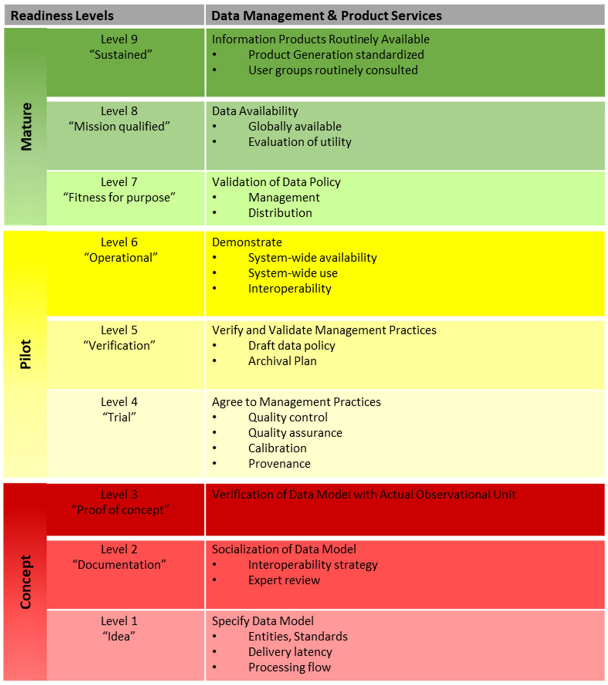
[1] a term broadly defined as a set of value-adding activities that one or more communities perform in creating and distributing goods and services (Longhorn and Blakemore, 2007)



	Readiness Levels	Data Management & Product Services
Mature	Level 9 "Sustained"	Information Products Routinely Available • Product Generation standardized • User groups routinely consulted
	Level 8 "Mission qualified"	Data Availability • Globally available • Evaluation of utility
	Level 7 "Fitness for purpose"	Validation of Data Policy • Management • Distribution
Pilot	Level 6 "Operational"	Demonstrate • System-wide availability • System-wide use • Interoperability
	Level 5 "Verification"	Verify and Validate Management Practices • Draft data policy • Archival Plan
	Level 4 "Trial"	Agree to Management Practices • Quality control • Quality assurance • Calibration • Provenance
Concept	Level 3 "Proof of concept"	Verification of Data Model with Actual Observational Unit
	Level 2 "Documentation"	Socialization of Data Model • Interoperability strategy • Expert review
	Level 1 "Idea"	Specify Data Model • Entities, Standards • Delivery latency • Processing flow

FIGURE 1
FOO Readiness level for Data Management and Information Products, adapted from Figure 9 in Lindstrom et al. (2012).

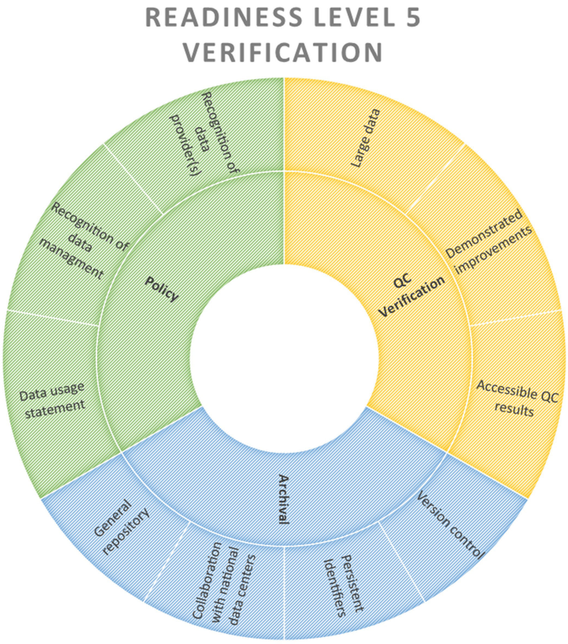


FIGURE 2
Score assignment scheme for readiness level 5 (Verification).

version (Pfeil et al., 2013; Sabine et al., 2013), was released in 2011 following a call from the international marine carbon community to create a quality-controlled, publicly available synthesis product of surface ocean CO_2 for the global oceans and coastal seas (IOCCP, 2007; Doney et al., 2009). SOCATv2 and SOCATv3 followed in 2013 (Bakker et al., 2014) and 2015 (Bakker et al., 2016), respectively. After the official launch of the SOCAT submission system in September 2015 (SOCAT and SOCOM, 2015), annual product releases have been accomplished. SOCATv2022 includes more than 40 million individual measurements from 1957 to 2021 from more than 100 data contributors (Bakker et al., 2022). The data product consists of 1) the collection of all individual data set files, 2) global and regional synthesis data products, 3) global (monthly, yearly and decadal) gridded products on a 1° latitude by 1° longitude grid and 4) a coastal monthly gridded product on a quarter degree grid. The main synthesis products (2, 3, 4) are based on surface water fCO_2 with an estimated accuracy of better than 5 µatm (33.7 million data points), while fCO_2 values with an accuracy of 5 to 10 µatm are made available separately (6.4 million data points). Recent SOCAT products contain searchable information on the organization where data providers are based, a step towards attributing data sets to funding agencies and countries.

While SOCAT synthesis products are made available *via* ERDDAP (Section 4.1.1.1), metadata of individual data sets in SOCAT are not yet machine-readable. Planned metadata automation will contribute to the initiative led by the Intergovernmental Oceanographic Commission of UNESCO towards a federated data system for the UN Sustainable Development Goal (SDG, UN, 2015) 14.3 ("Minimize and address the impacts of ocean acidification, including through enhanced scientific cooperation at all levels"). SOCAT also considers to include additional variables to the product, such as atmospheric CO_2, dissolved inorganic carbon (DIC), total alkalinity (TA), pH, nutrients, methane (CH_4) and nitrous oxide (N_2O) concentrations (SOCAT and SOCOM, 2015; Bakker et al., 2016).

TABLE 1 Data quality levels.

Level	Characteristics
0	Uncalibrated
1	Calibrated data with passed automated check (known as 'sanity check')
2	Scientific 1st level QC for precision and accuracy has been performed
3	External scientific QC for precision and accuracy has been performed

3.1.1 Software developments

3.1.1.1 ERDDAP

The open source software ERDDAP is used as the backbone for SOCAT data quality-control as well as providing access to data and data product. To effectively improve data interoperability, it is not enough to ensure that data are freely and openly available, though both are necessary. To reach a more diverse set of users, including domain and non-domain experts, it is critical to provide effective data services that are easy to use, support multiple data formats, and provide access to humans and machines. One tool that provides all of these capabilities is the open source software ERDDAP.

There are several benefits of using ERDDAP as a data server. Among its many features, it (i) supports dozens of popular formats; (ii) provides standards-based metadata and data services and formats; (iii) supports federated access of distributed ERDDAP data services; (iv) supports both human and machine interactions; (v) supports sub-setting of large datasets; (vi) provides improved discovery of datasets through commercial search engines; and (vii) provides support for archival of datasets. The GOOS Observations Coordination Group has adopted ERDDAP as the FAIR-compliant data server of choice for the global ocean networks.

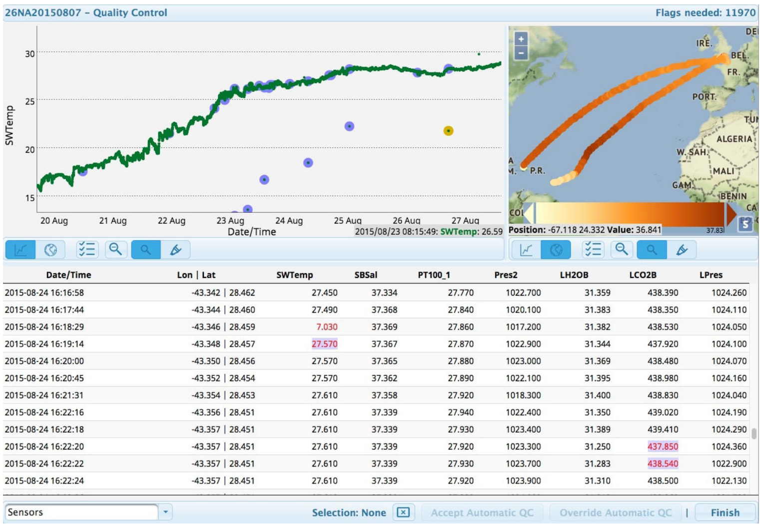
Serving data through a tool such as ERDDAP may also help better understand data access patterns. The most accurate method of understanding data usage relies on citations, particularly when using Digital Object Identifiers (DOIs). Using a tool such as ERDDAP also make it possible to gather usage statistics on how data is being accessed, which is a useful additional metric towards a more complete and accurate view of data usage. The usage tracking capabilities of ERDDAP can thus provide a mechanism to track user access, which can largely eliminate the requirements for users to log in.

3.1.1.2 QuinCe

The European Research Infrastructure ICOS is developing QuinCe (Steinhoff et al., 2019), as a standardized online tool to ingest, process and QC underway surface ocean fCO_2 measurements from diverse instruments using community-agreed algorithms. While presently QuinCe is only available to a few data providers, in future it will allow data providers to process their data transparently. That includes a record trail that links all applied changes to the original data, i.e. full data provenance is established. QuinCe can automatically export all data in several formats to data centers, near-real-time products, delayed mode products, and the SOCAT data submission system (or dashboard). QuinCe also automatically performs calibrations, data processing, and basic QC of underway instrument data from different platforms (allowing all text formats as input). An interactive user interface with time-series plots, cruise maps and a data table enables the data provider to perform detailed manual QC (Figure 3). The interactive control also enables additional manual scientific 1st QC, i.e. outlier detection, of the level 1 fCO_2 data, which results in level 2 fCO_2 data (World Ocean Circulation Experiment flagging scheme applied). For future traceability, QuinCe records all QC decisions.

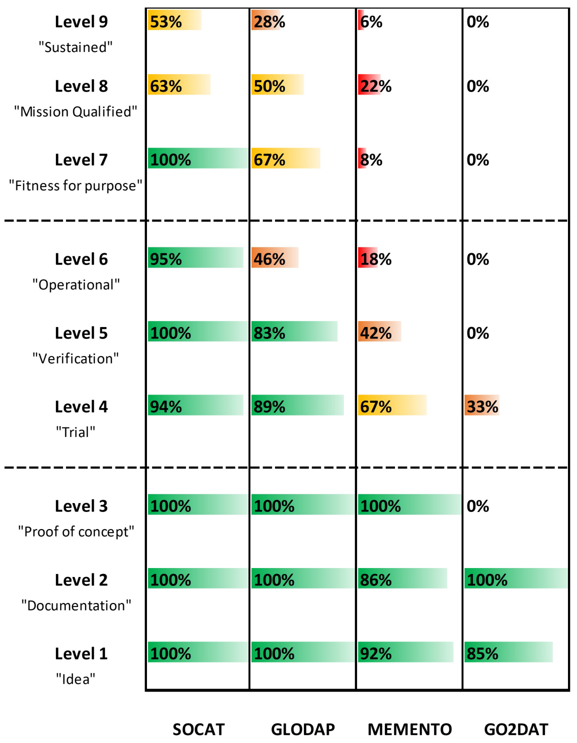
3.1.2 FOO readiness

SOCAT has implemented a clear concept and management structure "[…] to integrate, use and disseminate observational outcomes and understand their impacts […]" (Pearlman et al.,



Date/Time	Lon | Lat	SWTemp	SBSal	PT100_1	Pres2	LH2OB	LCO2B	LPres
2015-08-24 16:16:58	-43.342 | 28.462	27.450	37.334	27.770	1022.700	31.359	438.390	1024.260
2015-08-24 16:17:44	-43.344 | 28.460	27.490	37.368	27.840	1020.100	31.383	438.350	1024.110
2015-08-24 16:18:29	-43.346 | 28.459	7.030	37.369	27.860	1017.200	31.382	438.530	1024.050
2015-08-24 16:19:14	-43.348 | 28.457	27.570	37.367	27.870	1022.900	31.344	437.920	1024.100
2015-08-24 16:20:00	-43.350 | 28.456	27.570	37.365	27.880	1023.000	31.369	438.480	1024.070
2015-08-24 16:20:45	-43.352 | 28.454	27.570	37.362	27.890	1022.100	31.395	438.980	1024.160
2015-08-24 16:21:31	-43.354 | 28.453	27.610	37.358	27.920	1018.300	31.400	438.830	1024.040
2015-08-24 16:22:16	-43.356 | 28.451	27.610	37.339	27.940	1022.400	31.350	439.020	1024.190
2015-08-24 16:22:18	-43.357 | 28.451	27.610	37.339	27.930	1023.400	31.389	439.410	1024.290
2015-08-24 16:22:20	-43.357 | 28.451	27.610	37.339	27.920	1023.300	31.250	437.850	1024.360
2015-08-24 16:22:22	-43.357 | 28.451	27.610	37.339	27.930	1023.700	31.283	438.540	1022.900
2015-08-24 16:22:24	-43.357 | 28.451	27.610	37.339	27.920	1023.900	31.310	438.500	1022.130

FIGURE 3
A screenshot of the main Quality Control page of QuinCe, showing data from sensors in plot and map form together with a table of all sensor and calculated values. Flagged values from automatic and manual QC are highlighted.



	SOCAT	GLODAP	MEMENTO	GO2DAT
Level 9 "Sustained"	53%	28%	6%	0%
Level 8 "Mission Qualified"	63%	50%	22%	0%
Level 7 "Fitness for purpose"	100%	67%	8%	0%
Level 6 "Operational"	95%	46%	18%	0%
Level 5 "Verification"	100%	83%	42%	0%
Level 4 "Trial"	94%	89%	67%	33%
Level 3 "Proof of concept"	100%	100%	100%	0%
Level 2 "Documentation"	100%	100%	86%	100%
Level 1 "Idea"	100%	100%	92%	85%

FIGURE 4
FOO readiness level scores of SOCAT, GLODAP, MEMENTO and GO_2DAT. Green (> 80%); yellow (51% – 80%); orange (25% - 50%); red (<25%).

2019). SOCAT's well-documented data-flow concept includes all processes from archival to provision yielding (machine-readable) entities with common standards, e.g. common data formats and units. It has been tested and applied to several fCO_2 observing platforms, resulting in 100% scores for readiness levels 1-3 (Figure 4).

A best practice protocol and cook-books for the different procedures exist (Dickson et al., 2007; Wanninkhof et al., 2013; Bakker et al., 2016; Lauvset et al., 2018). The seamless data integration, data flow (SOCAT dashboard) and data extraction (Live Access Server, ERDDAP) enable version-controlled data archival and provision. This seamless data managment also enables traceable data calibration and quality control (level 1-3). Moreover, clearly outlined and defined criteria for the external QC (expert panel), i.e. 2nd QC, exist and the thorough metadata requirements enable the assignment of uncertainty categories. The growth of fCO_2 data points in successive SOCAT versions and the widespread use of the SOCAT synthesis products have verified the data management practices. 40 million data points from multiple fCO_2 platforms show the system-wide use- and availability of SOCAT's data streams. Further, the recent availability of SOCAT data through ERDDAP achieves high interoperability and in combination with the SOCAT front end, SOCAT has demonstrated making fCO_2 data FAIR and operational. SOCAT has passed the "Pilot" phase with scores higher than 94% for readiness levels 4 – 6. To obtain a 100% score for readiness level 4, improved data quality control for the accompanying variables, e.g. surface salinity is still needed. Also, SOCAT could benefit from a fully encompassing and transparent uncertainty propagation estimation (Merchant et al., 2017) instead of the presently "post-assigned" accuracy categories.

SOCAT's high level of automation sets it apart from other products. This process begins with a web-based data submission tool that allows scientists to submit data to the SOCAT system using the formats they are familiar with – typically ASCII/CSV files. This is critical as it allows the data producers to interact with the SOCAT system without having to convert their data to complicated formats. The overall effect is to lessen the workload of the data providers, data managers and quality controllers. Once submitted and quality-controlled, data are accessible through easy-to-use interactive viewers and access to the various gridded products is also available. Through regular provision of global FAIR fCO_2 data to "down-the-line" end-user services, such as the Global Carbon Budget (e.g. Le Quéré et al., 2018; Friedlingstein et al., 2022), SOCAT is a key step in the value chain of the EOV inorganic carbon (Guidi et al., 2020). It contributes to the ocean carbon sink's quantification and our understanding of ocean acidification. SOCAT thus addresses the United Nations Framework Convention on Climate Change Paris agreement and the UN SGD 14.3 (ocean acidification). Being used for numerous applications and cited 792 times (since 2013; Google Scholar) as of March 2023, prove SOCAT's utility and that it is fit for purpose. Altogether this yields a 100% score for readiness level 7. However, the evaluation of SOCAT's utility could strongly benefit from implementing enhanced data usage metrics (Section 4.1.1.1). Also, the existence of seasonal biases (more summer data) and regional gaps (e.g. Southern Ocean), even though mainly linked to the FOO components "Requirements" and "Observation", leave room for improvements towards a full "Mission qualified", resulting in a 63% score for readiness level 8. Lastly, even though SOCAT has standardized the product generation, erased many bottlenecks in the data stream and is a community-driven product with constant interaction with the data providers, SOCAT is not yet a sustained data product. Above all, this is due to the non-sustained and *ad-hoc* funding situation.

Additionally, the lack of easily available tools for transforming raw data from instruments and sensors into a state suitable for inclusion in SOCAT is only now starting to be addressed through efforts such as QuinCe (Section 4.1.1.2), leading to an intermediate score for readiness level 9 (53%). Wide spread adoption and integration of tools like QuinCe could help enhance machine-to-machine data submission into products like SOCAT, eliminating many of the manual processes currently required.

3.2 GLODAP

The Global Ocean Data Analysis Project was initiated to enable the quantification of the anthropogenic ocean carbon sink (e.g. Key et al., 2004; Sabine et al., 2004; Gruber et al., 2019). To this end, GLODAP focuses on collecting and synthesizing interior ocean data from hydrographic cruises with carbon-relevant data. GLODAP defines carbon-relevant as data that includes at least one measurement of the following: inorganic carbon sub-variables (pH, DIC, TA and/or fCO_2), carbon isotopes (C14 and/or C13) or transient tracers (CFC11, CFC12, CFC113, CCl_4 and/or SF_6). Through multiple layers of quality control, aiming to remove biases between cruises, GLODAP makes cruise data from various sources, from individual projects to numerous larger campaigns, consistent and comparable. With its high internal consistency of the core variables (DIC, TA, pH, nutrients, O_2, salinity and transient tracers), particularly of DIC and TA (± 4 µmol kg^{-1}), GLODAP has also become a relevant source for other scientific applications and observing platforms. One prominent example is BGC Argo floats, which rely heavily on GLODAP's high-quality data for validation. The first version of GLODAP, GLODAPv1 (Key et al., 2004), was released in 2004. It mainly included data from the World Ocean Circulation Experiment and Joint Global Ocean Flux Study campaigns as well as other historical cruise data from the Geochemical Ocean Sections Study, Transient Tracers in the Oceans, South Atlantic Ventilation Experiment, and INDIen Gaz Ocean expeditions. In combination with the CARbon dioxide IN the Atlantic Ocean (CARINA) product (Tanhua et al., 2009; Key et al., 2010) and the PACIFIc ocean Interior CArbon (PACIFICA, Suzuki et al., 2013) product, "[…] these products formed the natural basis for GLODAPv2" (Key et al., 2015; Olsen et al., 2016). Version 2 benefitted from advancements in data handling, which eventually enabled yearly updates starting in 2019. In addition to the annual updates, GLODAP plan to provide regular full decadal version releases, in concert with the GO-SHIP program (Olsen et al., 2019; Sloyan et al., 2019; Olsen et al., 2020; Lauvset et al., 2021). GLODAPv2.2022 (Lauvset et al., 2022) includes more than 1.4 million samples from 1085 cruises from 1972 to 2021. The data product consists of three pillars: 1) data from the individual cruises in a consistent format with coherent QC and unit conversion, 2) a bias-adjusted data product, and 3) a global 1°x1° mapped climatology. The latter is produced only for the full version releases (the last of which was in 2016).

For the future, "[the] GLODAP team now strive for advancements on two fronts towards a semi-automated system that reduces the work intensity and associated errors. Firstly, implementing a uniform, semi-automatic and standards-compliant data ingestion system that will facilitate the data submission and quality control (QC) procedures. […] Secondly, upgrading to a modern and versatile data extraction system that provide users more flexibility and options […] "(Tanhua et al., 2021).

3.2.1 FOO readiness

GLODAP has implemented a clear concept and management structure as well as a well-documented data flow, which includes all processes from archival to provision. Its entities apply the common World Ocean Circulation Experiment standards, i.e. have common and consistent data formats, units and semantics. The complete data flow has been tested and applied to 14 core variables for more than 1000 cruises, resulting in 100% scores for readiness levels 1-3 (Figure 4).

Best practice protocols and standard operating procedures for the observations of the core parameters exist and are well-established (GO-SHIP). Also, the applied interpolation and calculation schemes follow the most recent literature recommendations. The application of multiple tools, including the AtlantOS QC software (Velo et al., 2021), the crossover toolbox (Tanhua et al., 2010; Lauvset and Tanhua, 2015) and comparisons to CANYON-B (Bittig et al., 2018) combined with annual expert meetings, an online adjustment table and a consistent flagging scheme, yield a traceable and system-wide quality control (level 1-3). The improvement in consistency is further given and documented for each product. The strong and exponential data point growth has verified the data management practices and shows GLODAP's system-wide use and availability. However, to completely pass the pilot phase several shortcomings must be dealt with. First, one inorganic carbon sub-variable (fCO_2) and one carbon isotope (delC14, i.e. radiocarbon content expressed in Δ14C notation) are not subject to 2nd QC. Further, the data ingestion system is dependent on rather rudimentary communication by email and the collaboration with local data centers is not all-encompassing and automated. This dependency on manual work in the ingestion system results in deficits in the version control of the original data, which in turn leads to some archived data being out of synchronization with GLODAP. Data access services and machine-readable metadata, both crucial for full interoperability, are also not incorporated in the data flow. Lastly, the given consistency estimates might be closely linked to uncertainty assignments, but they are not the same and an encompassing and transparent uncertainty estimation is still warranted. GLODAP passes Level 4 and 5 with scores of 89% and 83%, but the missing features are especially punished in level 6 "Operational" with a mediocre score of 46%.

Regarding the more mature levels, GLODAP still obtains relatively high scores. Most of all GLODAP has proven its utility and to be fit-for-purpose being cited 641 times (since 2016; Google Scholar) as of March 2023 and being used for multiple end-user services. Most prominently, GLODAP has become the primary data source for quantifying the ocean carbon sink (Sabine et al., 2004; Gruber et al., 2019; Friedlingstein et al., 2020). The Cruise Summary Table and a fair usage statement ensure that the data provider's credibility is maintained. Nevertheless, mainly the relatively low level of automation in combination with no sustained funding hinder higher scores for all three "Mature" levels with 67%, 50% and 28% for level 7 – 9, respectively.

3.3 MEMENTO

The MarinE MethanE and NiTtrous Oxide database compiles N_2O and CH_4 measurements and - if available - associated data (such as atmospheric mole fractions, water temperature, salinity, dissolved O_2 and nutrients) from the open and coastal oceans. It provides calculated global and regional concentration fields for the surface and deep ocean in common units and estimates of the air-sea flux density of both gases. Initially starting with a database for

N_2O only (Freing and Bange, 2007) a joint initiative between the Surface Ocean Lower Atmosphere Study and European CoOperation in Science and Technology Action 735 (European CoOperation in the Field of Scientific and Technical Research) resulted in the development of MEMENTO (Bange et al., 2009). MEMENTO's main rationale is to help researchers to quantify the temporally and spatially variable N_2O and CH_4 oceanic distributions and their exchange with the atmosphere. N_2O and CH_4 are important atmospheric trace gases that act as strong greenhouse gases in the troposphere and as precursors of ozone depletion in the stratosphere (WMO, 2018; IPCC, 2021). The MEMENTO data product was used, for example, to model N_2O production and consumption processes on global and regional scales (Freing et al., 2012; Suntharalingam et al., 2012; Zamora et al., 2012). Recently, data from MEMENTO were also used to estimate the global N_2O and CH_4 emissions from the ocean (Weber et al., 2019; Yang et al., 2020). Being publicly available since 2009, MEMENTO cooperates with the Scientific Committee on Ocean Research working group 14.3 since 2014. By November 2021, MEMENTO included more than 120000 N_2O and more than 23000 CH_4 measurements from over 200 measurement campaigns covering the past 57 years of observations.

Besides the ongoing data update, MEMENTO wants to "continuously improve it by including additional meta-information, allowing additional data formats, and implementing new data quality control criteria." Further goals include the implementation of "[…] standard procedures that are developed within the [SCOR] working group for measuring N_2O and CH_4." (Kock and Bange, 2015) and an enhanced data archive structure that is more user-friendly.

3.3.1 FOO readiness

MEMENTO has implemented a clear concept, management structure and data flow, successfully applied to both core parameters. Scores of 92%, 86% and 100% for readiness levels 1-3, respectively, reflect that MEMENTO meets most of the required concept phase criteria. Most importantly, all entities, including original data and metadata, are provided using common standards (format, semantics and units). 100% scores are not obtained because MEMENTO misses two features that are relevant for interoperability. First, the data are not openly available and require registration. Second, MEMENTO's data management concept does not include archiving original data sets (such as bottle files, etc.) of individual cruises. Still, MEMENTO clearly passes the concept phase.

With a strong emphasis on the consistency and quality of the included data, MEMENTO meets all QC and quality assurance requirements of readiness level 4. But the important and heavily weighted traceability of applied changes, i.e. the provenance criteria, is not fulfilled. This missing feature, which limits the level 4 score to 67%, means that MEMENTO has not passed the first pilot phase level. Readiness levels 5 and 6 reveal further shortcomings of MEMENTO regarding the pilot phase criteria. These include the lack of transparency and verification of the QC, limited archiving features, lack of established links to data centers and version control, as well as the lack of interoperability. Especially the latter strongly affects level 6 scores, which in turn is heavily influenced by the missing DOI of the product. MEMENTO stays below the 50% mark for both levels with 42% and 18%.

Nonetheless, MEMENTO already meets some of the crucial criteria of the higher "Maturity" levels. It has addressed its societal drivers and is cited 89 times (since 2009; Google Scholar) as of March 2023. Moreover, it does provide a gridded product covering the entire globe. However, the low level of automation and other deficits, such as relatively low utility scores and non-sustained funding, strongly limit the scores for readiness level 7-9, with all levels being below 25%.

3.4 GO_2DAT

The main scientific rationale of the Global Ocean Oxygen Database and ATlas (GO_2DAT) lies in the understanding and prediction of ocean O_2 changes at daily to climate scales: "A better knowledge base of the spatial and temporal variations in marine O_2 will improve our understanding of the ocean O_2 budget, and allow for better quantification of the Earth's carbon and heat budgets, net global primary production and for adopting sustainable fisheries and aquaculture management." (Grégoire et al., 2021).

The first version of GO_2DAT is "under construction", but in the recently published roadmap towards GO_2DAT (Grégoire et al., 2021), the GO_2DAT team envisions a consistent and FAIR cross-platform database that targets all available O_2 measurements from the coastal and open ocean from both Eulerian and Lagrangian platforms. Thus, GO_2DAT shall include O_2 measurements from ships (Winkler data and CTD-O_2 sensor data), Argo floats, gliders, moorings, underway sensors and benthic boundary layer data. To tackle the lack of uniformity in data treatments a key characteristic of GO_2DAT will be the definition of a "community-agreed, fully documented metadata format and a consistent quality control procedure and quality flagging (QF) system". In addition to the database, several regularly updated "stacked" gridded products of O_2 concentration, O_2 partial pressure (pO_2) and the degree of saturation with respect to atmospheric O_2 for the coastal and global ocean with sub-seasonal to multi-decadal resolution, are planned.

GO_2DAT datasets and products will improve our understanding and estimation of the deoxygenation trend and mechanisms. Since 1950 the open ocean O_2 content has decreased (medium confidence) by a few percent (i.e. 0.5-3%) (IPCC, 2019) and the Oxygen Minimum Zones, which are permanent features of the open ocean, are expanding. However, models and observation-based products disagree on the amount and spatial distribution of deoxygenation. Different data sets and mapping procedures explain only part of these differences. In the global coastal ocean, the reference distribution of hypoxic sites is that assembled by Diaz and Rosenberg (2008), showing the worldwide distribution of regions affected by hypoxia at least once, as referred to in the literature. This effort has been valuable but should be updated and amended with the large volume of (sometimes disparate) quantitative information on coastal O_2 concentrations, including inventories of the frequency, timing, duration, intensity and spatial extension of the hypoxic events, and links to the original data contained in a globally accessible database.

3.4.1 FOO readiness

Given the recently published community-agreed roadmap (Grégoire et al., 2021), GO$_2$DAT already passes the readiness levels 1 "Idea" and 2 "Documentation". The roadmap describes in detail the encompassing entities and the data flow. The ingestion and archival system are clearly outlined and envisioned to build upon synchronized two-way data links between existing assembly centers (e.g. national data centers or regional hubs such as EMODnet) and an envisioned GO$_2$DAT global data assembly center. The importance of metadata is emphasized in that "GO$_2$DAT will ensure that data in each level are assigned an uncertainty and that sufficient metadata to interpret this uncertainty exists […] to assess the suitability of the data for a particular purpose (e.g. mean state, variability, climate trend assessment)." (Grégoire et al., 2021). Similarly, the need for automated assignment of persistent identifiers (i.e. DOIs) to submitted datasets, enabling data tracking and download statistics, is described. The envisioned data flow features that will ensure interoperability are also depicted. These include detailed descriptions on the harmonization and standardization procedures and also general concepts of the envisioned QC. The GO$_2$DAT team formulates its aim of annual releases of synthesized and mapped O$_2$ data, including sub-products restricted to a defined set of O$_2$ measuring techniques. The team also describes an envisioned interactive web platform, including data visualization tools, where the data products are easy to find and openly accessible. This front-end is envisioned to foster communication between users, data generators and product developers, directly implementing the FOO feedback cycle. The well-documented concept results in 85% for readiness level 1 and full compliance, i.e. 100%, for level 2. However, the concept idea has neither been proven nor verified yet. Hence, GO$_2$DAT does not comply with any criteria of readiness levels 3 and above, except that quality assurance protocols for all targeted O$_2$ observing platforms exist (33% for readiness level 4).

4 Discussion and conclusion

4.1 Synthesis of data product assessment

The new criteria catalog and scoring system were successfully applied to the four selected data synthesis products. The so-determined readiness level scores and maturity of each product are listed in Table 2. SOCAT is the most mature product, reaching the "Mature" status by being "Fit for purpose". GLODAP passes the "Verification" level and represents the only product in the "Pilot" phase. MEMENTO and GO$_2$DAT are in the "Concept" phase. However, MEMENTO also complies with the "Proof of Concept" level. GO$_2$DAT is the most recent initiative with the publication of a community-agreed roadmap (Grégoire et al., 2021). At this stage, its maturity is capped at the "Documentation" level. Nonetheless, all living products provide consistent and comparable level 3 data.

During the assessment, we could identify some critical and common approaches, which all four products share, independent of their different foci and state of development. To begin with, it is a pre-requisite for the success of a product to follow a clear mandate, i.e. to have a clear mission. Since the four products are community-driven, this is implicitly fulfilled. All products recognize the importance of not only the synthesis itself but also the importance of accompanying original data and metadata. Also, the importance of known and common standards and a clearly outlined QC is reflected in the individual data products' workflow. And even though the actual 2nd QC methods of how to reach level 3 data differ from in-depth metadata checks (SOCAT) to bias corrections (GLODAP and MEMENTO), all products (in-)directly foster the usage of best practices by "rewarding" high-quality data in one way or another.

The diverging readiness levels of the products can mostly be linked to the varying implementations of critical features. Two themes that are reoccurring in the evaluation process are i) the extent to which the principles of FAIR and ii) the degree to which automation processes are incorporated at multiple readiness levels in the criteria catalog. Most prominently incorporated by SOCAT's automated ingestion and extraction system. In particular its built-in version control, as well as interoperable data access for humans and

TABLE 2 Main characteristics and FOO readiness of GLODAP, SOCAT, MEMENTO and GO$_2$DAT. Acronyms: Ships Of OPportunity (SOOP); Research Vessel (RV); Autonomous Surface Vehicle (ASV); Autonomous Underwater Vehicle (AUV); Fixed Ocean Station (FOS);.

	Observing Platform	BGC EOV focus	Temporal Coverage	Spatial Coverage	Status	FOO Readiness
SOCAT	SOOP, RV, Yachts, moorings, drifters, ASV	Inorganic Carbon (fCO$_2$ for pCO$_2$)	1957 – 2021	Global, surface	Living Product	Fit-for-purpose (Level 7)
GLODAP	RV	Inorganic carbon (DIC, TA, pH, fCO$_2$ for pCO$_2$)	1972 –2021	Global, full depth	Living Product	Verification (Level 5)
MEMENTO	RV	N$_2$O (CH$_4$)	1965 – 2020	Global, full depth	Living Product	Proof of Concept (Level 3)
GO$_2$DAT	RV, AUV, FOS, SOOP, benthic platforms	O$_2$	1957 – 2021	Global, full depth	Published Roadmap	Documentation (Level 2)

machines (ERDDAP), fulfill multiple criteria throughout the readiness level catalog. Similarly, GLODAP's cruise summary table and adjustment table provide good examples of how to increase a product's maturity. These features should be used as blueprints for other synthesis products. Lastly, we want to stress one essential feature that no product has: long-term funding. This lack hinders the products from becoming fully sustainable and mature and directly puts the mandate of delivering comparable, consistent, high-quality ocean BGC observations at risk.

Generally, the readiness concept and the criteria catalog developed here provide - for the first time - an objective basis to assess the maturity of information and data products. The result of the assessment, i.e. the ranking, is in line with the number of citations of the different data products, serving as an independent proxy for the readiness of each product and proving the reliability of the FOO readiness levels. We have chosen to distribute the impact on the final scores equally among individual features and key characteristics, see Section 3.1. Of course, discussions of this equal weighting approach are appropriate, and we want to encourage the community to improve the scoring scheme. Also, we are aware of the risks associated with applying the readiness level approach to data products with clearly different foci. It is indeed easier for a product with a narrow focus, e.g. one type of observing platform and one key variable only, to obtain a mature level than for a product with multiple variables from multiple observing platforms. However, the latter product might tackle a bigger task or mandate. For this reason, we want to stress that the readiness level of a product should not be confused with the importance and utility of the product. The readiness should rather be used to identify steps a product needs to take to realize its full potential.

4.2 Outlook

The assessment excluded further data management efforts related to EOV BGC data which do not provide consistent and synthesized data of multiple data sources, e.g. the highly advanced BGC Argo database. These efforts also display important elements of the marine BGC data landscape but the here applied readiness level assessment is tailored specifically towards data synthesis products. However, the capabilities of ERDDAP diffuse the delimitation between more general databases and synthesis

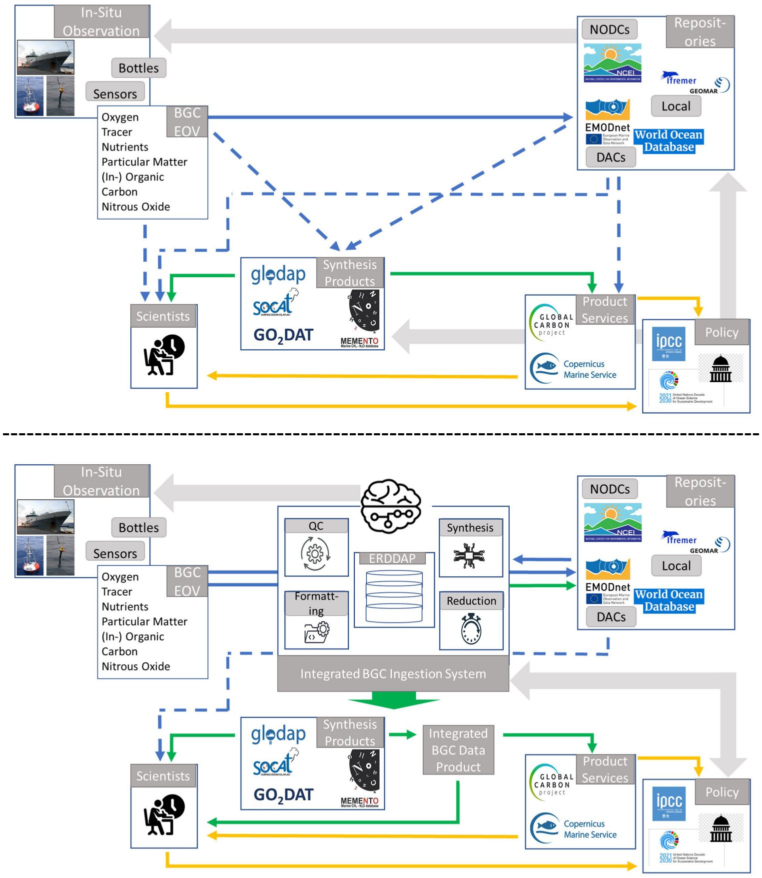


FIGURE 5
Top) Schematic of the current BGC data management system; Bottom) Schematic of the envisioned BGC data management system. Blue arrows show heterogenic (individual source) data flows; Green arrows show FAIR, consistent and QC'd data flows; Yellow arrows show information and service flows. Solid lines indicate strong and well-established links whereas dotted lines indicate rather weaker links with common data gaps. Grey arrows represent feedback between the FOO ocean data value chain pillars "Requirements", "Observations" and "Data and Information". For readability not all feedbacks are shown, e.g. the direct feedback between "Requirements" and "Observations" is not shown.

products increasingly. Widening the scope of this assessment to also include BGC EOV databases such as BGC Argo displays a future challenge.

In our vision, the ocean observation system should be independent of project-based research funds along the entire ocean observing value chain. We are in support of a sustained financing model, which could be realized through "[…] an international entity with a subscription-based or a binding Nationally Defined Contributions model, with a backbone/core ocean observing capability […]" (European Marine Board, 2021, page 14). Such a financing model would have to include the management of BGC data and would resolve the lack of long-term funding experienced by synthesis products.

4.2.1 An overarching BGC EOV data management system

Presently, much work is put into the data providers and the synthesis product management teams (Figure 5, top). The former must not only measure and analyze but provide their data to and comply with the requirements of multiple data repositories and products. The latter must mine data from multiple and very heterogenic sources. This leads to much manual labor with respect to data QC and formatting, but it also leads to long durations from the observation to the data provision and common data gaps. A typical consequence of the present data system is that unnecessary repetition of similar work- and data flows is applied occasionally to the same dataset.

Regarding the readiness of the entire spectrum of marine BGC observations, we need to obtain an overarching, more mature, sustainable BGC data management system with more reliable and FAIR data. A system that fully embraces the guideline "measure once – use many times" (Lindstrom et al., 2012; Snowden et al., 2019), crosses the bridge between the different BGC observing systems and products and can incorporate data with high resolution in space (horizontal and in-depth) and time (high frequency and long-term).

We envision a transparent and consistent seamless one-submission-only data flow management structure that is easy for the data providers and users alike and efficient as a system (Figure 5, bottom). ERDDAP services are at the heart of the centralized system, which is connected to all repositories with a two-way ingestion scheme. Further, a set of QuinCe alike software tools is implemented to automate and streamline the entire BGC EOV data processes from formatting to reduction to QC (level-0 to level-2) to submission. In our vision, this centralized system enables machine-to-machine data transfer for all data types (real-time, near-real-time and delayed mode) and data quality levels. It diminishes the need for manual data handling and results in interoperable data. Data would be consistent, more quickly available and all changes applied in the data life cycle would be easy to track. Importantly, this system allows scientists to work in the data formats they are most comfortable with but also supports higher level, self-describing data formats such as netCDF. This is crucial in that it supports data interoperability using data and metadata standards and conventions but does not require data producers to be data management experts. The synthesis products could focus purely on 2nd QC tasks to provide level 3 data. To complete the data system, an integrated BGC data product could combine all the different synthesis products and provide intercomparable and FAIR cross-platform and cross BGC EOV data to scientists and down-the-line services. Here, the interoperability and comparability of the different products will be enhanced to the full extent. On top of erasing existing semantic differences between the different products, the data would undergo another layer of QC. The "integrated BGC QC" would be purely dedicated to analyzing (and assigning) the given BGC EOV uncertainties of the different products. This additional QC leads to a consistent application of uncertainties for BGC EOV data from various sources (i.e. platform, measurement- and analysis type). Hence, data are made truly comparable, independent of their origin. And through a one-stop shop the data are easy to take up by different users.

The overarching system also improves the ability to identify data gaps in space and time and can partially guide the GOOS BGC observational strategy, implementing the FOO feedback loop on a larger and more encompassing scale (Figure 5, bottom). But above all, the system is set up to increase the FOO readiness of all BGC EOV observations and data products.

This vision should not be seen isolated from existing BGC data management efforts, which pursue a similar target. By no means do we aim at reinventing the wheel with yet another portal. The envisioned system should rather highlight what is needed for sustainable BGC data and guide the future development of existing BGC data management efforts accordingly.

Data availability statement

The original contributions presented in the study are included in the article/Supplementary Material. Further inquiries can be directed to the corresponding author.

Author contributions

NL and TT conceived the study, NL coordinated the author contributions, wrote and edited the manuscript, NL and TT contributed to tables and figures. TT, BF, BP, HB, SL, MG, DB, SJ, KO'B and AK contributed to the manuscript ideas and text. All authors contributed to the article and approved the submitted version.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

Supplementary material

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fmars.2023.1078908/full#supplementary-material

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Glossary

ASCII	American Standard Code for Information Interchange
ASV	Autonomous Surface Vehicle
AtlantOS	Atlantic Ocean Observing Systems
AUV	Autonomous Underwater Vehicle
BGC	BioGeoChemical
CANYON	CArbonate system and Nutrients concentration from hYdrological properties and Oxygen using a Neural-network
CARINA	CARbon dioxide IN the Atlantic Ocean
CSV	Comma Separated Value
CTD	Conductivity, Temperature and Depth
DIC	Dissolved Inorganic Carbon
DOI	Digital Object Identifier
EMODnet	European Marine Observation and Data Network
EOV	Essential Ocean Variable
FAIR	Findable Accessible Interoperable Reusable
FOO	Framework of Ocean Observation
FOS	Fixed Ocean Station
GLODAP	Global Ocean Data Analysis Project
GO_2DAT	Global Ocean Oxygen Database and Atlas
GOOS	Global Ocean Observing System
ICOS	Integrated Carbon Observing System
IOCCP	International Ocean Carbon Coordination Project
IPCC	Intergovernmental Panel on Climate Change
MEMENTO	MarinE MethanE and NiTrous Oxide
PACIFICA	PACIFic ocean Interior Carbon
QC	Quality Control
QF	Quality Flagging
RV	Research Vessel
SCOR	Scientific Committee on Oceanic Research
SDG	Sustainable Development Goal
SOCAT	Surface Ocean CO_2 Atlas
SOCOM	Surface Ocean pCO_2 Mapping intercomparison
SOOP	Ship Of Opportunity Program
TA	Total Alkalinity
UNESCO	United Nations Educational, Scientific and Cultural Organization
WMO	World Meteorological Organization.

4

GLODAPv2.2022: the latest version of the global interior ocean biogeochemical data product

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GLODAPv2.2022: the latest version of the global interior ocean biogeochemical data product

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Abstract. The Global Ocean Data Analysis Project (GLODAP) is a synthesis effort providing regular compilations of surface-to-bottom ocean biogeochemical bottle data, with an emphasis on seawater inorganic carbon chemistry and related variables determined through chemical analysis of seawater samples. GLODAPv2.2022 is an update of the previous version, GLODAPv2.2021 (Lauvset et al., 2021). The major changes are as follows: data from 96 new cruises were added, data coverage was extended until 2021, and for the first time we performed secondary quality control on all sulfur hexafluoride (SF_6) data. In addition, a number of changes were made to data included in GLODAPv2.2021. These changes affect specifically the SF_6 data, which are now subjected to secondary quality control, and carbon data measured on board the RV *Knorr* in the Indian Ocean in 1994–1995 which are now adjusted using certified reference material (CRM) measurements made at the time. GLODAPv2.2022 includes measurements from almost 1.4 million water samples from the global oceans collected on 1085 cruises. The data for the now 13 GLODAP core variables (salinity, oxygen, nitrate, silicate, phosphate, dissolved inorganic carbon, total alkalinity, pH, chlorofluorocarbon-11 (CFC-11), CFC-12, CFC-113, CCl_4, and SF_6) have undergone extensive quality control with a focus on systematic evaluation of bias. The data are available in two formats: (i) as submitted by the data originator but converted to World Ocean Circulation Experiment (WOCE) exchange format and (ii) as a merged data product with adjustments applied to minimize bias. For the present annual update, adjustments for the 96 new cruises were derived by comparing those data with the data from the 989 quality-controlled cruises in the GLODAPv2.2021 data product using crossover analysis. SF_6 data from all cruises were evaluated by comparison with CFC-12 data measured on the same cruises. For nutrients and ocean carbon dioxide (CO_2) chemistry comparisons to estimates based on empirical algorithms provided additional context for adjustment decisions. The adjustments that we applied are intended to remove potential biases from errors related to measurement, calibration, and data handling practices without removing known or likely time trends or variations in the variables evaluated. The compiled and adjusted data product is believed to be consistent to better than 0.005 in salinity, 1 % in oxygen, 2 % in nitrate, 2 % in silicate, 2 % in phosphate, 4 μmol kg^{-1} in dissolved inorganic carbon, 4 μmol kg^{-1} in total alkalinity, 0.01–0.02 in pH (depending on region), and 5 % in the halogenated transient tracers. The other variables included in the compilation, such as isotopic tracers and discrete CO_2 fugacity (fCO_2), were not subjected to bias comparison or adjustments.

The original data, their documentation, and DOI codes are available at the Ocean Carbon and Acidification Data System of NOAA NCEI (https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2022/, last access: 15 August 2022). This site also provides access to the merged data product, which is provided as a single global file and as four regional ones – the Arctic, Atlantic, Indian, and Pacific oceans – under https://doi.org/10.25921/1f4w-0t92 (Lauvset et al., 2022). These bias-adjusted product files also include significant ancillary and approximated data, which were obtained by interpolation of, or calculation from, measured data. This living data update documents the GLODAPv2.2022 methods and provides a broad overview of the secondary quality control procedures and results.

1 Introduction

The oceans mitigate climate change by absorbing both atmospheric CO_2 corresponding to a significant fraction of anthropogenic CO_2 emissions (Friedlingstein et al., 2019; Gruber et al., 2019) and most of the excess heat in the Earth system caused by the enhanced greenhouse effect (Cheng et al., 2017, 2020). The objective of GLODAP (Global Ocean Data Analysis Project; http://www.glodap.info, last access: 27 June 2022) is to provide high-quality and bias-corrected water column bottle data from the ocean surface to the sea floor. These data should be used to document the state and the evolving changes in physical and chemical ocean properties, e.g., the inventory of anthropogenic CO_2 in the ocean, natural oceanic carbon, ocean acidification, ventilation rates, oxygen levels, and vertical nutrient transports (Tanhua et al., 2021). The core quality-controlled and bias-adjusted variables of GLODAP are salinity, dissolved oxygen, inorganic macronutrients (nitrate, silicate, and phosphate), seawater CO_2 chemistry variables (dissolved inorganic carbon – TCO_2, total alkalinity – TAlk, and pH on the total hydrogen ion, or H^+, scale), the halogenated transient tracers chlorofluorocarbon-11 (CFC-11), CFC-12, CFC-113, carbon tetrachloride (CCl_4), and sulfur hexafluoride (SF_6).

Other chemical tracers are measured on many cruises included in GLODAP, such as dissolved organic carbon and nitrogen, as well as stable and radioactive isotope ratios. In many cases, a subset of these data is distributed as part of the GLODAP data product; however, such data have not been extensively quality controlled or checked for measurement biases in this effort. For some of these variables better sources of data exist, for example the product by Jenkins et al. (2019) for helium isotope and tritium data. GLODAP also includes some common derived variables to facilitate interpretation, such as potential density anomalies and apparent oxygen utilization (AOU). A full list of variables included in the data product is provided in Table 1.

The oceanographic community largely adheres to principles and practices for ensuring open access to research data, such as the FAIR (Findable, Accessible, Interoperable, Reusable) initiative (Wilkinson et al., 2016), but the plethora of file formats and different levels of documentation, combined with the need to retrieve data on a per cruise basis from different access points, limit the realization of their full scientific potential. In addition, the manual data retrieval is time consuming and prone to data handling errors (Tanhua et al., 2021). For biogeochemical data there is the added complexity of different levels of standardization and calibration and even different units and scales used for the same variable such that the comparability between datasets is often poor. Standard operating procedures have been developed for some variables (Dickson et al., 2007; Hood et al., 2010; Becker et al., 2020), and certified reference materials (CRMs) exist for seawater TCO_2 and TAlk measurements (Dickson et al., 2003) and reference materials for nutrients in seawater (RMNS, certified based on International Organization for Standardization Guide 34; Aoyama et al., 2012; Ota et al., 2010). Despite all this, biases in data still exist. These can arise from poor sampling and preservation practices, calibration procedures, instrument design and calibration, and inaccurate calculations. The use of CRMs does not by itself ensure accurate measurements of seawater CO_2 chemistry (Bockmon and Dickson, 2015), and the RMNS have only become available recently and are not universally used. For salinity and oxygen, the lack of calibration of the data from conductivity–temperature–depth (CTD) profiler mounted sensors is an additional and widespread problem, particularly for oxygen (Olsen et al., 2016). For halogenated transient tracers, uncertainties in standard gas composition, extracted water volume, and purge efficiency typically provide the largest sources of uncertainty. In addition to bias, occasional outliers occur. In rare cases poor precision – many multiples worse than that expected with current measurement techniques – can render a set of data of limited use. GLODAP deals with these issues by presenting the data in a uniform format, including any metadata either publicly available or submitted by the data originator, and by subjecting the data to rigorous primary and secondary quality control assessments, focusing on precision and consistency, respectively. The secondary quality control focuses on deep data, in which natural variability is minimal. Adjustments are applied to the data to minimize cases of bias that could be confidently established relative to the measurement precision for the variables and cruises considered. Key metadata are provided in the header of each data file, and original unadjusted data along with full cruise reports submitted by the data providers (where available) are accessible through the GLODAPv2 cruise summary table hosted by the Ocean Carbon and Acidification Data System (OCADS) at the National Oceanographic and Atmospheric Administration (NOAA) National Centers for Environmental Information (NCEI) (https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2022/cruise_table_v2022.html, last access: 15 August 2022).

This most recent GLODAPv2.2022 data product builds on earlier synthesis efforts for biogeochemical data obtained from research cruises, namely, GLODAPv1.1 (Key et al., 2004; Sabine et al., 2005), Carbon dioxide in the Atlantic Ocean (CARINA) (Key et al., 2010), Pacific Ocean Interior Carbon (PACIFICA) (Suzuki et al., 2013), and notably GLODAPv2 (Olsen et al., 2016). GLODAPv1.1 combined data from 115 cruises with biogeochemical measurements from the global ocean. The vast majority of these were the sections covered during the World Ocean Circulation Experiment and the Joint Global Ocean Flux Study (WOCE/JGOFS) in the 1990s, but data from important "historical" cruises were also included, such as from the Geochemical Ocean Sections Study (GEOSECS), Transient Traces in the Ocean (TTO), and South Atlantic Ventilation Experiment (SAVE). GLO-

Table 1. Variables in the GLODAPv2.2022 comma separated (csv) product files, their units, short and flag names, and corresponding names in the individual cruise exchange files. In the MATLAB product files that are also supplied a “G2” has been added to every variable name (e.g., G2cruise).

Variable	Units	Product file name	WOCE flag name[a]	Second QC flag name[b]	WHP-exchange name
EXPOCODE		expocode			
Digital object identifier		doi			
Assigned sequential cruise number		cruise			
Basin identifier[c]		region			
Station		station			STNNBR
Cast		cast			CASTNO
Year		year			DATE
Month		month			DATE
Day		day			DATE
Hour		hour			TIME
Minute		minute			TIME
Latitude		latitude			LATITUDE
Longitude		longitude			LONGITUDE
Bottom depth	m	bottomdepth			
Pressure of the deepest sample	dbar	maxsampdepth			DEPTH
Niskin bottle number		bottle			BTLNBR
Sampling pressure	dbar	pressure			CTDPRS
Sampling depth	m	depth			
Temperature	°C	temperature			CTDTMP
potential temperature	°C	theta			
Salinity		salinity	salinityf	salinityqc	CTDSAL/SALNTY
Potential density anomaly	kg m^{-3}	sigma0	(salinityf)		
Potential density anomaly, ref 1000 dbar	kg m^{-3}	sigma1	(salinityf)		
Potential density anomaly, ref 2000 dbar	kg m^{-3}	sigma2	(salinityf)		
Potential density anomaly, ref 3000 dbar	kg m^{-3}	sigma3	(salinityf)		
Potential density anomaly, ref 4000 dbar	kg m^{-3}	sigma4	(salinityf)		
Neutral density anomaly	kg m^{-3}	gamma	(salinityf)		
Oxygen	µmol kg^{-1}	oxygen	oxygenf	oxygenqc	CTDOXY/OXYGEN
Apparent oxygen utilization	µmol kg^{-1}	aou	aouf		
Nitrate	µmol kg^{-1}	nitrate	nitratef	nitrateqc	NITRAT
Nitrite	µmol kg^{-1}	nitrite	nitritef		NITRIT
Silicate	µmol kg^{-1}	silicate	silicatef	silicateqc	SILCAT
Phosphate	µmol kg^{-1}	phosphate	phosphatef	phosphateqc	PHSPHT
TCO_2	µmol kg^{-1}	tco2	tco2f	tco2qc	TCARBON
TAlk	µmol kg^{-1}	talk	talkf	talkqc	ALKALI
pH on total scale, 25 °C, and 0 dbar of pressure		phts25p0	phts25p0f	phtsqc	PH_TOT
pH on total scale, in situ temperature, and pressure		phtsinsitutp	phtsinsitutpf	phtsqc	
fCO_2 at 20 °C and 0 dbar of pressure	µatm	fco2	fco2f		FCO2/PCO2
fCO_2 temperature[d]	°C	*f*co2temp	(fco2f)		FCO2_TMP/PCO2_TMP
CFC-11	pmol kg^{-1}	cfc11	cfc11f	cfc11qc	CFC-11
pCFC-11	ppt	pcfc11	(cfc11f)		
CFC-12	pmol kg^{-1}	cfc12	cfc12f	cfc12qc	CFC-12
pCFC-12	ppt	pcfc12	(cfc12f)		
CFC-113	pmol kg^{-1}	cfc113	cfc113f	cfc113qc	CFC-113
pCFC-113	ppt	pcfc113	(cfc113f)		
CCl_4	pmol kg^{-1}	ccl4	ccl4f	ccl4qc	CCL4
$pCCl_4$	ppt	pccl4	(ccl4f)		
SF_6	fmol kg^{-1}	sf6	sf6f	sf6qc	SF6
pSF_6	ppt	psf6	(sf6f)		
$\delta^{13}C$	‰	c13	c13f	c13qc	DELC13
$\Delta^{14}C$	‰	c14	c14f		DELC14
$\Delta^{14}C$ counting error	‰	c14err			C14ERR
^{3}H	TU	h3	h3f		TRITIUM
^{3}H counting error	TU	h3err			TRITER
$\delta^{3}He$	%	he3	he3f		DELHE3

Table 1. Continued.

Variable	Units	Product file name	WOCE flag name[a]	Second QC flag name[b]	WHP-exchange name
^{3}He counting error	%	he3err			DELHER
He	nmol kg^{-1}	he	hef		HELIUM
He counting error	nmol kg^{-1}	heerr			HELIER
Ne	nmol kg^{-1}	neon	neonf		NEON
Ne counting error	nmol kg^{-1}	neonerr			NEONER
δ^{18}O	‰	o18	o18f		DELO18
Total organic carbon	µmol L^{-1}[e]	toc	tocf		TOC
Dissolved organic carbon	µmol L^{-1}[e]	doc	docf		DOC
Dissolved organic nitrogen	µmol L^{-1}[e]	don	donf		DON
Dissolved total nitrogen	µmol L^{-1}[e]	tdn	tdnf		TDN
Chlorophyll *a*	µg kg^{-1}[e]	chla	chlaf		CHLORA

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

DAPv2, which forms the basis for the update presented here, was released in 2016 with data from 724 scientific cruises, including those from GLODAPv1.1, CARINA, and PACIFICA, as well as data from 168 additional cruises. GLODAPv2 not only combined all previous efforts, but it also created ocean-wide consistency across all cruise data through an inversion analysis. A particularly important source of additional data was the cruises executed within the framework of the “repeat hydrography” program (Talley et al., 2016), instigated in the early 2000s as part of the Climate and Ocean – Variability, Predictability and Change (CLIVAR) program and since 2007 organized as the Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP) (Sloyan et al., 2019). GLODAPv2 is updated regularly using the “living data process” of *Earth System Science Data* to document significant additions and modifications to the data product.

There are two types of GLODAP updates: full and intermediate. Full updates involve a reanalysis, notably crossover and inversion, of the entire dataset (both historical and new cruises) in which all data points are subject to potential adjustment. This was carried out for the creation of GLODAPv2. For intermediate updates, recently available data are added following quality control procedures to ensure their consistency with the cruises included in the latest GLODAP release. Except for obvious outliers and similar types of errors (Sect. 3.3.1), the data from previous releases are not changed or adjusted during intermediate updates. Note that the GLODAP mapped climatologies (Lauvset et al., 2016) are not updated for these intermediate products. A naming convention has been introduced to distinguish intermediate from full product updates. For the latter the version number will change, while for the former the year of release is appended. The exact version number and release year (if appended) of the product used should always be reported in studies rather than making a generic reference to GLODAP.

Creating and interpreting inversions, as well as other checks of the entire dataset needed for full updates, are too demanding in terms of time and resources to be performed every year or every 2 years. The aim is to conduct a full analysis (i.e., including an inversion) again after the third GO-SHIP survey has been completed. This completion is currently scheduled for 2024, and we anticipate that GLODAPv3 will become available a few years thereafter (pending funding). In the interim, the fourth intermediate update is presented here, which adds data from 96 cruises to the last update, GLODAPv2.2021 (Lauvset et al., 2021).

2 Key features of the update

GLODAPv2.2022 contains data from 1085 cruises covering the global ocean from 1972 to 2021, compared to 989 for the period 1972–2020 for the previous GLODAPv2.2021 (Lauvset et al., 2021). Information about the 96 cruises added to this version is provided in Table A1 in the Appendix. Cruise sampling locations are shown alongside those of GLODAPv2.2021 in Fig. 1, while the coverage in time is shown in Fig. 2. Not all cruises have data for all the above-mentioned 13 core variables. For example, cruises with only seawater CO_2 chemistry or transient tracer data are still included even without accompanying nutrient data due to their value towards the computation of carbon inventories. In a few cases, cruises without any of these properties are included because they do contain data for other carbon-related tracers such as carbon isotopes, with the intention of ensuring their wider availability. The added cruises are from 2003 to 2021, with the majority being more recent than 2018. The largest data contribution comes from the Coastal Ocean Data Analysis Product in North America (CODAP-NA; Jiang et al., 2021), which is a comprehensive compilation of carefully quality-assessed coastal carbon data covering all continental shelves of North America, from Alaska to Mexico in the west and from Canada to the Caribbean in the east. Another large addition are the 29 new cruises from the RV *Keifu Maru II* and RV *Ryofu Maru III* in the western North Pacific (Oka et al., 2018, 2017). In the Arctic Ocean we update the time series from Weather Station M in the Norwegian Sea with an additional 10 years of data and add five new Arctic cruises from RV *Healy*. In the Indian Ocean the 2019 repeat of GO-SHIP line I08N by the RV *Mirai* is included. In addition, we are for the first time including the cruises in the GEOTRACES intermediate data product where seawater CO_2 chemistry data are available (https://www.geotraces.org/geotraces-intermediate-data-product-2021/, last access: 23 June 2022). The GEOTRACES mission is "to identify processes and quantify fluxes that control the distributions of key trace elements and isotopes in the ocean, and to establish the sensitivity of these distributions to changing environmental conditions", but several cruises that measure trace elements and isotopes also measure CO_2 chemistry, and these have now been included in GLODAPv2. All new data in GLODAPv2.2022 include seawater CO_2 chemistry, and additionally, 10 new cruises include halogenated transient tracers.

All new cruises were subjected to primary (Sect. 3.1) and secondary (Sect. 3.2) quality control (QC). These procedures are very similar to those used for GLODAPv2.2021 and previous versions, aiming to ensure the consistency of the data from the 96 new cruises with the previous release of the GLODAP data product (in this case, the GLODAPv2.2021 adjusted data product). For the first time we also apply secondary QC routines to SF_6 data, thus increasing the number of core variables from 12 to 13.

For GLODAPv2.2021 we added a basin identifier to the product files, where 1 is the Atlantic Ocean, 4 the Arctic Mediterranean Sea (i.e., the Arctic Ocean plus the Nordic Seas), 8 the Pacific Ocean, and 16 the Indian Ocean. These regions are abbreviated AO, AMS, PO, and IO, respectively, in the adjustment table. Data in the Mediterranean Sea, Caribbean Sea, and Gulf of Mexico are classified as belonging to the Atlantic Ocean (1). The basin identifiers are unchanged in GLODAPv2.2022 and added to the product files to make it easier for users to identify which ocean basin an individual cruise belongs to without having to use one of the four regional files. Note that there is no overlap between the regional files or for our basin identifiers, and cruises in the Southern Ocean are placed in the basin where most of the data were collected. As in GLODAPv2.2021 we include the DOI for each cruise in all product files with the aim of easing access to the original data and metadata, as well as improving the visibility of data providers.

3 Methods

3.1 Data assembly and primary quality control

Data from the 96 new cruises were submitted directly to us or retrieved from data centers – typically OCADS (https://www.ncei.noaa.gov/products/ocean-carbon-acidification-data-system, last access: 9 August 2022), the CLIVAR and Carbon Hydrographic Data Office (https://cchdo.ucsd.edu, last access: 27 June 2022), and PANGAEA (https://pangaea.de, last access: 27 June 2022). Each cruise is identified by an expedition code (EXPOCODE). The EXPOCODE is guaranteed to be unique and constructed by combining the country code and platform code with the date of departure in the format YYYYMMDD. The country and platform codes were taken from the ICES (International Council for the Exploration of the Sea) library (https://vocab.ices.dk/, last access: 27 June 2022).

The individual cruise data files were converted to the WHP-exchange format: a comma-delimited ascii format for data from hydrographic cruises, with different and specific versions for CTD and bottle data. GLODAP only includes WHP-exchange in bottle format, with data and CTD data at bottle trip depths. An overview of the significant points is given below, with full details provided at https://exchange-format.readthedocs.io/ (v1.2.0 as of 22 March 2022, last access: 16 June 2022), derived from Swift and Diggs (2008). The first line of each exchange file specifies the data type – in the case of GLODAP this is "BOTTLE" – followed by a creation date time stamp in ISO8601 (YYYYMMDD) format, as well as the identification of the group and person who prepared the file. The latter follows a convention of including the division/group, the institution, and the initials of the person. The omnipresent "PRINUNIVRMK" thus acknowledges the enormous effort by Robert M. Key at Princeton University. Next follows the README section, which provides brief cruise-specific information, such as dates, ship, region, method plus quality notes for each variable measured, citation information, and references to any papers that used or presented the data. The README information is typically assembled from the information contained in the metadata submitted by the data originator. In some cases, issues noted during the primary QC and other information such as file update notes are included. The only rule for the README section is that it must be concise and informative, and each line must start with the comment character (#). The README is followed by variable names and units on separate lines and then the data. The names and units are standardized and provided in Table 1 for the variables included in GLODAP, with full specifications provided at https://exchange-format.readthedocs.io/en/latest/parameters.html (v1.2.0 as of 22 March 2022, last access: 16 June 2022). For consistency with previous updates and to ease the use of existing methods and code, GLODAP

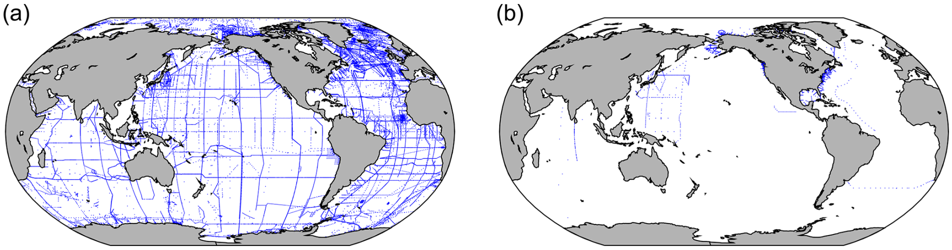

Figure 1. Location of stations in **(a)** GLODAPv2.2021 and for **(b)** the new data added in this update.

still uses the WHP-exchange format instead of adopting the new naming structure as outlined in Jiang et al. (2022).

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

Each data column (except temperature and pressure, which are assumed "good" if they exist) has an associated column of data flags (Joyce and Corry, 1994). For the original data exchange files, these flags conform to the WOCE definitions for water samples and are listed in Table 2. For the merged and adjusted product files these flags are simplified: questionable (WOCE flag 3) and bad (WOCE flag 4) data are removed, and their flags are set to 9. The same procedure is applied to data flagged 8 (very few such data exist); 1 (data not received) and 5 (data not reported) are also set to 9, while flags of 6 (mean of replicate measurements) and 7 (manual chromatographic peak measurement) are set to 2 if the data appear good. Also, in the merged product files a flag of 0 is used to indicate a value that could be measured but is approximated: for salinity, oxygen, phosphate, nitrate, and silicate, the approximation is conducted using vertical interpolation; for seawater CO_2 chemistry variables (TCO_2, TAlk, pH, and fCO_2), the approximation is conducted using the calculation from two measured CO_2 chemistry variables (Sect. 3.2.2). Importantly, the interpolation of CO_2 chemistry variables is never performed, and thus a flag value of 0 has a unique interpretation.

If no WOCE flags were submitted with the data, then they were assigned by us. Regardless, all incoming files were subjected to primary QC to detect questionable or bad data – this was carried out following Sabine et al. (2005) and Tanhua et al. (2010), primarily by inspecting property–property plots. For this task, the GLODAP primary quality control software (Velo et al., 2021) was used, as it presents a custom predefined schema of property–property plots designed by the consortium to ease the detection of outliers. Outliers showing up in two or more different such plots were generally defined as questionable and flagged. In some cases, outliers were detected during the secondary QC; the consequent flag changes have then also been applied in the GLODAP versions of the original cruise data files in agreement with the data submitter.

3.2 Secondary quality control

The aim of the secondary QC was to identify and correct any significant biases in the data from the 96 new cruises relative to GLODAPv2.2021 while retaining any signal due to temporal changes. To this end, secondary QC in the form of consistency analyses was conducted to identify offsets in the data. All identified offsets were scrutinized by the GLODAP reference group through a series of teleconferences during May 2022 to decide the adjustments to be applied to reduce the apparent offset (if any). To guide this process, a set of initial minimum adjustment limits was used (Table 3). These represent the minimum bias that can be confidently established relative to the measurement precision for the variables and cruises considered and are the same as those used for GLODAPv2.2021. In addition to the average magnitude of the offsets, factors such as the precision of the offsets, persistence towards the various cruises used in the comparison, regional dynamics, and the occurrence of time trends or other variations were considered. Thus, not all offsets larger than the initial minimum limits have been adjusted. A guiding principle for these considerations was to not apply an adjustment whenever in doubt. Conversely, in some cases when data and offsets were very precise and the cruise had been conducted in a region where variability is expected to be small, adjustments lower than the minimum limits were applied. Any adjustment was applied uniformly to all values for a variable and cruise; i.e., an underlying assumption is that cruises suffer from either no or a single and constant mea-

Table 2. WOCE flags in GLODAPv2.2022 exchange-format original data files (briefly; for full details see Swift, 2010) and the simplified scheme used in the merged product files.

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

[a] Flag set to 9 in product files. [b] Data are not included in the GLODAPv2.2022 product files and their flags set to 9. [c] Data are included, but flag is set to 2.

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

Variable	Minimum adjustment
Salinity	0.005
Oxygen	1 %
Nutrients	2 %
TCO_2	$4\,\mu mol\,kg^{-1}$
TAlk	$4\,\mu mol\,kg^{-1}$
pH	0.01
CFCs	5 %

surement bias. Adjustments for salinity, TCO_2, TAlk, and pH are always additive, while adjustments for oxygen, nutrients, and the halogenated transient tracers are always multiplicative. Except where explicitly noted (Sect. 3.3.1 and Table A2 in the Appendix) adjustments were not changed for data previously included in GLODAPv2.2021.

Crossover comparisons were the primary source of information used to identify offsets for salinity, oxygen, nutrients, TCO_2, TAlk, and pH (Sect. 3.2.2). As in GLODAPv2.2021 and GLODAPv2.2020 but in contrast to GLODAPv2 and GLODAPv2.2019, the evaluation of the internal consistency of the seawater CO_2 chemistry variables was not used for the evaluation of pH (Sect. 3.2.3). As in the two previous updates (2020 and 2021) we made extensive use of two predictions from two empirical algorithms – CArbonate system And Nutrients concentration from hYdrological properties and Oxygen using a Neural-network version B (CANYON-B) and CONsisTency EstimatioN and amounT (CONTENT) (Bittig et al., 2018) – for the evaluation of offsets in nutrients and seawater CO_2 chemistry data (Sect. 3.2.4). For previous versions we have also used multiple linear regression analyses and deep water averages, broadly following Jutterström et al. (2010), for additional information for the secondary QC of salinity, oxygen, nutrients, TCO_2, and TAlk data. In GLODAPv2.2022 we did not have to rely on the results of the multiple linear regression (MLR) analyses to make decisions about adjustments, and, in general, we are increasingly moving towards only using CANYON-B and CONTENT estimates (Sect. 3.2.4) as additional information when the crossover analysis is insufficient.

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

3.2.1 Merging of sensor and bottle data

Salinity and oxygen data can be obtained by analysis of water samples (bottle data) and/or directly from the CTD sensor pack. These two measurement types are merged and presented as a single variable in the product. The merging was conducted prior to the consistency checks, ensuring their internal calibration in the product. The merging procedures were only applied to the bottle data files, which commonly include values recorded by the CTD at the pressures where the water samples are collected. Whenever both CTD and bottle data were present in a data file, the merging step considered the deviation between the two and calibrated the CTD values if required and possible. Altogether seven scenarios (Table 4) are possible for each of the CTD conductivity and oxygen (O_2) sensor properties individually, in which the fourth never occurred during our analyses but is included to maintain consistency with GLODAPv2. For 39 % of the

96 new cruises both CTD and bottle data were included in the original cruise files for salinity and oxygen, and for all these cruises the two data types were found to be consistent. These new data have a lower proportion of cruises with both bottle and CTD measurements than GLODAPv2.2021 (75 % and 63 %, respectively, for salinity and oxygen). For salinity the remaining 61 % have only CTD data, while for oxygen 30 % have only CTD data and 21 % have only bottle data. Having both CTD and bottle values in the data files is highly preferred as the information is valuable for quality control (bottle mistrips, leaking Niskin bottles, and oxygen sensor drift are among the issues that can be revealed). The extent to which the bottle data (i.e., OXYGEN in the individual cruise exchange files) is mislabeled CTD data (i.e., should be CTDOXY) is uncertain. Regardless, all CTD and bottle data for salinity were consistent and did not need any further calibration, and only 3 out of the 96 cruises required calibration of the oxygen data.

3.2.2 Crossover analyses

The crossover analyses were conducted with the MATLAB toolbox prepared by Lauvset and Tanhua (2015) and with GLODAPv2.2021 as the reference data product. The toolbox implements the "running-cluster" crossover analysis first described by Tanhua et al. (2010). This analysis compares data from two cruises on a station-by-station basis and calculates a weighted mean offset between the two and its weighted standard deviation. The weighting is based on the scatter in the data such that data that have less scatter have a larger influence on the comparison than data with more scatter. Whether the scatter reflects actual variability or data precision is irrelevant in this context as increased scatter nevertheless decreases the confidence in the comparison. Stations are compared when they are within 2 arcdeg distance (∼ 200 km) of each other. To minimize the effects of natural variability only deep data are used. Either the 1500 or 2000 dbar pressure surface was used as the upper bound, depending on the amount of available data, their variation at different depths, and the region in question. Which one to use was determined on a case-by-case basis by comparing crossovers with the two depth limits and using the one that provided the clearest and most robust information. In regions where deep mixing or convection occurs, such as the Nordic, Irminger, and Labrador seas, the upper bound was always placed at 2000 dbar; while winter mixing in the first two regions is normally not deeper than this (Brakstad et al., 2019; Fröb et al., 2016), convection beyond this limit has occasionally been observed in the Labrador Sea (Yashayaev and Loder, 2017). However, using an upper depth limit deeper than 2000 dbar will quickly give too few data for robust analysis. In addition, even below the deepest winter mixed layers, properties do change over the time periods considered (e.g., Falck and Olsen, 2010), so this limit does not guarantee steady conditions. In the Southern Ocean deep convection beyond 2000 dbar seldom occurs, an exception being the processes accompanying the formation of the Weddell Polynya in the 1970s (Gordon, 1978). Deep and bottom water formation usually occurs along the Antarctic coasts, where relatively thin nascent dense water plumes flow down the continental slope. We avoid such cases, which are easily recognizable. To avoid removing persistent temporal trends, all crossover results are also evaluated as a function of time (see below).

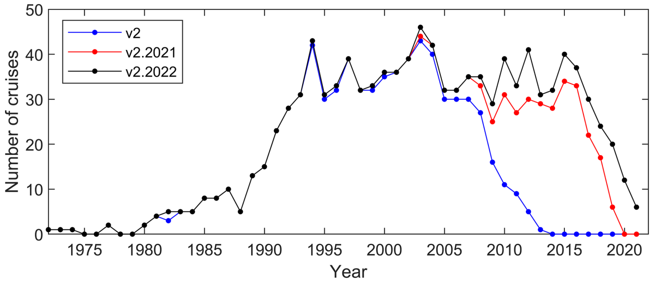

Figure 2. Number of cruises per year in GLODAPv2, GLODAPv2.2021, and GLODAPv2.2022.

As an example of crossover analysis, the crossover for silicate measured on the two cruises 49UF20190207, which is new to this version, and 49RY20110515, which was included in GLODAPv2, is shown in Fig. 3. For silicate the offset is determined as the ratio, in accordance with the procedures followed for GLODAPv2. The silicate values from 49UF20190207 are slightly higher, with a weighed mean offset of 1.02 ± 0.01 compared to those measured on 49RY20110515.

For each of the 96 new cruises, such a crossover comparison was conducted against all possible cruises in GLODAPv2.2021, i.e., all cruises that had stations closer than 2 arcdeg distance to any station for the cruise in question. The summary figure for silicate on 49UF20190207 is shown in Fig. 4. The silicate data measured on this cruise are 1.01 ± 0.00 higher when compared to the data measured on nearby cruises included in GLODAPv2.2021. This is smaller than the initial minimum adjustment limit for silicate of 2 % (Table 3) and as such does not automatically lead to an adjustment of the data in the merged data product. However, in this case the offset, while small, is very consistent and present in silicate data from many different cruises. Since we have also been able to identify a cause of the offset (see Sect. 4), an adjustment of 1 % has been applied. All other variables show very high consistency; thus, no adjustment is given to any other variable on cruise 49UF20190207 in GLODAPv2.2021. This is supported by the CANYON-B and CONTENT results (Sect. 3.2.4). Note that adjustments, when applied, are typically round numbers (e.g., −3 not −3.4 for TCO_2 and 0.005 not 0.0047 for pH) to avoid communicating that the ideal adjustments are accurately known.

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

Case	Description	Salinity	Oxygen
1	No data are available: no action needed.	0	7
2	No bottle values are available: use CTD values.	58	30
3	No CTD values are available: use bottle values.	0	19
4	Too few data of both types are available for comparison, and > 80 % of the records have bottle values: use bottle values.	0	0
5	The CTD values do not deviate significantly from bottle values: replace missing bottle values with CTD values.	38	37
6	The CTD values deviate significantly from bottle values: calibrate CTD values using linear fit and replace missing bottle values with calibrated CTD values.	0	1
7	The CTD values deviate significantly from bottle values, and no good linear fit can be obtained for the cruise: use bottle values and discard CTD values.	0	2

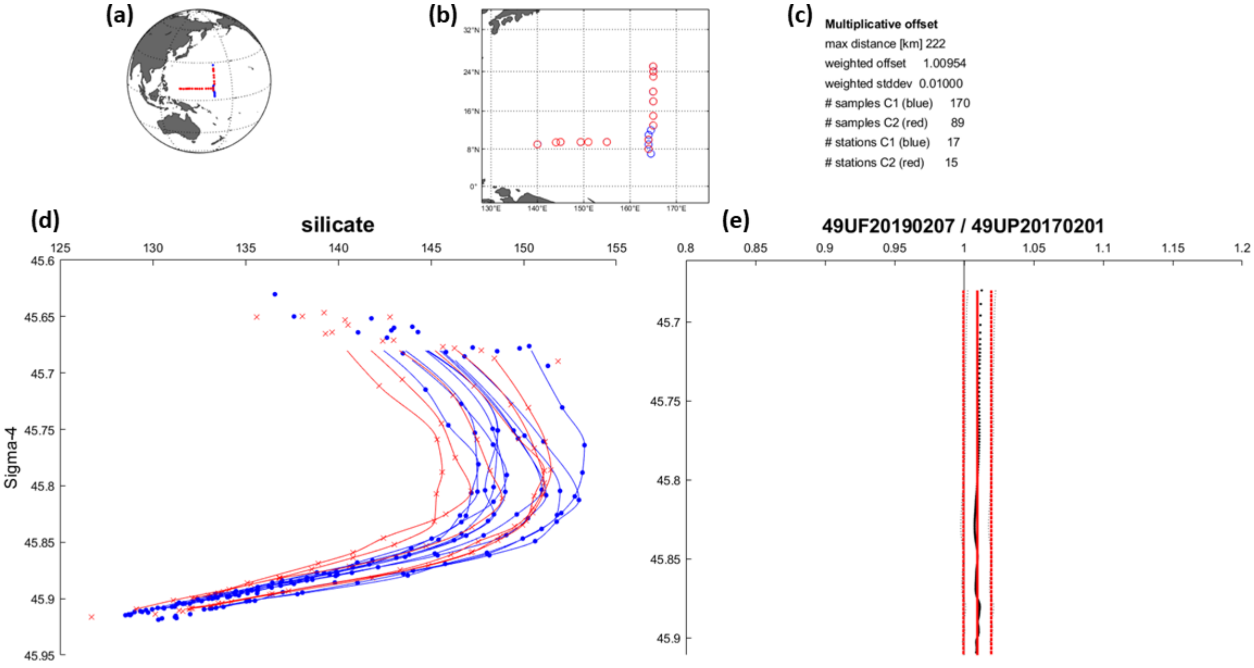

Figure 3. Example crossover figure for silicate for cruises 49UF20190207 (blue) and 49RY20110515 (red), as was generated during the crossover analysis. Panel **(a)** shows all station positions for the two cruises, and **(b)** shows the specific stations used for the crossover analysis. Panel **(d)** shows the data of silicate (µmol kg^{-1}) below the upper depth limit (in this case 2000 dbar) versus potential density anomaly referenced to 4000 dbar as points and the interpolated profiles as lines. Non-interpolated data either did not meet minimum depth separation requirements (Table 4 in Key et al., 2010) or are the deepest sampling depth. The interpolation does not extrapolate. Panel **(e)** shows the mean silicate difference profile (black, dots) with its standard deviation, as well as also the weighted mean offset (straight red lines) and weighted standard deviation. Summary statistics are provided in **(c)**.

3.2.3 pH scale conversion and quality control

Altogether 60 of the 96 new cruises included measured, spectrophotometric pH data, and only one required an adjustment (Sect. 4). We also excluded (flag −777) pH on one cruise as a result of the QC work. All except one cruise reported pH data on the total scale and at 25 °C. For the one cruise reporting pH on the seawater scale the data were converted following established routines (Olsen et al., 2020). For details on scale and temperature conversions in previous versions of GLODAPv2, we refer to Olsen et al. (2020). In contrast to quality control of pH data in GLODAPv2 (Olsen et al., 2016), the evaluation of the internal consistency of CO_2 system vari-

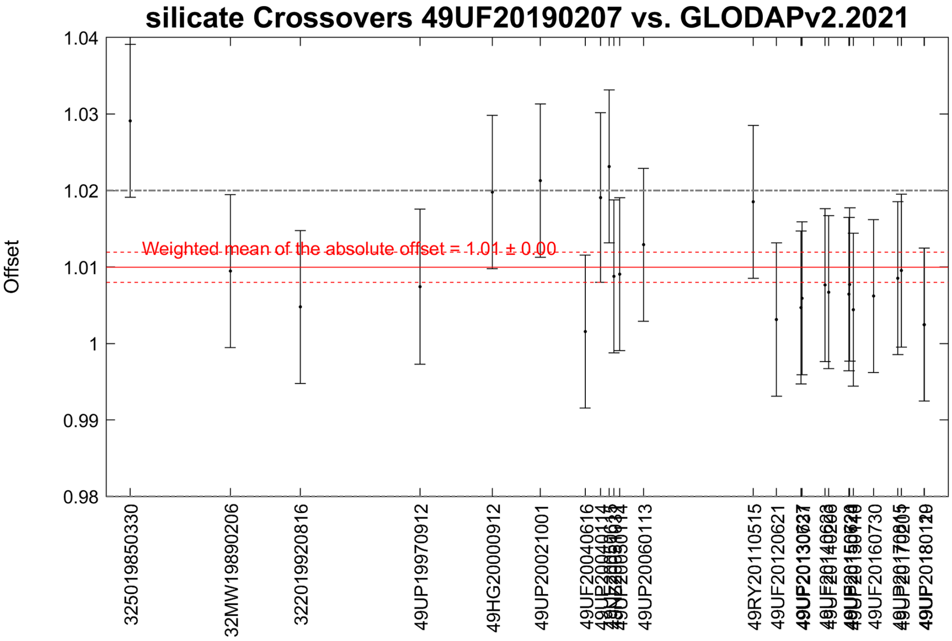

Figure 4. Example summary figure for silicate crossovers for 49UF20190207 versus the cruises in GLODAPv2.2021 (with cruise EXPOCODE listed on the x axis sorted according to the year the cruise was conducted). The black dots and vertical error bars show the weighted mean offset and standard deviation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

ables has not been used for the secondary quality control of the pH data in the GLODAPv2 updates of 2020 and onwards. For the 60 new cruises with pH in GLODAPv2.2022 only crossover analysis was used, supplemented by CONTENT and CANYON-B comparisons (Sect. 3.2.4). Recent literature has demonstrated that internal consistency evaluation procedures are subject to errors owing to an incomplete understanding of the thermodynamic constants, major ion contents, measurement biases, and potential contribution of organic compounds or other unknown protolytes to alkalinity. These complications lead to pH-dependent offsets in calculated pH compared with cruise spectrophotometric pH measurements (Álvarez et al., 2020; Carter et al., 2018; Fong and Dickson, 2019; Takeshita et al., 2020). The pH-dependent offsets may be interpreted as biases and generate false corrections (Álvarez et al., 2020; García-Ibáñez et al., 2022). The offsets are particularly strong at pH levels below 7.7, where calculated and measured pH values are different by on average between 0.01 and 0.02. For the North Pacific this is a problem as pH values below 7.7 can occur at the depths used during the QC (> 1500 dbar for this region; Olsen et al., 2016). Since any correction, which may be an artifact, would be applied to the full profiles, we use a minimum adjustment of 0.02 for the North Pacific pH data in the merged product files. Elsewhere, the inconsistencies that may have arisen are smaller, since deep pH is typically higher than 7.7 (Lauvset et al., 2020), and at such levels the difference between calculated and measured pH is less than 0.01 on average (Álvarez et al., 2020; Carter et al., 2018). Outside the North Pacific, we believe that the pH data are consistent to within 0.01. Avoiding CO_2 chemistry internal consistency considerations for these intermediate products helps to reduce the problem, but since the reference dataset (as also used for the generation of the CANYON-B and CONTENT algorithms) may have these issues, a future full re-evaluation, envisioned for GLODAPv3, is needed to address the problem completely.

3.2.4 CANYON-B and CONTENT analyses

CANYON-B and CONTENT (Bittig et al., 2018) were used to support decisions regarding the application of adjustments (or not). CANYON-B is a neural network for estimating nutrients and seawater CO_2 chemistry variables from temperature, salinity, and oxygen content. CONTENT additionally considers the consistency among the estimated CO_2 chemistry variables to further refine them. These approaches were developed using the data included in the GLODAPv2 data product (i.e., the 2016 version without any more recent updates). Their advantage compared to crossover analyses for evaluating consistency among cruise data is that effects of water mass changes on ocean properties are represented in the nonlinear relationships in the underlying neural network. For example, if elevated nutrient values measured on a cruise are not due to a measurement bias but actual aging of the water masses that have been sampled and as such accompanied by a decrease in oxygen content, the measured values and the CANYON-B estimates are likely to be similar. Vice versa, if the nutrient values are biased, the measured values and CANYON-B predictions will be dissimilar.

Used in the correct way and with caution this tool is a powerful supplement to the traditional crossover analyses which form the basis of our analyses. Specifically, we gave no weight to comparisons in which the crossover analyses had suggested that the salinity and/or O_2 data were biased, as this would lead to error in the predicted values. We also considered the uncertainties of the CANYON-B and CONTENT estimates. These uncertainties are determined for each predicted value, and for each comparison the ratio of the difference (between measured and predicted values) to the local uncertainty was used to gauge the comparability. As an example, the CANYON-B and CONTENT analyses of the data obtained for 49UF20190207 are presented in Fig. 5. The CANYON-B and CONTENT results confirmed the crossover comparisons for silicate discussed in Sect. 3.2.2 showing an inconsistency of 1.01. For the other variables, the inconsistencies are low and agree with the crossover results (not shown here but results can be accessed through the adjustment table).

Another advantage of the CANYON-B and CONTENT comparisons is that these procedures provide estimates at the level of individual data points; e.g., pH values are determined for every sampling location and depth where temperature, salinity, and O_2 data are available. Cases of strong differences between measured and estimated values are always examined. This has helped us to identify primary QC issues for some cruises and variables, for example a case of an inverted pH profile on cruise 32PO20130829, which was identified and amended in GLODAPv2.2020.

3.2.5 Halogenated transient tracers and SF_6

For the halogenated transient tracers (CFC-11, CFC-12, CFC-113, and CCl_4; CFCs for short), an inspection of surface saturation levels and an evaluation of relationships between the tracers for each cruise were used to identify biases rather than crossover analyses. Crossover analysis is of limited value for these variables given their transient nature and low contents at depth. As for GLODAPv2, the procedures were the same as those applied for CARINA (Jeansson et al., 2010; Steinfeldt et al., 2010).

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

As TTD, we use an inverse Gaussian function, which can be described by two parameters: the mean age (Γ) and the width (Δ) (Hall et al., 2002). Typically, the ratios of Δ / Γ are chosen as a fixed parameter, and Γ is varied. Here, we use a range of Γ between 0 and 2000 years and two values for Δ / Γ: 0.5 and 2. This range of TTD parameters reproduces simultaneous observation of different tracers, like CFC-12 and SF_6, when calculating the tracer contents from the TTD and the atmospheric mixing ratio (Steinfeldt et al., 2009). Typically, for the same CFC-12 value derived from the TTD, the corresponding SF_6 value increases with the Δ / Γ ratio of the TTD, and it also increases with decreasing saturation (α). As range for the expected SF_6 to CFC-12 relation we use the TTD with $\Delta / \Gamma = 0.5$ and $\alpha = 1$ as the lower boundary and the TTD with $\Delta / \Gamma = 0.5$ and 80 % saturation as the upper boundary. In some cases, like deep water formation or an ice-covered region, the tracer saturation might be lower, as the minimum of 65 % from Steinfeldt et al. (2009) indicates, but the majority of the data is actually located between our assumed lower and upper boundaries (see results for cruise 096U20160426 in Fig. 6). A few exceptions are found for cruises in the Southern Ocean, as has already been shown in Stöven et al. (2015). Note that in 1996, a SF_6 release experiment was performed in the Greenland Sea (Watson et al., 1999). This leads to a large excess of SF_6 compared to CFC-12 in the Nordic Seas, which is clearly visible in our analyses and hampers the quality control of the SF_6 data in this region.

3.3 Merged product generation

The merged product file for GLODAPv2.2022 was created by updating cruises and correcting known issues in the GLODAPv2.2021 merged file and then appending a merged and bias-corrected file containing the 96 new cruises – sorted according to EXPOCODE, station, and pressure – to this updated GLODAPv2.2021 file. GLODAP cruise numbers were assigned consecutively, starting from 4001, so they can be distinguished from the GLODAPv2.2021 cruises, which ended at 3043. The merging was otherwise performed following the procedures used for previous GLODAP versions (Olsen et al., 2019, 2020; Lauvset et al., 2021).

3.3.1 Updates and corrections for GLODAPv2.2021

For GLODAPv2.2022 we made several updates to cruises included in GLODAPv2.2021 (and earlier versions). The major updates were (i) to perform secondary quality control on all

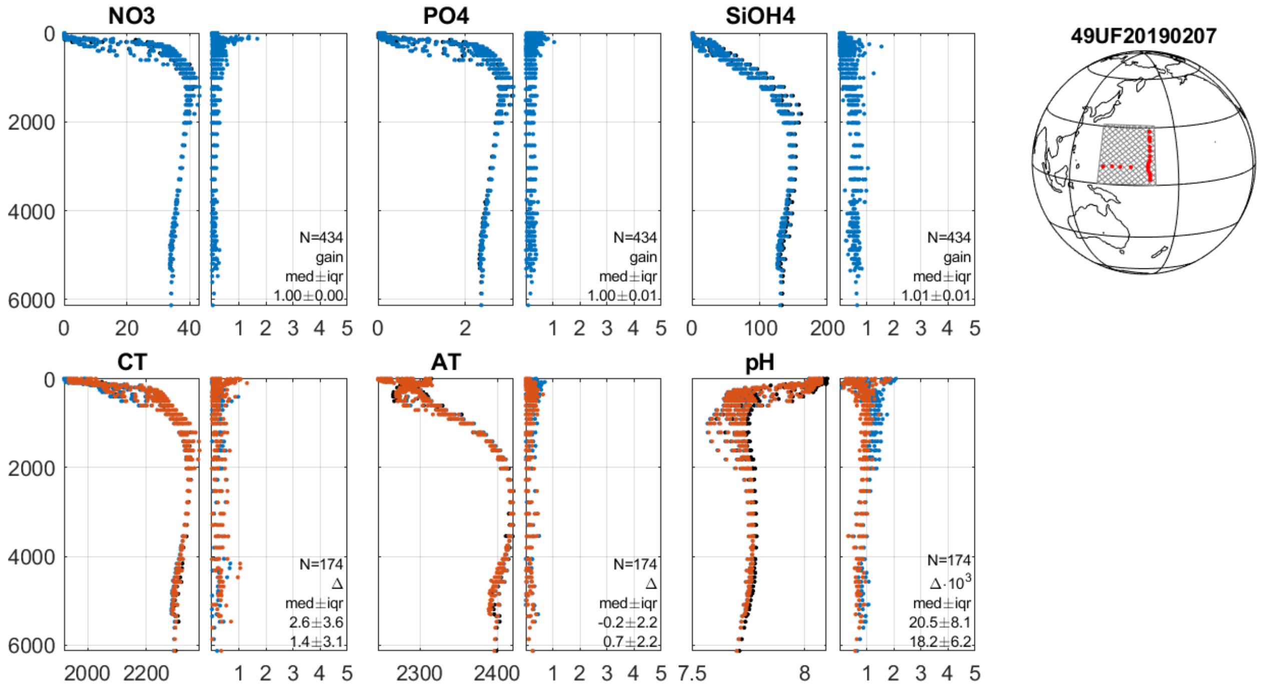

Figure 5. Example summary figure for CANYON-B and CONTENT analyses for 49UF20190207. Any data from regions where CONTENT and CANYON-B were not trained are excluded. The top row shows the nutrients and the bottom row the seawater CO_2 chemistry variables. All are shown versus sampling pressure (dbar), and the unit is micromoles per kilogram ($\mu mol\,kg^{-1}$) for all except pH, which is on the total scale at in situ temperature and pressure. Black dots (which to a large extent are hidden by the predicted estimates) are the measured data, blue dots are CANYON-B estimates, and red dots are the CONTENT estimates. Each variable has two figure panels. The left shows the depth profile, while the right shows the absolute difference between measured and estimated values divided by the CANYON-B and CONTENT uncertainty estimate, which is determined for each estimated value. These values are used to gauge the comparability; a value below 1 indicates a good match, as it means that the difference between measured and estimated values is less than the uncertainty of the latter. The statistics in each panel are for all data deeper than 500 dbar, and N is the number of samples considered. A multiplicative adjustment and its interquartile range are given for the nutrients. For the seawater CO_2 chemistry variables the numbers in each panel are the median difference between measured and predicted values for CANYON-B (upper) and CONTENT (lower). Both are given with their interquartile range.

Table 5. Possible outcomes of the secondary QC and their codes in the online adjustment table.

Secondary QC result	Code
The data are of good quality, are consistent with the rest of the dataset, and should not be adjusted	0/1*
The data are of good quality but are biased: adjust by adding (for salinity, TCO_2, TAlk, pH) or by multiplying (for oxygen, nutrients, CFCs) the adjustment value	Adjustment value
The data have not been quality controlled, are of uncertain quality, and are suspended until full secondary QC has been carried out	−666
The data are of poor quality and excluded from the data product	−777
The data appear of good quality, but their nature, being from shallow depths and coastal regions without crossovers or similar, prohibits full secondary QC	−888
No data exist for this variable for the cruise in question	−999

* The value of 0 is used for variables with additive adjustments (salinity, TCO_2, TAlk, pH) and 1 for variables with multiplicative adjustments (for oxygen, nutrients, CFCs). This is mathematically equivalent to “no adjustment” in both cases.

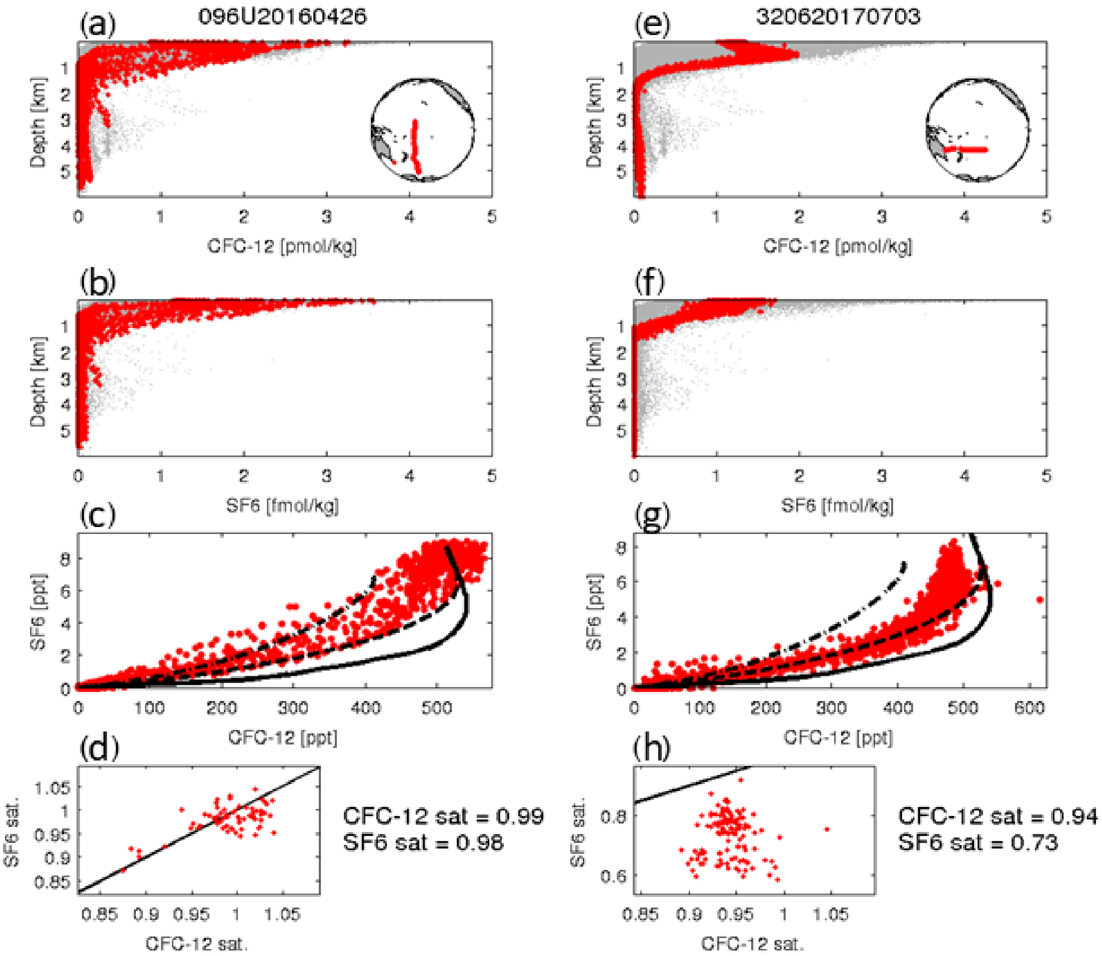

Figure 6. Example of plots used as basis for the SF_6 QC procedure. Shown are results for cruises 096U20160426 (left) and 320620170703 (right). **(a, e)** CFC-12 versus pressure for the specific cruise (red), together with all data from the corresponding GLODAP region (Pacific in this case, grey). **(b,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

Table 6. Summary of secondary QC results for the 96 new cruises, in number of cruises per result and per variable.

	Sal.	Oxy.	NO_3	Si	PO_4	TCO_2	TAlk	pH	CFC-11	CFC-12	CFC-113	CCl_4	SF_6
With data	96	90	91	92	93	93	94	60	5	6	1	0	2
No data	0	6	5	4	3	3	2	36	91	90	95	96	94
Unadjusted[a]	35	33	33	5	33	35	34	28	3	4	1	0	2
Adjusted[b]	0	2	0	29	1	0	1	1	1	1	0	0	0
−888[c]	61	55	58	58	58	58	59	30	1	1	0	0	0
−666[d]	0	0	0	0	1	0	0	0	0	0	0	0	0
−777[e]	0	0	0	0	0	0	0	1	0	0	0	0	0

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

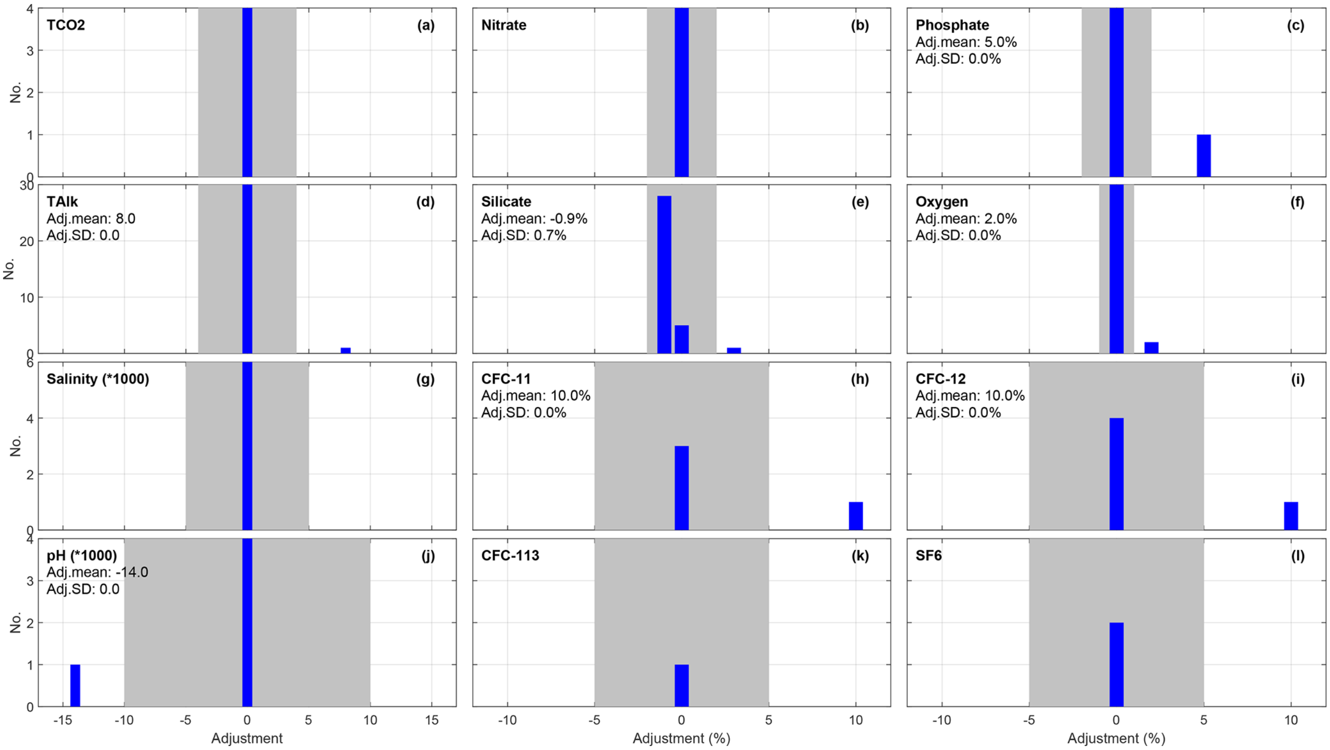

Figure 7. Distribution of applied adjustments for each core variable that received secondary QC, in micromoles per kilogram (μmol kg^{-1}) for TCO_2 and TAlk and unitless for salinity and pH (but multiplied by 1000 in both cases so a common x axis can be used), while for the other properties adjustments are given in percent ((adjustment ratio -1)$\times$100). Grey areas depict the initial minimum adjustment limits. The figure includes numbers for data subjected to secondary quality control only. Note also that the y-axis scale is set to render the number of adjustments visible, so the bar showing zero offset (the 0 bar) for each variable is cut off (see Table 6 for these numbers).

SF_6 data (see Sect. 3.2.5) and (ii) to apply small adjustments to TCO_2 and TAlk data measured on board the RV *Knorr* in 1994–1995 (EXPOCODES 316N199*; Table A2). These adjustments are derived from offsets in the CRM measurements which were previously reported but never applied to the seawater measurements (Christopher Sabine and Douglas Wallace, personal communication, 2022; Johnson et al., 2002). These offsets are lower than the minimum adjustment limits defined for GLODAP. Applying these adjustments achieves procedural consistency with other CO_2 chemistry data that are usually corrected for CRM offsets before being subjected to secondary QC.

For TAlk the original CRM offsets were derived from Table 2 in Millero et al. (1998), who reported repeated CRM measurements on different titration cells for each cruise. The mean measured CRM value across all cells was calculated and compared to the published reference value for the same batch, and, if necessary, the offsets obtained from multiple CRM batches measured on one cruise were averaged. For TCO_2 the original CRM offsets were calculated from Table 3 in Johnson et al. (1998), who reported offsets for two measurement systems, which were here averaged. Johnson et al. (2002) report that their TCO_2 measurements were affected by changes in pipette volumes, which they were able to correct for in the CRM measurements. However, these volume corrections were most likely not applied to the seawater measurements (Douglas Wallace, personal communication, 2022; Johnson et al., 2002), and we therefore use the CRM offsets reported before correcting for the changes in pipette volume. For both TAlk and TCO_2 we calculate and use the mean CRM offset across all Indian Ocean cruises on the RV *Knorr* from 1994–1995 (-3.5 μmol kg^{-1} for TAlk and 1.7 μmol kg^{-1} for TCO_2) as a bulk adjustment value for the seawater measurements on these cruises. The GLODAP policy for avoiding small adjustments does not apply in this instance because there is a documented reason for the adjustment beyond improving internal consistency of the GLODAPv2 data product. Encouragingly, we also note that applying these adjustments improves the consistency with more recent (post-2000) Indian ocean data in GLODAPv2: for TAlk the mean absolute offset decreased from 2.8 μmol kg^{-1} for the unadjusted data to -0.7 μmol kg^{-1} for the adjusted data, while for TCO_2 the mean absolute offset decreased from -2.3 μmol kg^{-1} for the unadjusted data to -0.6 μmol kg^{-1} for the adjusted data, respectively.

Table A2 in the Appendix shows a list of the cruises that have been updated, as well as what the update consists of.

In addition, several minor omissions and errors have been identified and corrected.

- An error was corrected in the QC flagging of calculated CO_2 chemistry variables when fCO_2 was used as one of the inputs (changed from 1 to 0).
- CFC-12 data were added to cruise 06M320150501.
- Missing bottle number were added to cruises 29AH20160617 and 29HE20190406.
- For cruise 316N19831007 the WOCE flag on TAlk was changed from 2 to 0.
- Oxygen concentrations of 49UP19970912 have been adjusted 1.5 % upward.
- pH values of 49HG19960807 have been adjusted downward by 0.05.
- The time series from Weather Station M in the Norwegian Sea was updated with data from 2008–2021.
- In addition to DOIs for all original data files, DOIs for the included data products (CODAP-NA and GEOTRACES) have been added to the product files.
- An extra column “G2expocode” has been added, listing the EXPOCODE for each entry.

4 Secondary quality control results and adjustments

The secondary QC has five possible outcomes which are summarized in Table 5, along with the corresponding codes that appear in the online adjustment table and that are also occasionally used as shorthand for decisions in the text below. Some cruises were not applicable for full secondary QC. Specifically, in some cases data were too shallow or geographically too isolated for full and conclusive consistency analyses. In other cases, the results of these analyses were inconclusive, but we have no reason to believe that the data in question are of poor quality. A secondary QC flag has been included in the merged product files to enable their identification, with “0” used for variables and cruises not subjected to full secondary QC (corresponding to code −888 in Table 5) and “1” for variables and cruises that were subjected to full secondary QC. The secondary QC flags are assigned per cruise and variable, not for individual data points, and are independent of – and included in addition to – the primary (WOCE) QC flag on individual measurements. For example, interpolated (salinity, oxygen, nutrients) or calculated (TCO_2, TAlk, pH) values, which have a primary QC flag of 0, may have a secondary QC flag of 1 if the measured data these values are based on have been subjected to full secondary QC. Conversely, individual data points may have a secondary QC flag of 0 even if their primary QC flag is 2 (good data). Prominent examples for this version are the CODAP-NA data (Jiang et al., 2021), which as a primarily coastal dataset typically has quite shallow sampling depths that rendered conclusive secondary QC impossible. As a consequence, most, but not all, of these data are included with a secondary QC flag of 0.

The secondary QC actions for the 13 core variables and the distribution of adjustments applied on the 96 new cruises are summarized in Table 6 and Fig. 7, respectively. For most variables only a small fraction of the data were adjusted: no salinity, TCO_2, or nitrate data, 1.1 % TAlk data and phosphate data, 2.2 % of oxygen data, and 31 % of silicate data. The large percentage of silicate data requiring adjustment in this version is due to a consistent 1 % offset in the silicate data from the Japan Meteorological Agency (JMA) after 2018 (compared to older data from JMA). This offset has been traced to a change in the batch of Merck silicate standard solution used. In GLODAPv2.2022 this offset has been corrected by adjusting the new data (after 2018) to be consistent with the older data. For the CFCs, CFC-11 required adjustment for one out of the five new cruises and CFC-12 required adjustment on one out of six new cruises. For the total of 82 cruises with SF_6 data in GLODAPv2.2022, two cruises (06MT20060712 and 325020080826) could not be subjected to secondary quality control (−888), and five cruises received an upward adjustment (see example for cruise 320620170703 in Fig. 6). The magnitude of the adjustment was calculated using the saturation of CFC-12 as a benchmark. Additionally, for two cruises (49K619990523 and 58GS20090528), the SF_6 values are out of the TTD-derived range, as are the surface saturations. In these cases, the SF_6 data are discarded (QC flag −777). Of the 96 new cruises in GLODAPv2.2022 only two include SF_6, and neither required an adjustment. Overall, the magnitudes of the various adjustments applied are small, and the tendency observed during the production of the three previous updates remains, namely that the large majority of recent cruises are consistent with earlier releases of the GLODAP data product. A total of 60 out of the 96 new cruises included measured pH data, but only one received an adjustment (and one was flagged −777). However, the new crossover and inversion analysis of all pH data in the northwestern Pacific that was planned following the release of GLODAPv2.2020 has not yet been performed. Such an analysis is planned for the next full update of GLODAP, i.e., GLODAPv3. Therefore, the conclusion from GLODAPv2.2020 remains that some caution should be exercised if looking at trends in ocean pH in the northwestern Pacific using GLODAPv2.2022 or earlier versions.

For the nutrients, adjustments were applied to maintain consistency with data included in GLODAPv2.2021 and earlier versions. An alternative goal for the adjustments would be maintaining consistency with data from cruises that employed reference materials (RMNS) to ensure accuracy of nutrient analyses. Such a strategy was adopted

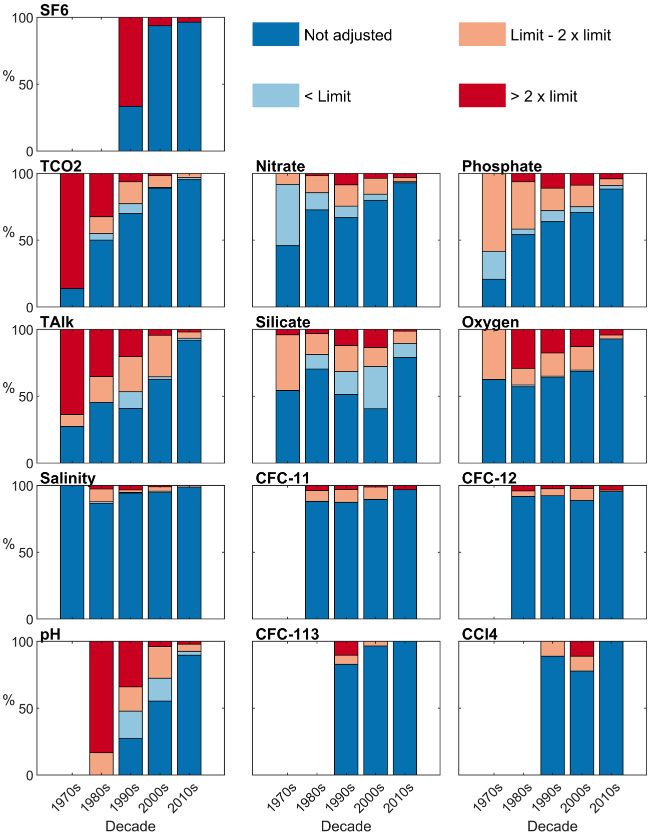

Figure 8. Magnitude of applied adjustments relative to minimum adjustment limits (Table 3) per decade for the 1085 cruises included in GLODAPv2.2022.

by Aoyama (2020) for preparation of the Global Nutrients Dataset 2013 (GND13) and is being considered for GLODAP as well. However, as this would require a re-evaluation of the entire dataset, this will not occur until the next full update of GLODAP. For now, we note the overall agreement between the adjustments applied in these two efforts (Aoyama, 2020) and that most disagreements appear to be related to cases where no adjustments were applied in GLODAP.

The improvement in data consistency resulting from the secondary QC process is evaluated by comparing the weighted mean of the absolute offsets for all crossovers before and after the adjustments have been applied. This “consistency improvement” for core variables is presented in Table 7. The data for CFCs were omitted from these analyses for previously discussed reasons (Sect. 3.2.5). Globally, the improvement is modest. Considering the initial data quality, this result was expected. However, this does not imply that the data initially were consistent everywhere. Rather, for some regions and variables there are substantial improvements when the adjustments are applied. For example, oxygen, silicate, and phosphate in the Atlantic Ocean all show a considerable improvement.

Table 7. Improvements resulting from quality control of the 96 new cruises per basin and for the global dataset. The values in the table are the weighted mean of the absolute offset of unadjusted and adjusted data versus GLODAPv2.2021. The total number of valid crossovers in the global ocean for the variable in question is *n*. The values in this table represent the inter-cruise consistency in the GLODAPv2.2022 product.

	Arctic			Atlantic			Indian			Pacific			Global			
	Unadj.		Adj.	Unadj.		Adj.	Unadj.		Adj.	Unadj.		Adj.	Unadj.		Adj.	*n* (global)
Sal (×1000)	NA	⇒	NA	4.6	⇒	4.6	0.7	⇒	0.7	1.2	⇒	1.2	1.3	⇒	1.3	1105
Oxy (%)	NA	⇒	NA	1.5	⇒	0.8	0.5	⇒	0.5	0.4	⇒	0.4	0.5	⇒	0.4	1064
NO_3 (%)	NA	⇒	NA	1.7	⇒	1.7	0.7	⇒	0.7	0.4	⇒	0.4	0.4	⇒	0.4	940
Si (%)	NA	⇒	NA	3.0	⇒	2.6	0.9	⇒	0.9	1.4	⇒	0.6	1.4	⇒	0.6	916
PO_4 (%)	NA	⇒	NA	2.0	⇒	1.1	0.7	⇒	0.7	0.7	⇒	0.7	0.7	⇒	0.7	936
TCO_2 ($\mu mol\, kg^{-1}$)	NA	⇒	NA	7.3	⇒	7.3	2.0	⇒	2.0	1.8	⇒	1.8	2.4	⇒	2.4	544
TAlk ($\mu mol\, kg^{-1}$))	NA	⇒	NA	4.5	⇒	3.1	5.2	⇒	5.2	1.8	⇒	1.8	1.9	⇒	1.8	515
pH (×1000)	NA	⇒	NA	11.6	⇒	11.6	NA	⇒	NA	5.5	⇒	5.3	5.5	⇒	5.4	462

NA – not available

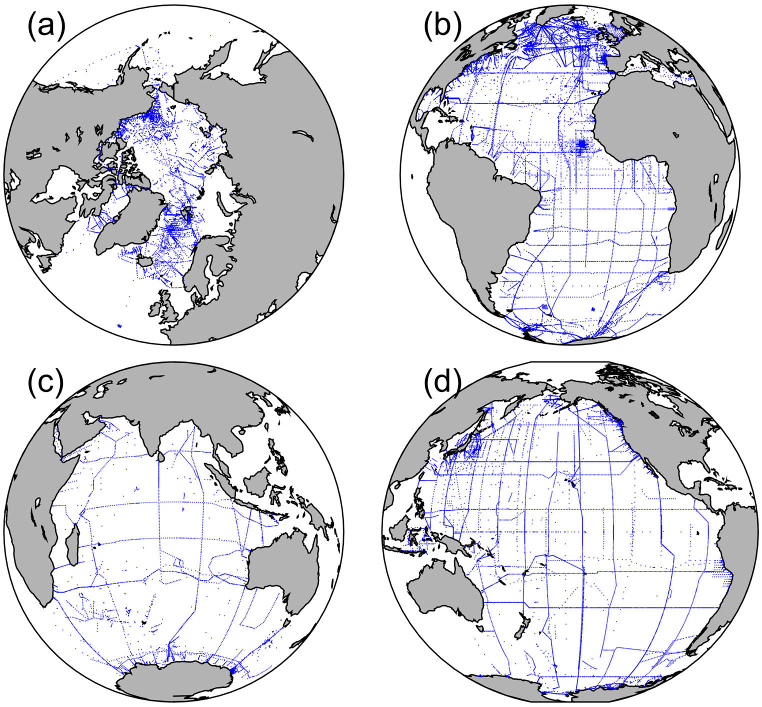

Figure 9. Locations of stations included in the **(a)** Arctic, **(b)** Atlantic, **(c)** Indian, and **(d)** Pacific ocean product files for the complete GLODAPv2.2022 dataset.

The various iterations of GLODAP provide insight into initial data quality covering more than 4 decades. Figure 8 summarizes the applied absolute adjustment magnitude per decade. These distributions are broadly unchanged compared to GLODAPv2.2021 (Fig. 7 in Lauvset et al., 2021). Most TCO_2 and TAlk data from the 1970s needed an adjustment, but this fraction steadily declines until only a small percentage is adjusted in recent years. This is encouraging and demonstrates the value of standardizing sampling and measurement practices (Dickson et al., 2007), the widespread use of CRMs (Dickson et al., 2003), and instrument automation. The pH adjustment frequency also has a downward trend; however, there remain issues with the pH adjustments, and this is a topic for future development in GLODAP, with the support from the Ocean Carbon & Biogeochemistry (OCB) Ocean Carbonate System Intercomparison Forum (OCSIF, https://www.us-ocb.org/ocean-carbonate-system-intercomparison-forum/, last access: 27 June 2022) working group (Álvarez et al., 2020). For the nutrients and oxygen, only the phosphate adjustment frequency decreases from decade to decade. However, we do note that the more recent data from the 2010s receive the fewest adjustments. This may reflect recent increased attention that seawater nutrient measurements have received through an operation manual (Becker et al., 2020; Hydes et al., 2010), availability of RMNS (Aoyama et al., 2012; Ota et al., 2010), and the Scientific Committee on Oceanic Research (SCOR) working group no. 147 towards comparability of global oceanic nutrient data (COMPONUT). For silicate, the fraction of cruises receiving adjustments peaks in the 1990s and 2000s. This is related to the 2 % offset between US and Japanese cruises in the Pacific Ocean that was revealed during production of GLODAPv2 and discussed in Olsen et al. (2016). For salinity and the halogenated transient tracers, the number of adjusted cruises is small in every decade.

5 Data availability

The GLODAPv2.2022 merged and adjusted data product is archived at the OCADS of NOAA NCEI (https://doi.org/10.25921/1f4w-0t92, Lauvset et al., 2022). These data and ancillary information are also available via our web pages and https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2022/ (last access: 15 August 2022). The data are available as comma-separated ascii files (*.csv) and as binary MATLAB files (*.mat) that use the open-source Hierarchical Data Format version 5 (HDF5). The data product is also made available as an Ocean Data View (ODV) file which can be easily explored using the "webODV Explore" online data service (https://explore.webodv.awi.de/, webODV Explore, 2022). Regional subsets are available for the Arctic, Atlantic, Pacific, and Indian oceans. There are no data overlaps between regional subsets, and each cruise exists in only one basin file even if data from that cruise

Table 8. Table listing the number of data points in GLODAPv2.2022, as well as the number of data with various combinations of variables.

Variables	Number of records
All core (salinity, oxygen, nitrate, silicate, phosphate, TCO_2, TAlk, pH, CFC-11, CFC-12, CFC-113, CCl_4, and SF_6)	174
All core except SF_6	2029
Salinity, oxygen, nitrate, silicate, phosphate, CFC-11, CFC-12, CFC-113, CCl_4, and SF_6 plus two of TCO_2, TAlk, and pH	636
Salinity, oxygen, nitrate, silicate, phosphate, TCO_2, TAlk, and pH	168 330
CFC-11, CFC-12, CFC-113, CCl_4, and SF_6	926
At least one transient tracer species or SF_6	427 913
SF_6	98 951
Two out of the three CO_2 chemistry core variables (TCO_2, TAlk, pH)	448 024
Measured fCO_2	33 844
Salinity, oxygen, nitrate, silicate, and phosphate	861 650
Salinity and oxygen	1 165 389
No salinity	27 906
Total in GLODAPv2.2022	1 381 248

cross basin boundaries. The station locations in each basin file are shown in Fig. 9. The product file variables are listed in Table 1. As well as being included in the .csv and .mat files, lookup tables for matching the EXPOCODE and DOI of a cruise with GLODAP cruise number are provided with the data files. A “known issues document” accompanies the data files and provides an overview of known errors and omissions in the data product files. It is regularly updated, and users are encouraged to inform us whenever any new issues are identified. It is critical that users consult this document whenever the data products are used.

All material produced during the secondary QC is available via the online GLODAP adjustment table hosted by GEOMAR, Kiel, Germany, at https://glodapv2-2022.geomar.de/ (GLODAP, 2022a) and can also be accessed through http://www.glodap.info (GLODAP, 2022b). This is similar in form and function to the GLODAPv2 adjustment table (Olsen et al., 2016) and includes a brief written justification for any adjustments applied.

The original cruise files, with updated flags determined during additional primary GLODAP QC, are available through the GLODAPv2.2022 cruise summary table (CST) hosted by OCADS: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2022/cruise_table_v2022.html (GLODAP, 2022c). Each of these files has been assigned a DOI, which is included in the data product files but not listed here. The CST also provides brief information on each cruise and access to metadata, cruise reports, and its adjustment table entry.

While GLODAPv2.2022 is made available without any restrictions, users of the data should adhere to the fair data use principles: for investigations that rely on a particular (set of) cruise(s), recognize the contribution of GLODAP data contributors by at least citing both the cruise DOI and any articles where the data are described, as well as, preferably, contacting principal investigators to explore opportunities for collaboration and co-authorship. To this end, DOIs are provided in the product files, as well as relevant articles and principal investigator names in the cruise summary table. Contacting principal investigators comes with the additional benefit that the principal investigators often possess expert insight into the data and/or specific region under investigation. This can improve scientific quality and promote data sharing.

This paper should be cited in any scientific publications that result from usage of the product. Citations provide the most efficient means to track use, which is important for attracting funding to enable the preparation of future updates.

6 Summary

GLODAPv2.2022 is an update of GLODAPv2.2021. Data from 96 new cruises have been added to supplement the earlier release and extend temporal coverage by 1 year. GLODAP now includes 48 years, 1972–2021, of global interior ocean biogeochemical data from 1085 cruises. The total number of data records is 1 381 248 (Table 8). Records with measurements for all 13 core variables (salinity, oxygen, nitrate, silicate, phosphate, TCO_2, TAlk, pH, CFC-11, CFC-12, CFC-113, CCl_4, and SF_6) are very rare (174), and requiring only two out of the three core seawater CO_2 chemistry variables, in addition to all the other core variables, is still very rare with only 636 records (Table 8). A major limiting factor to having all core variables is the simultaneous availability of data for all four transient tracer species and SF_6. In GLODAPv2.2022 there are 98 951 records with SF_6 data and 427 913 records with at least one transient tracer or SF_6. A total of 2 % (27 906) of all data records do not have salinity. There are several reasons for this, the main one being the inability to vertically interpolate due to a separation that is too large between measured samples. Other reasons for missing salinity include salinity not being reported and missing depth or pressure.

As for previous versions there is a bias toward summertime in the data in both hemispheres; most data are collected during April through November in the Northern Hemisphere,

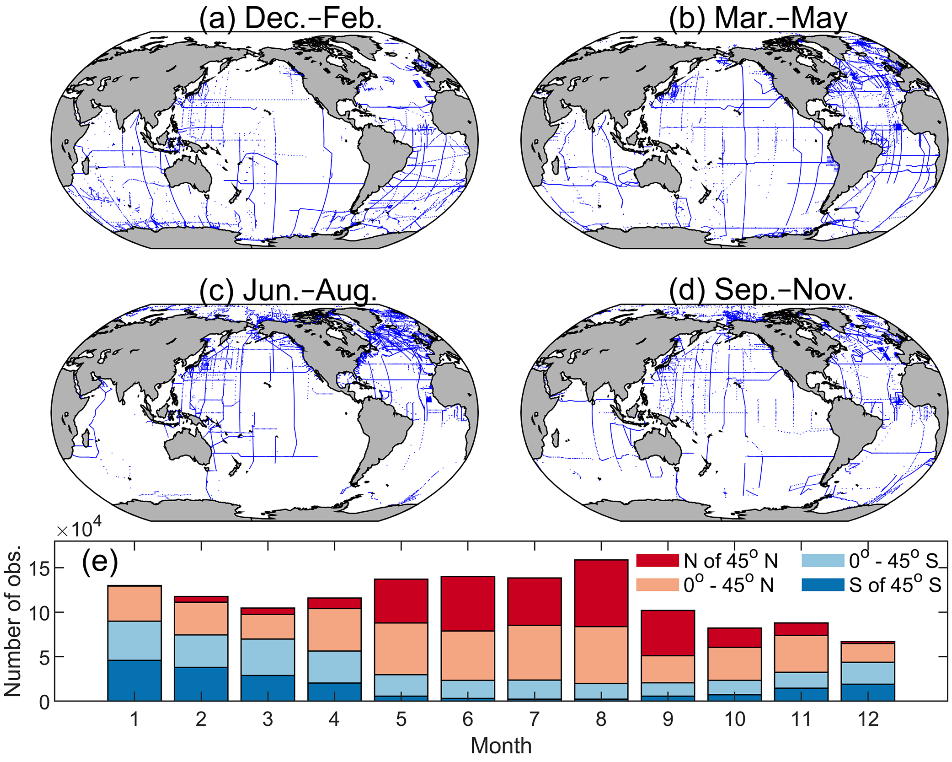

Figure 10. Distribution of data in GLODAPv2.2022 in **(a)** December–February, **(b)** March–May, **(c)** June–August, and **(d)** September–November, as well as **(e)** number of observations for each month in four latitude bands.

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

Except for salinity and oxygen, the core data were collected exclusively through chemical analyses of collected water samples. The data of the 13 core variables were subjected to primary quality control to identify questionable or bad data points (outliers) and secondary quality control to identify systematic measurement biases. The data are provided in two ways: as a set of individual exchange-formatted original cruise data files with assigned WOCE flags and as globally and regionally merged data product files with adjustments applied to the data according to the outcome of the consistency analyses. Importantly, no adjustments were applied to data in the individual cruise files, while primary QC changes were applied.

The consistency analyses were conducted by comparing the data from the 96 new cruises to the previous data product GLODAPv2.2021. Adjustments were only applied when the offsets were believed to reflect biases relative to the earlier data product release related to measurement calibration and/or data handling practices and not to natural variability or anthropogenic trends. For GLODAPv2.2022 a special case is the RV *Knorr* cruises in 1994–1995 in which the adjustment reflects offsets in CRM measurements that have not previously been corrected for. The adjustment table at https://glodapv2-2022.geomar.de/ (last access: 15 August 2022) lists all applied adjustments and provides a brief justification for each. The consistency analyses rely on deep ocean data (> 1500 or 2000 dbar depending on region), but supplementary CANYON-B and CONTENT analyses consider data below 500 dbar. Data consistency for cruises with exclusively shallow sampling was not examined. All new pH data for this version were comprehensively reviewed using crossover analysis, and only one required adjustment, while another had to be flagged bad (−777) and removed from the product. Regardless, full reanalysis of all available pH data, particularly in the North Pacific, will be conducted for GLODAPv3.

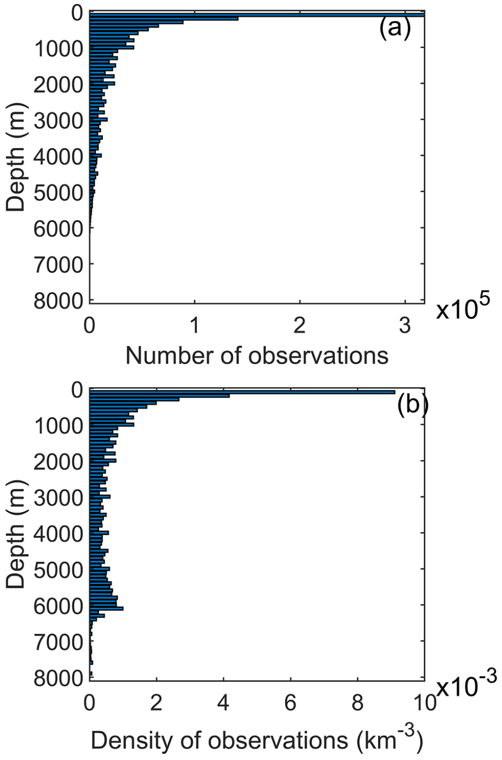

Figure 11. Number **(a)** and density **(b)** of observations in 100 m depth layers. The latter was calculated by dividing the number of observations in each layer by its global volume calculated from ETOPO2 (National Geophysical Data Center, 2006). For example, in the layer between 0 and 100 m there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

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

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

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

Appendix A: Supplementary tables

Table A1. Cruises included in GLODAPv2.2022 that did not appear in GLODAPv2.2021. Complete information on each cruise, such as variables included, and chief scientist and principal investigator names is provided in the cruise summary table at https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2022/cruise_table_v2022.html (last access: 15 August 2022).

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

Table A1. Continued.

No.	EXPOCODE	Region	Alias	Start	End	Ship
4051	33HQ20090403	Pacific	HLY0902	20090403	20090512	*Healy*
4052	33HQ20100907	Arctic	HLY1003	20100907	20100927	*Healy*
4053	33HQ20121005	Arctic	HLY1203	20121005	20121025	*Healy*
4054	33HQ20170826	Arctic	HLY1702	20170826	20170915	*Healy*
4055	33HQ20180807	Arctic	HLY1801	20180807	20180824	*Healy*
4056	33HQ20190806	Arctic	HLY1901	20190806	20190822	*Healy*
4057	33RO20120721	Atlantic	RB-12-03, GOMECC2	20120722	20120813	*Ronald H. Brown*
4058	33RO20170718	Atlantic	GOMECC3	20170718	20170820	*Ronald H. Brown*
4059	33WA20141201	Atlantic	WS1418	20141201	20141205	*F.G. Walton Smith*
4060	33WA20150921	Atlantic	WS15264	20150921	20150925	*F.G. Walton Smith*
4061	49HH20091106	Indian	KH09-05	20091106	20100109	*Hakuho Maru*
4062	49NZ20191205	Indian	MR19-04 (Leg 2), GO-SHIP I08N	20191205	20191227	*Mirai*
4063	49UF20190207	Pacific	ks201902	20190207	20190320	*Keifu Maru II*
4064	49UF20190424	Pacific	ks201904	20190424	20190526	*Keifu Maru II*
4065	49UF20190604	Pacific	ks201905	20190604	20190710	*Keifu Maru II*
4066	49UF20190716	Pacific	ks201906	20190716	20190908	*Keifu Maru II*
4067	49UF20190916	Pacific	ks201907	20190916	20191022	*Keifu Maru II*
4068	49UF20200108	Pacific	ks202001	20200108	20200126	*Keifu Maru II*
4069	49UF20200201	Pacific	ks202002	20200201	20200323	*Keifu Maru II*
4070	49UF20200605	Pacific	ks202004	20200605	20200614	*Keifu Maru II*
4071	49UF20200619	Pacific	ks202005	20200619	20200724	*Keifu Maru II*
4072	49UF20200730	Pacific	ks202006	20200730	20200820	*Keifu Maru II*
4073	49UF20201021	Pacific	ks202008	20201021	20201201	*Keifu Maru II*
4074	49UF20210202	Pacific	ks202102	20210202	20210312	*Keifu Maru II*
4075	49UF20210407	Pacific	ks202103	20210407	20210509	*Keifu Maru II*
4076	49UF20210515	Pacific	ks202104	20210515	20210627	*Keifu Maru II*
4077	49UP20181122	Pacific	rf201808to09	20181122	20181225	*Ryofu Maru III*
4078	49UP20190110	Pacific	rf201901	20190110	20190223	*Ryofu Maru III*
4079	49UP20190228	Pacific	rf201902	20190228	20190326	*Ryofu Maru III*
4080	49UP20190408	Pacific	rf201903	20190208	20190511	*Ryofu Maru III*
4081	49UP20190516	Pacific	rf201904	20190516	20190606	*Ryofu Maru III*
4082	49UP20190612	Pacific	rf201905	20190612	20190803	*Ryofu Maru III*
4083	49UP20190811	Pacific	rf201906	20190811	20190926	*Ryofu Maru III*
4084	49UP20191125	Pacific	rf201908	20191125	20191222	*Ryofu Maru III*
4085	49UP20200227	Pacific	rf202002	20200227	20200323	*Ryofu Maru III*
4086	49UP20200605	Pacific	rf202005	20200605	20200715	*Ryofu Maru III*
4087	49UP20200730	Pacific	rf202006	20200730	20200909	*Ryofu Maru III*
4088	49UP20201019	Pacific	rf202008	20201019	20201109	*Ryofu Maru III*
4089	49UP20210113	Pacific	rf202101	20210113	20210223	*Ryofu Maru III*
4090	49UP20210301	Pacific	rf202102	20210301	20210321	*Ryofu Maru III*
4091	49UP20210425	Pacific	rf202104	20210425	20210528	*Ryofu Maru III*
4092	58HB20201110	Atlantic		20201110	20211116	*Hans Brattstrøm*
4093	64PE20100428	Atlantic	PE319	20100428	20100526	RV *Pelagia*
4094	64PE20100611	Atlantic	PE321	20100611	20100708	RV *Pelagia*
4095	740H20111224	Atlantic	JC068	20111224	20120127	*RRS James Cook*
4096	74EQ20101018	Atlantic	D357	20101018	20101122	*RRS Discovery*

Table A2. List of cruises included in GLODAPv2.2021 which have been updated as part of GLODAPv2.2022. Complete information on each cruise, such as variables included, and chief scientist and principal investigator names is provided in the cruise summary table at https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system/oceans/GLODAPv2_2022/cruise_table_v2022.html (last access: 15 August 2022).

No.	EXPOCODE	Region	Alias	Update	Adjustment
26	06M220090714	Atlantic	CLIVAR AR07W_2009, MSM12_3	Performed second QC on SF$_6$	1.0
55	06MT20030626	Atlantic	06MT591	Performed second QC on SF6	1.0
57	06MT20030831	Atlantic	06MT593	Performed second QC on SF6	1.0
58	06MT20040311	Atlantic	06MT605	Performed second QC on SF6	1.0
62	06MT20060712	Atlantic	MT68_3_2006	Performed second QC on SF6	−888
63	06MT20091026	Atlantic	MT80/1_2009	Performed second QC on SF6	1.0
64	06MT20110405	Atlantic	MT84_3	Performed second QC on SF6	1.0
263	316N20020530	Arctic	NS02, KN166_11	Performed second QC on SF6	1.0
273	318M20091121	Pacific	CLIVAR P06_2009	Performed second QC on SF6	1.0
295	320620110219	Pacific	CLIVAR S04P_2011	Performed second QC on SF6	1.0
307	325020080826	Pacific	CLIVAR_TN224_2008	Performed second QC on SF6	−888
324	32OC20080510	Atlantic	32OC446	Performed second QC on SF6	1.0
329	33AT20120324	Atlantic	CLIVAR_A22_2012	Performed second QC on SF6	1.0
330	33AT20120419	Atlantic	CLIVAR_A20_2012	Performed second QC on SF6	1.0
345	33RO20071215	Pacific	CLIVAR P18_2007	Performed second QC on SF6	1.0
346	33RO20100308	Atlantic	CLIVAR A13.5_2010, RB_07-05	Performed second QC on SF6	1.0
347	33RO20110926	Atlantic	CLIVAR A10_2011, RB-11-02	Performed second QC on SF6	1.0
355	33RR20090320	Indian	CLIVAR I05_2009	Performed second QC on SF6	1.0
434	49HG19971110	Pacific	NH97	Performed second QC on SF6	1.2
435	49HG19980812	Pacific	NH98	Performed second QC on SF6	1.2
461	49K619990523	Pacific	49EWMI9905_1	Performed second QC on SF6	−777
631	58AA20010527	Arctic	58AA0113, TRACTOR 13	Performed second QC on SF6	1.0
635	58GS20090528	Arctic	SARS09, CLIVAR 75N_2009	Performed second QC on SF6	−777
674	740H20081226	Atlantic	JC30	Performed second QC on SF6	1.0
702	74JC19960720	Arctic	74JC9608	Performed second QC on SF6	1.0
703	74JC20100319	Atlantic	JR239, ANDREX-2	Performed second QC on SF6	1.0
706	77DN20020420	Arctic	77DN0204	Performed second QC on SF6	1.0
708	77DN20050819	Arctic	ODEN05, AOS-2005	Performed second QC on SF6	1.0
724	ZZIC2005SWYD	Arctic	SWITCHYARD	Performed second QC on SF6	1.0
1002	06AQ20120107	Atlantic	ANT-XXVIII/3	Performed second QC on SF6	1.0
1003	06AQ20120614	Arctic	ARK XXVII/1	Performed second QC on SF6	1.0
1005	06AQ20150817	Arctic	PS-94, ARK-XXIX/3	Performed second QC on SF6	1.0
1007	06M220080723	Atlantic	MSM09-1	Performed second QC on SF6	1.0
1008	06M220170104	Atlantic	MSM60-1 SAMOC	Performed second QC on SF6	1.0
1011	06M320150501	Atlantic	M116/1	Performed second QC on SF6	1.0
1012	06M220081031	Atlantic	MSM10/1	Performed second QC on SF6	1.0
1013	06MT20091126	Atlantic	MT80/2	Performed second QC on SF6	1.1
1014	06MT20101014	Atlantic	M83/1	Performed second QC on SF6	1.0
1016	06MT20140317	Atlantic	M105	Performed second QC on SF6	1.0
1020	096U20160426	Pacific	IN2016_V03, P15S	Performed second QC on SF6	1.0
1025	18HU20130507	Atlantic	AR07W_2013	Performed second QC on SF6	1.0
1026	18HU20140502	Atlantic	AR07W_2014	Performed second QC on SF6	1.0
1027	18HU20150504	Atlantic	AR07W_2015	Performed second QC on SF6	1.0
1029	18MF20120601	Atlantic	AR07W_2012	Performed second QC on SF6	1.0
1033	316N20111106	Atlantic	GT11, NAT-11	Performed second QC on SF6	1.0
1035	318M20130321	Pacific		Performed second QC on SF6	1.0
1036	320620140320	Pacific	GO-SHIP P16S_2014	Performed second QC on SF6	1.0
1038	325020131025	Pacific	TGT303, P21_2013	Performed second QC on SF6	1.0
1040	33HQ20150809	Arctic	HLY1502	Performed second QC on SF6	1.0
1041	33RO20130803	Atlantic	A16N_2013	Performed second QC on SF6	1.0
1042	33RO20131223	Atlantic	RB1307, A16S_2013	Performed second QC on SF6	1.0
1043	33RO20150410	Pacific	GO-SHIP P16N_2015 Leg 1	Performed second QC on SF6	1.0
1044	33RO20150525	Pacific	GO-SHIP P16N_2015 Leg 2	Performed second QC on SF6	1.0

Table A2. Continued.

No.	EXPOCODE	Region	Alias	Update	Adjustment
1045	33RO20161119	Pacific	RB1606, GO-SHIP P18_2016	Performed second QC on SF6	1.0
1046	33RR20160208	Indian	I08S_2016	Performed second QC on SF6	1.0
1050	49NZ20121128	Indian	P14S_S04_2012; MR12-05 Leg 2	Performed second QC on SF6	1.0
1051	49NZ20130106	Indian	S04I_2013	Performed second QC on SF6	1.0
1053	49NZ20140717	Pacific	MR14-04, GO-SHIP P01_2014	Performed second QC on SF6	1.0
1054	49NZ20151223	Indian	MR15-05, I10_2015	Performed second QC on SF6	1.0
1055	49NZ20170208	Pacific	MR16-09, P17E	Performed second QC on SF6	1.0
1103	58GS20150410	Atlantic	AR07E_2015	Performed second QC on SF6	1.0
1104	58GS20160802	Arctic	75N_2016	Performed second QC on SF6	1.0
2003	06M220130509	Atlantic	MSM28	Performed second QC on SF6	1.0
2005	06M220150502	Atlantic	MSM42	Performed second QC on SF6	1.0
2006	06M220150525	Atlantic	MSM43	Performed second QC on SF6	1.0
2008	096U20180111	Indian	SR03.2018	Performed second QC on SF6	1.0
2011	29AH20160617	Atlantic	OVIDE-16	Performed second QC on SF6	1.0
2020	316N20101015	Atlantic	KN199-04	Performed second QC on SF6	1.0
2023	316N20150906	Atlantic	Davis Strait 2015	Performed second QC on SF6	1.0
2026	35TH20080825	Atlantic	SUBPOLAR08	Performed second QC on SF6	1.0
2027	45CE20170427	Atlantic	CE17007	Performed second QC on SF6	1.0
3002	06M220160331	Atlantic	MSM53	Performed second QC on SF6	1.0
3003	06MT20160828	Atlantic	M130	Performed second QC on SF6	1.0
3004	06MT20170302	Pacific	M135	Performed second QC on SF6	1.0
3005	06MT20180213	Atlantic	M145	Performed second QC on SF6	1.0
3029	320620170703	Pacific		Performed second QC on SF6	1.2
3030	320620170820	Pacific		Performed second QC on SF6	1.1
3031	320620180309	Pacific	NBP18_02	Performed second QC on SF6	1.0
3033	325020190403	Indian	TN366	Performed second QC on SF6	1.0
3034	33RO20180423	Indian		Performed second QC on SF6	1.0
3041	49NZ20191229	Indian	MR19-04 (Leg 3)	Performed second QC on SF6	1.0
3042	58JH20190515	Arctic	JH2019205	Performed second QC on SF6	1.0
249	316N19941201	Indian	316N145_5	Performed second QC on TCO2	1.7
249	316N19941201	Indian	316N145_5	Performed second QC on TAlk	−3.5
250	316N19950124	Indian	316N145_6	Performed second QC on TCO2	1.7
250	316N19950124	Indian	316N145_6	Performed second QC on TAlk	−3.5
251	316N19950310	Indian	316N145_7	Performed second QC on TCO2	1.7
251	316N19950310	Indian	316N145_7	Performed second QC on TAlk	−3.5
252	316N19950423	Indian	316N145_8	Performed second QC on TCO2	1.7
252	316N19950423	Indian	316N145_8	Performed second QC on TAlk	−3.5
253	316N19950611	Indian	316N145_9	Performed second QC on TCO2	1.7
253	316N19950611	Indian	316N145_9	Performed second QC on TAlk	−3.5
254	316N19950715	Indian	316N145_10	Performed second QC on TCO2	1.7
254	316N19950715	Indian	316N145_10	Performed second QC on TAlk	−3.5
255	316N19950829	Indian	316N145_11, 316N145_12	Performed second QC on TCO2	1.7
255	316N19950829	Indian	316N145_11, 316N145_12	Performed second QC on TAlk	−3.5
256	316N19951111	Indian	316N145_13	Performed second QC on TCO2	1.7
256	316N19951111	Indian	316N145_13	Performed second QC on TAlk	−3.5
257	316N19951202	Indian	316N145_14, 316N145_15	Performed second QC on TCO2	1.7
257	316N19951202	Indian	316N145_14, 316N145_15	Performed second QC on TAlk	−3.5
433	49HG19960807	Pacific	NH96-2	Performed second QC on pH	−0.05
574	49UP19970912	Pacific	RF97-09	Performed second QC on oxygen	1.015
1011	06M320150501	Atlantic	M116/1	Added CFC-12 data	
656	58P320011031	Arctic	Station M	Added new data from 2008 until 2021	
2011	29AH20160617	Atlantic	OVIDE-16	Added bottle numbers	
2013	29HE20190406	Atlantic	FICARAM_XIX	Added bottle numbers	
239	316N19831007	Atlantic	AJAX	Changed TAlk WOCE flag from 2 to 0	

Note on former version. Former versions of this article were published on 15 August 2016, 25 September 2019, 23 December 2020, and 3 December 2021 and are available at https://doi.org/10.5194/essd-8-297-2016, https://doi.org/10.5194/essd-11-1437-2019, https://doi.org/10.5194/essd-12-3653-2020, and https://doi.org/10.5194/essd-13-5565-2021.

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

Competing interests. At least one of the (co-)authors is a member of the editorial board of *Earth System Science Data*. The peer-review process was guided by an independent editor, and the authors also have no other competing interests to declare.

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A vision for FAIR ocean data products

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A vision for FAIR ocean data products

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The ocean is mitigating global warming by absorbing large amounts of excess carbon dioxide from human activities. To quantify and monitor the ocean carbon sink, we need a state-of-the-art data resource that makes data submission and retrieval machine-compatible and efficient.

Human activities such as combustion of fossil fuel, land use change, and cement production increased the atmospheric carbon dioxide (CO_2) concentration to 418 ppm in April 2021. This level is almost 50% higher than at the beginning of the industrial age. The greenhouse effect of atmospheric CO_2 and other gases has led to significant warming and increased stratification in the ocean, and has consequences for ecosystems and marine ecosystem services. Notably, atmospheric CO_2 concentrations would now be around another 76 ppm higher than current levels[1] if the ocean had not taken up a significant fraction of our emissions from the atmosphere[2].

The ocean is one of the largest carbon pools on the planet, second only to the Earth's crust. The ocean contains about 38,000 Gigatonnes of carbon and thereby dwarfs the cumulative emissions of fossil CO_2 since the Industrial Revolution from fossil fuel combustion (about 440 GtC to 2019) and land-use change (about 210 GtC)[1]. As such, the accumulation rate of carbon in the surface ocean of about 1 μmol kg^{-1} year^{-1} driven by anthropogenic CO_2 emissions is much smaller than the natural variations in dissolved inorganic carbon content, over a range of 500 μmol kg^{-1} regionally and 100 μmol kg^{-1} seasonally[3]. Thus, any emission-driven trends in ocean carbon concentrations or changes in biogeochemical cycles are expressed amid large

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natural variability in these seawater properties across a range of spatial and temporal scales. Accurately quantifying a small change against a large and variable background requires precise and accurate measurements made over decades.

The GLobal Ocean Data Analysis Project (GLODAP)[4,5], initiated in 2004 and subsequently updated[6–8], has been instrumental in delivering carbon-relevant interior ocean data that support well-quantified estimates of the ocean carbon sink. The project delivers near-global data coverage; standardized quality control procedures; a high degree of internal consistency; common data formats; and open and free access to the available data. Compared to its first version, the GLODAP data inventory has more than tripled in size (Fig. 1).

In order to continue to serve its purpose, GLODAP needs to advance both its data ingestion systems and its data extraction systems to become more streamlined and automated. In order to decrease the amount of routine manual work as well as the potential for errors, data submission workflows must become uniform, semi-automated, and compatible with machine-learning techniques for quality control. The data extraction system also needs to accommodate a wider range of filtering to fine-tune requests from users.

Global ocean carbon data

Faced with the challenge of quantifying the ocean's storage of anthropogenic carbon, the ocean community began to systematically measure marine inorganic carbon concentrations in the 1970 and 1980's[4]. These efforts ramped up significantly during the World Ocean Circulation Experiment and the Joint Global Ocean Flux Study (WOCE/JGOFS) during the 1990's, and have later been continued along selected WOCE lines in the repeat hydrographic programs including the Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP)[9].

The primary focus of GLODAP is synthesizing seawater inorganic carbon chemistry data from these global cruise campaigns. However, data for ocean hydrography, dissolved oxygen, transient tracers, inorganic nutrients, and a range of other variables are included to facilitate interpretation. A unique feature of GLODAP is the addition of several layers of quality control and adjustments conducted to minimize inconsistencies and biases in the data[10] using a range of tools such as comparison of deep water values at nearby locations. GLODAP offers uniform data at three levels; (1) data from individual cruises in a uniform format with coherent quality control and unit conversion applied, (2) a bias adjusted data product, and 3) a global 1° × 1° mapped climatology[11].

The GLODAP data product has supported more than 2000 articles (and counting) since the year 2000, evidencing its extensive use by the scientific community and the trust placed in it. Seminal contributions on the oceanic anthropogenic carbon content and temporal evolution would not have been possible without GLODAP[2,12,13]. The knowledge from these studies informs, for instance, the Intergovernmental Panel for Climate Change (IPCC) assessments, and the Sustainable Development Goals (SDG) of the UN Agenda 2030 and the Global Climate Observing System (GCOS) indicators on ocean acidification. GLODAP is also an essential reference data set for autonomous observing networks, such as Biogeochemical-Argo: "The long-term success of a global chemical sensor observing system will depend on support from an ongoing, shipboard hydrographic program to produce a high-quality data set for deep waters at the global scale."[14].

With the growth in the amount of data, the ongoing need to provide information on the ocean carbon sink to inform global carbon emission-reduction efforts, and the emerging need to monitor impacts of initiatives in geoengineering and sustainable use of the oceans, the importance of GLODAP will only increase. However, despite receiving short-term funds from a range of projects, GLODAP is a largely unfunded community effort organized and executed by the GLODAP team. Such a situation is unsustainable, and there is significant risk that the effort will diminish or disappear in the next few years. The building and supporting of infrastructure will be critical to ensure that GLODAP continues to provide a valuable service to the global community.

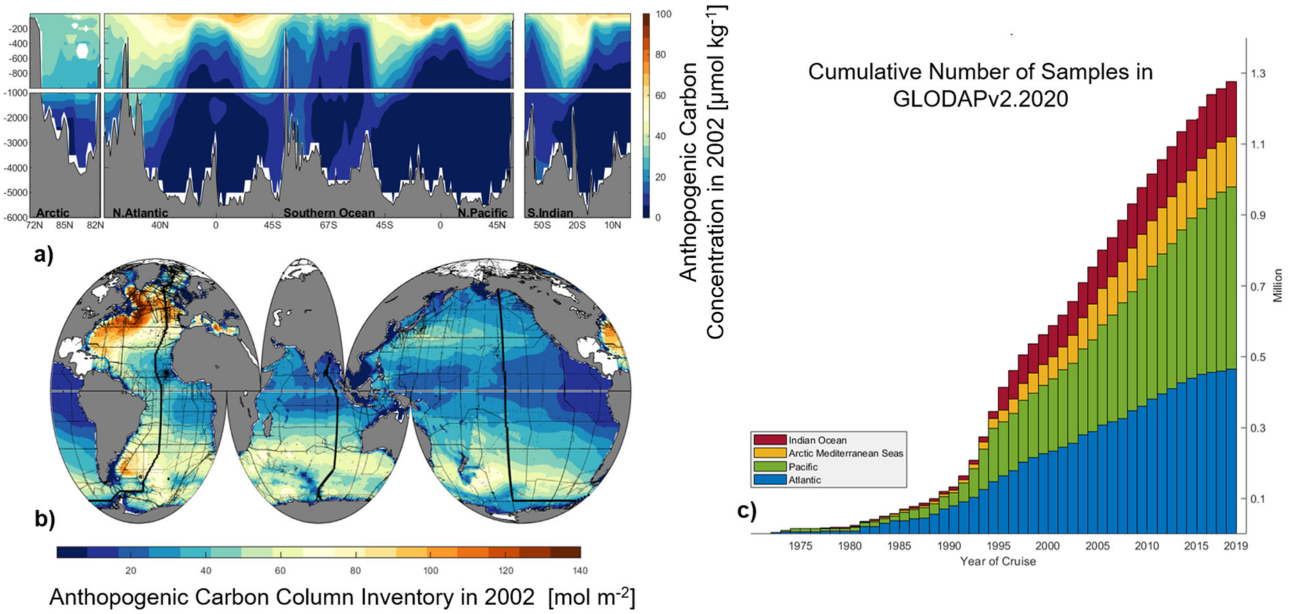

Fig. 1 Key outputs and metrics of GLODAP. a Interior ocean concentration of anthropogenic carbon along a section indicated with a black line in panel (**b**). **b** Integrated column inventory of anthropogenic carbon[22]. Both panels used transient tracer data and the Transit Time Distribution method to calculate anthropogenic carbon[23] content. **c** Cumulative number of samples in GLODAPv2.2020 over time.

Improved efficiency and service

The current GLODAP workflow requires substantial manual work that necessitates dedicated time from, and funding for, data experts, and that introduces opportunities for data handling errors. GLODAP has matured over the last decade with a set of well-documented protocols and development of dedicated software, as well as a backbone of data management support. However, the GLODAP team now strives for advancements on both data input and output, toward a semi-automated system that will reduce the manual work intensity and associated errors.

First, the team aims to implement a uniform, semi-automatic, and standards-compliant data ingestion system that will facilitate the data submission and quality control procedures. This will enable direct interaction with data providers, leading to improvements in data handling, data quality control, and documentation. The envisaged changes will also enable rapid application of novel quality control approaches using machine-learning techniques.

Second, we want to upgrade to a versatile data extraction system. Such a system will provide more flexibility and options to users, such as requesting output with originally submitted data (without adjustments), or only sub-sets of the data in various formats.

These upgrades will streamline repository workflows to insure the data products are FAIR (findable, accessible, interoperable, and reusable)[15], while reducing the burden of data management on scientists. Nevertheless, there will remain a need for experts to spend time on quality control and internal consistency adjustments.

Branch out to keep data accessible

We expect that the improvements will encourage submission of data through building a community of data providers, and will simplify and streamline the process of providing regular updates of the GLODAP products. At the same time, access to GLODAP data will increase. Workflow improvements would allow for enhanced data access systems supporting machine-to-machine services, and better integrated data visualization products[16,17].

The GO-SHIP repeat hydrography effort currently provides the backbone of GLODAP thanks to its high data quality and rapid availability. However, many other datasets reach GLODAP through the extensive network of the GLODAP team; some of these datasets will be functionally lost if not collated by GLODAP. An automated system can aid rescue these data for reuse, by providing a streamlined process for scientists to submit data and metadata, and for users to access and visualize the data.

Upgrades of GLODAP will benefit from the data system that has already been developed for the Surface Ocean CO_2 Atlas (SOCAT)[18]. SOCAT successfully streamlined data submission, quality control, and release of an annual synthesis product, but faces the same resourcing challenges as GLODAP to sustain regular updates. Leveraging an existing, and proven, workflow translates to a significant reduction in both cost and labor of developing a similar system for GLODAP.

An investment for the planet's future

GLODAP needs continued support from the scientific community, but also needs support from funding agencies and stakeholders. Without the updated infrastructure and adequate sustained resourcing in place, GLODAP services may not be able to be maintained on a regular basis.

While the ocean currently takes up about 2.6 Gt of anthropogenic carbon annually, we must understand the evolution, efficiency, and regional patterns of the ocean carbon sink if we want to be able to predict the climate effect of future emissions, as well as to quantify and assess mitigation efforts. Furthermore, human activities affect ocean biogeochemistry in other ways as well, such as de-oxygenation[19], changes in nutrient supply[20], and ocean acidification[21], issues that all need high quality, consistent ocean biogeochemical data to quantify trends, and variability.

Co-located high-quality measurements of physical and biogeochemical parameters that allow for the separation of natural variability from anthropogenic changes—as delivered by GLODAP—are a key component to monitoring, understanding, and mitigating the human influence on the Earth's climate.

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Author contributions

T.T. and S.K.L. co-lead the writing team. S.K.L. and N.L. made the figure, A.O., M.A., N.L., S.D., H.C.B., P.J.B., B.R.C., L.C.C., R.A.F., M.H., M.I., E.J., A.K., A.M., F.F.P., B.P., C.S., R.S., M.T., B.T., A.V., R.W., E.B., K.O.B., and R.M.K. all contributed to the GLODAP project and the writing.

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Competing interests

The authors declare no competing interests.

Additional information

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6

Synthesis Product for Ocean Time-Series (SPOTS) – A ship-based biogeochemical pilot

Synthesis Product for Ocean Time-Series (SPOTS) – A ship-based biogeochemical pilot

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Abstract. The presented pilot for the "Synthesis Product for Ocean Time-Series" (SPOTS) includes data from 12 fixed ship-based time-series programs. The related stations represent unique marine environments within the Atlantic Ocean, Pacific Ocean, Mediterranean Sea, Nordic Seas, and Caribbean Sea. The focus of the pilot has been placed on biogeochemical essential ocean variables: dissolved oxygen, dissolved inorganic nutrients, inorganic carbon (pH, total alkalinity, dissolved inorganic carbon, and partial pressure of CO_2), particulate matter, and dissolved organic carbon. The time-series used include a variety of temporal resolutions (monthly, seasonal, or irregular), time ranges (10 – 36 years), and bottom depths (80 – 6000 m), with the oldest samples dating back to 1983 and the most recent one corresponding to 2021. Besides having been harmonized into the same format (semantics, ancillary data, units), the data were subjected to a qualitative assessment in which the applied methods were evaluated and categorized. The most recently applied methods of the time-series programs usually follow the recommendations outlined by the Bermuda Time-Series Workshop report (Lorenzoni and Benway, 2013) which is used as the main reference for "biogeochemical best-practices". However, measurements of dissolved oxygen and pH in particular, still show room for improvement. Additional data-quality descriptors include precision and accuracy estimates, indicators for data variability, and offsets compared to a reference and widely recognized data product for the global ocean: the "GLobal Ocean Data Analysis Project". Generally, these descriptors indicate a high level of continuity in measurement quality within time-series programs and a good consistency with the GLobal Interior Ocean Carbon Data, even though robust comparisons to the latter are limited. The data are available as (i) a merged comma-separated file that is compliant with the World Ocean Circulation Experiment (WOCE) exchange format and ii) a format dependent on user queries via the ERDDAP server of the Global Ocean Observing System (GOOS). The pilot increases the data utility, findability, accessibility, interoperability, and reusability following the FAIR philosophy, enhancing the readiness of biogeochemical time-series. It facilitates a variety of applications that benefit from the collective value of biogeochemical time-series observations and forms the basis for a sustained time-series living data product, SPOTS, complementing relevant products for the global interior ocean carbon data (GLobal Ocean Data Analysis Project), global surface ocean carbon data (Surface Ocean CO_2 Atlas; SOCAT), and global interior and surface methane and nitrous oxide data (MarinE MethanE and NiTrous Oxide product).

Aside from the actual data compilation, the pilot project produced suggestions for reporting metadata, implementing quality control measures, and making estimations about uncertainty. These recommendations aim at encouraging the community to adopt more consistent and uniform practices for analysis and reporting and at updating these practices regularly. The detailed recommendations, links to the original time-series programs, the original data, their documentation, and related efforts are available on the SPOTS website. This site also provides access to the data product (DOI: 10.26008/1912/bco-dmo.896862.1) and ancillary data.

1. Introduction

Continuing global anthropogenic carbon dioxide emissions in combination with increasing nutrient inputs into the ocean over the past decades have resulted in unprecedented changes in the ocean biogeochemistry (O'Brien et al., 2017; Friedligstein et al., 2022) and marine ecosystem states (e.g., Edwards et al., 2013; Barton et al., 2016). As climate change progresses, these complex changes will aggravate (Bopp et al., 2013; Cooley et al., 2022).

To disentangle natural variability, occurring on a range of temporal and spatial scales (Valdés and Lomas, 2017), and human-induced changes in marine ecosystems (Henson et al., 2016; Benway et al., 2019) decades of sustained fixed-location time-series observations are required. Following recommendations from international programs such as the Joint Global Ocean Flux Study (JGOFS, 1990) and Global Ocean Ecosystem Dynamics (GLOBEC, 1997), only few ship-based fixed ocean time-series programs have been established around the globe since the late 1980s. The ongoing observations of these programs have captured the evolving changes in ocean biogeochemistry and associated impacts on marine food webs, marine biodiversity, and ecosystems. Examples of observed changes include changes in the ocean's anthropogenic carbon inventory, oxygen levels, seawater pH, ventilation rates, and vertical nutrient transports (e.g., Bates et al., 2014; Tanhua et al., 2015; Neuer et al., 2017). Even though the collective value of multiple time-series data is greater than that provided by each individual time-series, ship-based time-series programs have primarily been launched to support the specific goals of individual programs and ancillary projects. The International Group of Marine Ecological Time Series (IGMETS, O'Brien et al., 2017) demonstrated the collective value by performing an integrative and collective assessment of over 340 ship-based time-series thereby increasing the range of space- and time scales that can be addressed and highlighting the importance of joint and multidisciplinary time-series observing programs (Valdés and Lomas, 2017).

Despite their indisputable importance and the wealth of ship-based time-series data, difficulties in data discoverability, accessibility, and interoperability presently limit ship-based time-series data utilization, the realization of their full scientific potential, and the overall recognition of the programs (Benway et al., 2019; Tanhua et al., 2021). Moreover, these challenges have prevented shipboard time-series from becoming a more formalized and endorsed component of the Global Ocean Observing System (GOOS, Moltmann et al., 2019). In addition to the lack of a community-agreed time-series data public release agreement that leads to free sharing of time-series data being uncommon, the lack of standardized formats, semantics, units, scales, standards, quality assurance- and control, metadata reporting, and user interfaces across and within time-series sites represent the main data challenges. The usage of different measurement protocols sometimes without comprehensive reporting of the corresponding variable-inherent uncertainties and the time-consuming manual data retrieval at multiple access points are further prone to data handling errors. Existing biogeochemical (BGC) data synthesis products have already tackled these challenges for other observation types and increased the utility of large amounts of individual datasets, e.g., the MarinE MethanE and NiTrous Oxide product (MEMENTO, Kock and Bange, 2015), the Global Ocean Data Analysis Project (GLODAP, Lauvset et al., 2022) and the Surface Ocean CO_2 Atlas (SOCAT, Bakker et al., 2016). However, neither IGMETS (O'Brien et al., 2017) nor OceanSites (Weller et al., 2016), a global network of long-term autonomous open ocean reference stations, have generated a global data synthesis product of time-series data that would complement existing BGC data synthesis products.

To address these shortcomings and to follow up on the Bermuda Time Series workshop from 2013 (Lorenzoni et al., 2013), both the Ocean Carbon and Biogeochemistry program and the EU Horizon 2020 project EuroSea convened workshops with several time-series operators. Resulting from these workshops a call was formulated for a pilot data synthesis product of well-established time-series programs that focuses on a limited set of variables. Further, a roadmap was created to develop a pilot product that aims at establishing a Findable Accessible Interoperable Reusable (FAIR, Wilkinson et al., 2016) data management plan for shipboard ocean time-series (Benway et al., 2020). This goes hand in hand with the GOOS Implementation Roadmap (GOOS, 2020) calling for more systematic and sustainable approaches for climate-relevant observations across ocean data platforms and networks (Belward et al., 2016), especially regarding the GOOS defined scientific applications: The ocean carbon content (Q1.1); ocean dead zones (Q2.1); rates of acidification (Q2.2); and ocean productivity (Q3.2).

Following these calls, we here describe the resultant Synthesis Product for Ocean Time-Series (SPOTS) pilot, synthesizing high-quality data from 12 global ship-based time-series sites with a focus on BGC essential ocean variables (EOV). This paper briefly presents the included time-series programs (Sect. 2), describes the methods applied to compile and assess the product (Sect. 3) and data quality assessment (Sect. 4), describes the final product (Sect. 5), elaborates on the stakeholder usability (Sect. 6), and describes the data access (Sect.7). Finally, the main findings of the effort are presented (Sect. 8) and next steps to guarantee the continuity and success of SPOTS are identified (Sect. 9).

2. Data Sources

The SPOTS pilot includes data from 12 fixed ship-based time-series programs (Fig. 1), all of which routinely measure BGC EOVs. All major climate zones are covered, although not all ocean biogeochemical zones are (Reygondeau et al., 2013). Existing datasets were extended whenever possible by publicly available and more recent data (Table S1.). In addition to capturing different marine environments (Sect. 2.1), the characteristics of the time-series programs also differ in terms of the station visit frequency, i.e. temporal resolution (monthly, seasonal, or irregular), the time range of the observational period, the bottom depth and whether a dedicated research vessel is used (Table 1). If a time-series program consists of two or more related stations, usually the deepest station was selected. The included data from GIFT and RADCOR display exceptions to this rule as for both sites data from three related stations were selected.

Table 1: Key metadata of participating time-series programs. Colors indicate ocean basins: Green: Pacific; Light blue: Atlantic; Orange: Marginal Seas; Dark Blue: Nordic Seas. S=Salinity (either bottle or CTD-data); O_2=Oxygen (either bottle or CTD-data); NO_3=Dissolved inorganic nitrate; NO_2=Dissolved nitrite; PO_4=Dissolved phosphate; $SiOH_4$=Dissolved silicate; NH_4=Dissolved ammonium; DIC=Dissolved inorganic carbon; TA=Total alkalinity; $p\text{CO}_2$=Partial pressure of carbon dioxide; POC=Particulate organic carbon; PON=Particulate organic nitrogen; POP=Particulate organic phosphorus; DOC=Dissolved organic carbon.

Time-Series Site	Location	Time Range	Temporal Resolution	Bottom Depth	# of Visits	Dedicated Vessel	Variables	Original DOI(s)
KNOT	44.0°N 155.0°E	1997–2020	1-3 cruises yr^{-1}	6000 m	21	No	S,O_2,NO_3,NO_2,$SiOH_4$,PO_4,NH_4,DIC,TA,pH	10.25921/tarq-6v91
K2	47.0°N 160.0°E	1999–2020	1-3 cruises yr^{-1}	6000 m	49	No	S,O_2,NO_3,NO_2,$SiOH_4$,PO_4,NH_4,DIC,TA,pH, DOC	10.25921/mpfz-sv16
ALOHA	22.8°N 158.0°W	1988–2019	Monthly	4750 m	311	Yes	S,O_2,NO_3,NO_2,$SiOH_4$,PO_4,DIC,TA,pH, POC,PON,POP,DOC	10.1575/1912/bco-dmo.3773.1
Munida	45.8°S 171.5°E	1998–2019	6 cruises yr^{-1}	1000 m	80	Yes	S,NO_3,$SiOH_4$,PO_4,DIC,TA	NA
GIFT	36.9°N 6.0°W	2005–2015	Seasonal	315 m – 842 m	26	Yes	S,O_2,NO_3,$SiOH_4$,PO_4, TA,pH, DOC	10.20350/digitalCSIC/10549
CVOO	17.6°N 24.3°W	2006–2019	1-3 cruises yr^{-1}	3600 m	42	Partly	S,O_2,NO_3,NO_2,$SiOH_4$,PO_4,NH_4,DIC,TA, POC,PON,POP	10.1594/PANGAEA.958597
RADCOR	43.4°N 8.4°E	2013–2020	Monthly	15 m – 80 m	80	Yes	S,O_2,NO_3,NO_2,$SiOH_4$,PO_4,DIC,TA,pH	NA
CARIACO	10.5°N 64.7°W	1995–2017	Monthly	1300 m	230	Yes	S,O_2,NO_3,NO_2,$SiOH_4$,PO_4,NH_4,TA,pH, POC,PON,POP,DOC	10.1575/1912/bco-dmo.3093.1
DYFAMED	42.3°N 7.5°E	1991–2017	Monthly	2400 m	190	No	S,O_2,NO_3,NO_2,$SiOH_4$,PO_4,,DIC,TA,pH	10.17882/43749
IrmingerSea	64.3°N 28.0°W	1983–2019	Seasonal	1000 m	131	Yes	S,O_2,NO_3,$SiOH_4$,PO_4, DIC,TA,$p\text{CO}_2$	10.3334/cdiac/otg.carina_irmingersea_v2; 10.25921/vjmy-8h90
IcelandSea	68.0°N 12.7°W	1983–2019	Seasonal	1850 m	146	Yes	S,O_2,NO_3,$SiOH_4$,PO_4, DIC,TA,$p\text{CO}_2$	10.3334/cdiac/otg.carina_icelandsea; 10.25921/qhed-3h84
OWSM	66.0°N 2.0°E	2001–2021	4-12 cruises yr^{-1}	2100 m	147	Until 2009	S,O_2,NO_3,$SiOH_4$,PO_4, DIC,TA	10.3334/cdiac/otg_tsm_ows_m_66n_2e

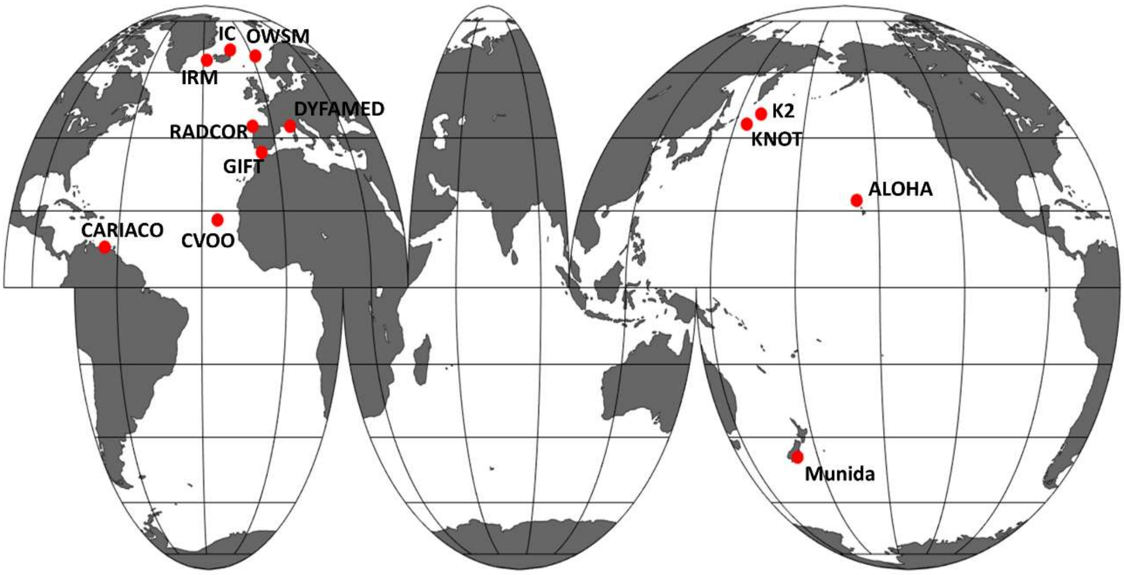

Figure 1: Locations of participating ship-based time-series stations.

2.1. Marine Environment of Time-Series Sites

2.1.1. A Long-term Oligotrophic Habitat Assessment (ALOHA)

The deep water (~4750 m) time-series station of the Hawaii Ocean Time-Series program (HOT), ALOHA (Karl and Church, 2019), is located 100 km north of Oahu, Hawaii, more than one Rossby radius (50 km) away from the steep topography associated with the Hawaiian Ridge. ALOHA serves as an open ocean benchmark and its research goals are aligned with the main objectives of the JGOFS and the World Ocean Circulation Experiment (WOCE). One of the principals of the HOT program is to observe seasonal and interannual variations in water mass characteristics and BGC variables. The monthly measurements since 1988 are representative of the oligotrophic North Pacific eastern subtropical gyre with Station ALOHA lying in the center of the North Pacific and North Equatorial Current. Typically, the site is characterized by a relatively deep permanent pycnocline (and nutricline), and a shallow mixed-layer depth. Intermittent local wind forcing caused by extratropical cyclones' cold fronts impacts the annual cycle of the surface waters (Karl et al., 1996).

2.1.2. CArbon Retention In A Colored Ocean (CARIACO)

The station of the CARIACO Oceanographic Time-Series Program (Muller-Karger et al., 2019) is located in the Cariaco Basin, a semi-enclosed tectonic depression located on the continental shelf off northern Venezuela in the southern Caribbean Sea. The Cariaco Basin is composed of two approximately 1400 m deep sub-basins that are connected to the Caribbean Sea by two shallow (140 m deep) channels. These channels allow for the open exchange of near-surface water. The restricted circulation below the 140 m sills, coupled with highly productive surface waters due to seasonal wind-driven coastal upwelling (around 450 g C m^{-2} y^{-1}; Muller-Karger et al., 2010), has led to sustained anoxia below around 250 m. The goal of the near-monthly measurements at CARIACO between 1995 and 2017 was to observe linkages between oceanographic processes and the production, remineralization, and sinking flux of particulate matter in the Cariaco Basin, and how these change over time. It also aimed at understanding climatic changes in the region.

2.1.3. Cape Verde Ocean Observatory (CVOO)

CVOO is located in the eastern tropical North Atlantic about 800 km from the west coast of Africa, which is influenced by the seasonal eastern boundary upwelling system, high Saharan dust deposition rates, and frequently passing eddies (Schütte et al., 2016). It is part of the Cape Verde Observatory, which also includes an operational atmospheric monitoring site. The combined observations aim at investigating long-term changes of greenhouse gas concentrations in the atmosphere and in the ocean in a key region for air-sea interaction. The irregular measurements of BGC variables at CVOO started in 2006 and are still ongoing, and the project strives for more regular measurements in the future by having a dedicated vessel available. The station has a bottom depth of 3600 m and lies in the center of the Cape Verde Fontal Zone, resulting in large variations of the present oligotrophic water masses. The frontal zone separates most of the eastern tropical North Atlantic from the anticyclonic subtropical gyre system in the North Atlantic (Stramma et al., 2005). This further results in an ocean shadow zone and an oxygen-poor layer between 400 m to 500 m (Stramma et al., 2008), which is being sampled at CVOO. Below the mixed layer, subtropical underwater from the subtropical gyre system, as well as North Atlantic Central Water and South Atlantic Central Water can be present (Tomczak 1981; Pastor et al., 2008).

2.1.4. DYFAMED

DYFAMED is located in the central part of the Ligurian Sea, about 50 km off Nice, on the Nice Corsica transect, and is representative of open sea western Mediterranean basin waters. Ongoing multidisciplinary monthly measurements at DYFAMED have been performed since 1991 observing: i) the evolution of the water mass properties, ii) the carbon export change, and iii) the variability of the biological species relative to climate forcing. The water column can be divided into three principal layers: deep, intermediate, and surface. The latter, typically for the Mediterranean trophic environment, experiences large seasonal variability. Further, the Northern Current front acts as a barrier to exchanges with the coastal zone of the Ligurian Sea and prevents DYFAMED from lateral inputs (Vescovali et al., 1998). Consequently, the primary production depends on inputs of nutrients from deeper waters and atmospheric inputs of nitrogen and some trace metals, particularly during summer (Miquel, 2011). The DYFAMED site is characterized by intermediate water (300-400m) that is lower in oxygen concentrations (Levantine Intermediate Water) and deep water that is richer in oxygen, primarily induced by vertical mixing occurring in winter during intense and cold winds (convection processes; Coppola et al., 2018).

2.1.5. Gibraltar Fixed Time series (GIFT)

Seasonal measurements at GIFT were established in 2005 to quantify the exchange of carbon between the Mediterranean Sea and the adjacent Atlantic Ocean and assess the temporal evolution of BGC fluxes. The three GIFT time-series stations (Flecha et al., 2019) are located along the longitudinal axis of the Strait of Gibraltar, which connects the two basins. The Strait is surrounded by the Gulf of Cadiz (west) and the Alboran Sea (east). Water circulation in the channel can be described as a bi-layer system characterized by an inward (eastward) flow of the North Atlantic Central Water in the upper layer and an outward (westward) flow of Mediterranean waters (predominantly formed by a mixture of the Levantine Intermediate Water and the Western Mediterranean Deep Water) at the bottom layer. The depth and thickness of each water mass vary along the Strait, due to topography in the channel and the influence of physical mechanisms. In particular, the Espartel sill (358 m depth) and the Camarinal sill (285 m depth) lead to large variability in the proportion of water flows' position. Therefore, sampling depths vary from one campaign to another due to the instant position of the incoming and outcoming flows that are identified by their thermohaline properties through the CTD casts.

2.1.6. Irminger Sea station (IRM-TS) and Iceland Sea station (IC-TS)

In 1983, seasonal measurements at the IRM-TS and the IC-TS (Olafsson et al., 2010) were initiated to observe the seasonal variability of carbon-nutrient chemistry in the North Atlantic off the Iceland shelf. The stations are located in two hydrographically different regions north and southwest of Iceland (Takahashi et al., 1985; Peng et al., 1987). The station in the northern Irminger Sea (IRM-TS) is characterized by relatively warm and saline ($S > 35$) Modified North Atlantic Water derived from the North Atlantic Drift. Winter mixing is induced by strong winds and loss of heat to the atmosphere. This location may also be described as representing the subpolar gyre (Hatún et al., 2005). The IS-TS is located in the central Iceland Sea north of the Greenland-Scotland Ridge. At the IC-TS cold Arctic Intermediate Water, formed from Atlantic Water and low salinity Polar Water, usually predominates and overlays Arctic Deep Water (Olafsson et al., 2009). The Polar Water influence in the surface layers is variable (Stefansson, 1962; Hansen and Østerhus, 2000). Both regions are important sources of North Atlantic Deep Water.

2.1.7. K2 and KNOT

The K2 and KNOT stations (Wakita et al., 2017) are located approximately 400 km northeast of Hokkaido Island, Japan in the subarctic western North Pacific. Since 2001 and 1997, respectively, irregular field observations have been conducted at these stations to investigate the inorganic carbon system dynamics in response to variations in hydrography and biological processes. The overarching goal is to investigate the response of the biological pump to climate forcing in the western subarctic Pacific gyre. The region is characterized by high primary productivity, abundant marine resources (FAO, 2016) and might be the first region of the ocean to become undersaturated with respect to calcium carbonate during winter (Orr et al., 2005). The sites are representative of the southwestern subarctic gyre with both stations lying offshore of the Oyashio Current and just north of the subpolar front. Seasonal cycles are present (e.g., Takahashi et al., 2006; Tsurushima et al., 2002; Wakita et al., 2013) with a highly productive biological pump from spring to fall and strong vertical mixing of deep waters that are rich in dissolved inorganic carbon (DIC) in winter.

2.1.8. Munida

This deep-water station is located in the Southwest Pacific Ocean 65 km off the southeast coast of New Zealand and is part the Munida Time Series Transect, which is sampled every two months. Measurements at Munida were established in 1998 to study the role of these waters in the uptake of atmospheric carbon dioxide, and the seasonal, interannual, and long-term changes of the carbonate chemistry. The subantarctic waters are a sink for atmospheric carbon dioxide (Currie et al., 2011), and the seasonal cycles of DIC are primarily driven by net community production (Brix et al, 2013; Jones et al., 2013) with modification by the annual cycle of sea surface temperature.

2.1.9. Ocean Weather Station Mike (OWSM)

OWSM is located in the Norwegian Sea at the western baroclinic branch of the northwards-flowing Norwegian Atlantic Current where the water depth is 2100 m (Skjelvan et al., 2008; 2022). Hydrographic measurements date back to 1948 while carbonate chemistry measurements started in 2001 to monitor long-term changes in the biogeochemistry. Between 2001 and 2009, the station was sampled monthly, and since 2010, the sampling frequency has been four to six times per year. The site encompasses the cold Norwegian Sea Deep Water and the Arctic Intermediate Water in addition to the relatively warm and saline Atlantic Water. Occasionally during late summer, fresh Norwegian Coastal Current Water meanders all the way out to OWSM, influencing the surface water at the station. Seasonal variability is observed in the uppermost ~200 m, and long-term trends of carbonate variables are observed at all water depths. Over time, the surface water CO_2 content at OWSM has increased at a faster rate than atmospheric pCO_2 at this site (Skjelvan et al., 2022).

2.1.10. A Coruña RADIALES (RADCOR)

The RADIALES program started in 1989 aiming to obtain reliable baselines for long-term studies on climate change and ecosystem dynamics in times of increasing anthropogenic disturbances along the northern and northwestern Spanish coasts (Valdés et al., 2021). The program consists of monthly multidisciplinary perpendicular sections covering the Cantabrian Sea and northwest coastal and neritic Spanish ocean. The A Coruña (NW Galician coast) section (RADCOR) started in 1990 (Bode et al., 2020) and CO_2 variables have been incorporated since 2013 in two stations, E2CO and E4CO. RADCOR is located on the northern edge of the Iberian Upwelling Region. Here, the classical pattern of seasonal stratification of the water column in temperate regions is masked by upwelling events from May to September. These upwelling events provide nutrients to support both primary and secondary production in summer. Nevertheless, upwelling is highly variable in intensity and frequency, demonstrating substantial interannual variability, mostly affecting the E2CO station (80 m), while the station closest to shore, E4CO (15 m), is more impacted by estuarine and benthic processes.

3. Methods

The data flow of the SPOTS pilot depicting the main steps of the synthesis is schematically illustrated in Fig. 2. In the following, the individual components of this data flow are described in detail.

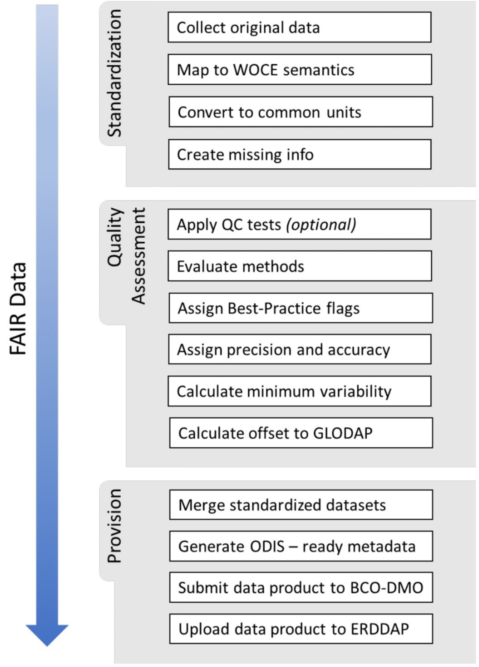

Figure 2: Schematic data flow of the SPOTS pilot

3.1. Data Collection

The data from the 12 participating time-series programs were retrieved from data centers or directly obtained from the responsible principal investigator (Table S1). In the latter case, merging, formatting, additional quality-control (QC), and archiving of existing data were carried out. Only bottle data for BGC EOVs, that had been measured by at least two of the participating programs were included in the pilot project, along with accompanying ancillary pressure, salinity, and temperature data. We have also developed a metadata template for BGC EOV ship-based time-series data (Table S2). The template has subsequently been used to collect all relevant metadata information from each participating time-series program. The collected metadata includes general information about the program, such as information about the principal investigator and the location and timeframe of related station(s). It also includes detailed information on the measured variables - e.g., units; sampling and analytical methods and associated instrumentation; calculation, calibration, and quality control procedures; and standards or (certified) reference materials used. The latter not only vary among the time-series programs, but can also vary within a time-series program over time.

3.2. Data Assembly

The SPOTS pilot was created by standardizing data format, units, header names, primary QC flags, times, locations, and fill values and subsequently merging the individual datasets of each time-series program into one file. Only data that received a WOCE quality flag 2 (Table S3) were included in the product. Existing data were altered as little as possible without interpolation or calculation of "missing" variables. Similarly, original station-, cast- and bottle numbers were kept or created artificially if non-existent to ensure consistency. The headers, units, and flags of the individual time-series datasets were standardized (Table S4) to conform with the WOCE exchange bottle data format (Swift and Diggs, 2008), a comma-delimited ASCII format for bottle data from hydrographic cruises. To enable an automated mapping to other existing vocabularies, we also mapped the WOCE headers to the Natural Environment Research Council (NERC) British Oceanographic Data Centre P01 vocabulary collection, as well as to the newly proposed BGC bottle standard by Liqing et al. (2022). We did not use the latter as "central" semantics due to restrictions of existing QC-tools (e.g., AtlantOS QC (Velo et al., 2022) and the crossover toolbox (Tanhua et al., 2010; Lauvset and Tanhua, 2015)) to WOCE semantics.

The standardization process also entailed unit conversions, most frequently from micromoles per liter (µmol L^{-1}; nutrients and dissolved organic carbon (DOC)) or from micrograms per kilogram (µg kg^{-1}; particulate matter) to micromoles per kilogram of seawater (µmol kg^{-1}). The default procedure to convert from volumetric to gravimetric units was to use seawater density at in-situ salinity, reported laboratory temperature (otherwise assuming 20°C as laboratory conditions), and pressure of 1 atm (following recommendations from Liqing et al., 2022). For some time-series datasets, the combined concentration of nitrate and nitrite was reported (Table S4). If explicit nitrite concentrations were provided, these were subtracted to obtain the nitrate values. If not, the combined concentration was renamed to nitrate assuming that the relative nitrite amount is negligible. For the HOT program specifically, low-level, high-sensitivity measurements of macronutrients (phosphate and nitrate) were available but not included in the pilot product. Particulate organic matter was derived by subtracting the particulate inorganic matter from the total particulate matter, if available. For particulate organic carbon and particulate organic nitrogen, the factors 1/12.01 and 1/14.01 (inverse standard atomic masses) were used, respectively, for the unit conversion to micromoles per kilogram. For the HOT program, particulate carbon and nitrogen measurements correspond to total particle concentrations (PC and PN), but are here assumed to approximate POC and PON. If neither temperature nor pressure was provided, all corresponding data entries were excluded from the product. The potential density anomaly[1] is the only calculated variable. Missing and excluded values were set to -999.

3.3. Qualitative Assessment of Data

3.3.1. Internally Applied Quality-Control (QC)

The majority of the programs have established their own routines for QC and correspondingly flag their data using different flagging schemes. We did not double-check the applied flags, nor did we run additional QC checks. The applied QC on the collected stations include statistical outlier checks on routinely measured pressure intervals using either a two- or three- (seasonal) sigma criteria, visual inspections of property-property plots (PPP), and application of crossovers using reference layers (Table S5). For example, K2 and KNOT used North Pacific Deep Water (NPDW), defined as the water mass between 27.69 σ_θ (around 2000 dbar) and 27.77 σ_θ (around 3500 dbar) (Wakita et al., 2017), as the reference layer for their internal crossover checks. For CVOO and Munida, we performed QC by applying a seasonal two-sigma criterium to the data, and for CVOO, we made additional use of comparisons to CANYON-B (Bittig et al., 2018) and crossovers. Since the QC procedures differ from program to program, we have provided recommendations for the QC of future data, so that the flags are applied more consistently across different programs (Sect. 6.3). Further, the standardization of the SPOTS pilot also entailed mapping to a central flagging scheme. We chose the WOCE bottle flag scheme (Table S3). Flags indicating replicate measurements (WOCE flag of 6) were set to 2, whereas all other flags were set to 9 and the corresponding values to -999.

3.3.2. Best-Practices (BP) Assessment

Given the inconsistencies in the applied internal quality checks and the fact that bias corrections following crossovers analyses are presently impossible to apply to all included time-series datasets[2], the comparability of the data for the SPOTS pilot was qualitatively assessed. The information on the applied methods of each time-series program, as provided through the metadata collection, was evaluated against, ideally, published Best Practices (BPs), and otherwise known standard operating procedures (SOPs). "BP Flags" were assigned accordingly to each cruise of a time-series program (Table 2).

Table 2: Meaning of assigned BP Flags.

Flag	Definition
0	No data
1	Methods meet all BP requirements (including "desired")
2	Methods only meet "required" BP requirements
3	Methods do not meet the BP requirements (or no metadata given)

The majority of the defined "BP requirements" used for the evaluation are based on the Bermuda Time-Series Workshop report (Lorenzoni and Benway, 2013), with additional implementation of: GO-SHIP manuals (Langdon et al., 2010; Becker et al., 2019); the CARIACO Methods Manual (Astor et al., 2013); HOT analytical methods (https://hahana.soest.hawaii.edu/hot/protocols/protocols.html), which are based on the Joint Global Ocean Flux

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[1] Calculated using the Matlab seawater toolbox (Morgan, 1994)

[2] Crossover require a "constant" reference layer over the entire span of measurements. Especially in coastal and shallow water formation regions this layer is nonexistent. Detrending might make this criterion redundant. However, detrending techniques rely on regular measurement intervals, which is not the case for most ship-based time-series sites.

Study protocols (IOC, 1994); the guide to BPs for ocean CO_2 measurements (Dickson et al., 2007); results from the Scientific Committee on Research Working Group 147 “Towards comparability of global oceanic nutrient data” (Bakker et al., 2016; Aoyama et al., 2015); and studies on preservation techniques for nutrients (e.g. Dore et al., 1996). The requirements were grouped into “Required” and “Desired” BP, see Table 3. To fulfill all requirements, i.e. receive a BP flag of 1, the metadata must show that the methods also met the corresponding “Desired” requirements. Only time-series programs that provided granular metadata, i.e. metadata differentiating between different methods applied in time, could obtain a BP flag of 1.

Table 3: BP requirements used for the method evaluation.

Variable		Required	Desired
Salinity		AutoSal	(Sub-) standard used regularly
			Temperature constant
			Glass bottles
Dissolved Oxygen		Winkler	Draw temperature used for mass calculation if difference to in situ temperature > 2.5°C
			Titration reagent assessed using CSK/OSIL primary standard
Nutrients	**All**	Autoanalyser; If stored: Frozen upright	Carrier Solution documented
			Calibrated against Reference Material
	Silicate	Autoanalyser; If stored and concentrations are above 40 µmol L^{-1}: Poisoned and kept cold	Carrier Solution documented
			Calibrated against Reference Material
Dissolved Inorganic Carbon		Coulometry	Calibrated against Certified Reference Material (Andrew Dickson, SIO)
			If stored: Poisoned, kept in dark and cool location
		Potentiometric (closed-cell); Calibrated against Certified Reference Material (Andrew Dickson, SIO); If stored: Poisoned and kept in a cold, dark location[3]	Not applicable
Total Alkalinity		Potentiometric Titration (multi-step)	Open Cell or curve fitting method documented
			Calibrated against Certified Reference Material (Andrew Dickson, SIO)
			If stored: Poisoned, kept in dark and cool location
		Spectrophotometric	Indicator dye: bromocresol green
			Calibrated against Certified Reference Material (Andrew Dickson, SIO)
			If stored: Poisoned, kept in dark and cool location
pH		Spectrophotometric with scale and temperature reported	Indicator dye: m-cresol purple
			Indicator dye: Purified
			If dye is not purified: Correction applied to impurities
Partial pressure of CO_2		Gas-chromatography	Temperature and standard reported
			If stored: Poisoned, kept in dark and cool location
		Infrared-based system	Temperature and standard reported
			If stored: Poisoned, kept in dark and cool location
Particulate Matter	**Carbon and Nitrate**	High temperature combustion with reported filter volume and pore size	Dried filters (60°C)
			Standards reported

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[3] Capped at a BP flag 2.

	Phosphorus	Ash hydrolysis with reported filter volume and pore size	Dried filters (60°C)
			Standards reported
Dissolved Organic Carbon		High temperature combustion	Filtered
			If stored: Frozen or acidified to and refrigerated
			Calibrated against Reference Material (Dennis Hansell, University of Miami)

3.4. Quantitative Assessment of Data

In addition to the qualitative BP assessment (Sect. 3.3), the bottle data of the time-series are described by our quantitative descriptors: 1) precision, 2) accuracy, 3) variability on the most consistent depth layer, and 4) consistency with GLODAP (Lauvset et al., 2022). Precision and accuracy were included in the SPOTS pilot dataset file, the latter two were not included and are only described here.

3.4.1. Precision and Accuracy

Precision and accuracy estimates, as provided by each time-series program's primary quality-assurance procedure, were assigned to the bottle data. The temporal resolution of these estimates varies from estimates given for each cruise, i.e. on a cruise-to-cruise basis, to estimates given for longer time periods (covering multiple cruises) without recorded changes in applied methodology (Table S6), depending on the individual time-series' internal procedure. If only one estimate was given for a variable for the entire time-series, that estimate was only assigned to the most recently applied method. The units correspond to the units of the respective variable.

Precision estimates are based on replicate samples and expressed as one standard deviation of the replicate measurements[4]. For the carbon variables, the assigned accuracy estimates represent the deviation from certified reference materials from the A. Dickson Laboratory (Scripps Institution of Oceanography). The pH accuracies of RADCOR are an exception, representing the difference from the theoretical TRIS buffer value at 25°C. For oxygen concentrations, the assigned accuracy estimates represent the accuracy of the KIO_3 primary standard normality assessed using a certified reference standard from either Ocean Scientific International Ltd (OSIL) or Wako Pure Chemical Industries (WAKO). For nutrient concentrations, the assigned accuracy estimates represent the deviation from reference material from either OSIL, WAKO, or QUASIMEME (Wells et al., 1997) or from certified reference material from Kanso Technos Co., Ltd. (KANSO). For particulate phosphorus concentrations, the assigned accuracy estimates represent deviations from National Institute of Science and Technology (NIST) apple leaves (0.159% P by weight). For DOC, the accuracy estimates represent deviations from deep seawater reference material from D. Hansell (RSMAS, University of Miami). The exact calculations to express the above deviations from reference materials differ slightly across the time-series programs (Table S7), thereby preventing combined precision and accuracy estimates to calculate a total uncertainty in a consistent manner. The estimates should not be confused with values provided by instrument manufacturers, which are ideal values and are usually well below real-world uncertainties.

3.4.2. Minimum Variability

To provide an internal consistency measure of measurement quality, we determined the minimum variability of each BGC variable for each time-series station on the pressure surface (+/- 100 dbar) with the least oxygen variability, i.e. the layer on which oxygen has the lowest coefficient of variation. We chose oxygen as natural variability in oxygen can be linked to either variation in ventilation, water mass changes, or changes in consumption and production by biological activity[5] (Sarmiento and Gruber, 2006; Keeling et al., 2010; Stramma and Schmidtko, 2019). As these natural oxygen changes are likely to be accompanied by changes in other BGC variables, we used the layer that is closest to an oxygen equilibrium as an approximation for the least natural variability in ocean BGC. In addition, this choice allowed us to use the salinity variability as an independent indicator of natural variability. For i) CARIACO, ii) GIFT, iii) Munida, and iv) RADCOR, this layer could not be determined properly, respectively, due to i) anoxic water masses below the mixed layer, ii) varying measurement depths, iii) no oxygen data and iv) a shallow bottom depth of 80 m. The minimum variabilities of the other variables

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[4] Exception: IRM- and IC TS using $V_{dub}*C_{mean}$ (following OSPAR, 2011), where V_{dub} is coefficient of variation calculated from dublicates and C_{mean} is the mean of the concentration measured.

[5] Not represented in the variability of salinity

were subsequently determined by calculating the coefficient of variation of all samples on the identified pressure surface. A minimum of 10 samples on the pressure surface was required.

3.4.3. Comparisons to GLODAP

The final quantitative descriptor indicates how well the time-series data compares to the GLODAP dataset (GLODAPv2.2021, Lauvset et al., 2021) and vice-versa, with no a prioi assumption of which is ‘correct’. To this end, we applied an adapted version of the GLODAP crossover routine to all individual cruises of the time-series programs. Generally, the crossover routine calculates a depth-independent offset between a cruise and a reference dataset based on multiple crossing cruises, i.e. “crossover-pairs”. The secondary quality control of GLODAP depends heavily on this routine to determine and correct for biases of new cruises, which results in the high internal consistency of the core GLODAP variables. In the following, we first describe the crossover routine of GLODAP in detail and subsequently highlight the modifications applied to the routine so that it fits our pilot product needs.

For a given variable the depth-independent offset of a new cruise against GLODAP is calculated using the following steps:

Step 1) Detect all GLODAP cruises that cross the to-be-compared cruise (denoted as Cruise A in the following), i.e. find all “crossover-pairs” of Cruise A in GLODAP. In the 2nd QC of GLODAP, a “crossover-pair” is defined by two cruises that have (at least) three stations within a 2° radius that include (at least) three samples below a minimum of 1500 dbar. These requirements ensure that the influence of natural signals on the calculated offsets is limited. That becomes especially important if the time period between Cruise A and a crossing GLODAP cruise (denoted as Cruise B in the following) is large.

Step 2) Interpolate the samples of Cruise A and Cruise B to the same standard depths. Usually, the concentrations are compared on sigma-4 surfaces[6]. Samples above the chosen minimum depth are ignored to exclude layers that are influenced by daily to interannual variability.

Step 3) Compare all existing samples of Cruise A and B that are on the same depth surface and from stations within 2°. For each depth surface, the individual offsets are averaged to obtain depth-dependent mean offsets and standard deviations. For nutrients and oxygen, the offsets are multiplicative, and for the carbon variables and salinity, the offsets are additive.

Step 4) Calculate the constant offset of Cruise A against Cruise B by inverse variance weighting all depth-dependent offsets. The resultant depth-independent offset is also known as the crossover-pair offset.

Step 5) Calculate the standard deviation of the crossover-pair offset by inverse variance weighting all depth-dependent standard deviations. This crossover-pair standard deviation reflects the similarity of the offsets within one depth surface and across all depth surfaces. The lower it is, the higher the confidence in the crossover-pair offset.

Step 6) Repeat Steps 2) to 5) for all identified crossover-pairs.

Step 7) Calculate the total offset of Cruise A against GLODAP by inverse variance weighting all calculated crossover-pair offsets. The resultant standard deviation describes the overall uncertainty in the total offset.

For our purposes, we applied an adapted version of the above-described crossover routine using GLODAP as the “reference dataset” against which each time-series station is compared. The term “reference dataset” does not imply that the quality of GLODAP is higher than the quality of the time-series programs, only that it represents a dataset with known consistency in time and space. Each cruise of a time-series station, i.e. station visit, represents another Cruise A in the above-outlined crossover steps.

For a given time-series station and variable, our adapted crossover routine starts with the identification of crossover-pairs for each station visit, similar to Step 1. However, since multiple time-series cruises only take one profile with fewer than three samples below 1500 dbar, we could not apply the same crossover-pair requirements. We kept the distance requirement of 2° and added a new temporal requirement, that only crossover cruises within +/- 45 days were included in the routine. That permitted relaxing the minimum depth requirement and dropping

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[6] In regions with a high probability of internal waves, in upwelling and water formation regions the offsets are calculated on pressure surfaces.

the requirement of the minimum number of profiles. Note that we excluded crossover-pairs of cruises that are included in both products (parts of: IC-TS, IRM-TS, and OWSM). Steps 2 to 6 of the routine are identical and repeated for all time-series station cruises. In the next step, all crossover pair offsets against the same GLODAP cruise, i.e. a particular Cruise B, are averaged. This step was necessary when multiple time-series cruises took place within 90 days and all were compared to the same Cruise B. Consequently, we obtained one depth-independent offset (and standard deviation) of the time-series station against each GLODAP cruise that meets the crossing requirements. In a final calculation, we determine the total offset of the time-series station against GLODAP by inverse variance weighting all obtained time-series station offsets. If the standard deviation of the time-series station offset against a particular cruise B was below the consistency estimates of GLODAPv2 (see Table 11 in Olsen et al., 2016), the latter ones were used as standard deviations (e.g. only one crossover pair exits between the entire time-series and a particular Cruise B). The routine was only applied to variables defined as core variables[7] in GLODAP. Negative (or lower than unity) offsets indicate lower values compared to GLODAP and vice versa.

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[7] Salinity, oxygen, nitrate, phosphate, silicate, DIC, total alkalinity and pH

4. Data Assessment Results

4.1. Best-Practices (BP) Evaluation

The results of the BP assessment indicate that the time-series programs have documented their methodology well and that the most recent methods generally follow BPs (Fig. 3 and Table 3). The proportion of data allocated a BP flag 1 is strongly dependent on the variable and program assessed. The assigned flags partly reflect that over the 40 years multiple method changes occurred (Fig. 4). Method changes are even more pronounced in programs without a dedicated vessel (Table 1). However, not all changes are captured by the assigned BP flags, e.g. instrument changes (Table S6). Note that the overall percentages in Fig. 3 are skewed towards ALOHA, as the number of ALOHA samples makes up around 60% of all samples of the product (Sect. 5).

Further, note that BPs are constantly evolving and consequently this assessment must be seen as "dynamical". In some cases, programs explicitly choose to not follow the most recent recommendations in favor of method consistency. E.g., unpublished internal analyses and discussions in the HOT program about possible advantages and disadvantages of a purified dye for the pH measurements (recommended following the Bermuda Time-Series Workshop report) resulted in not changing their dye. These additional analyses demonstrate the difficulties in determining BPs, but the knowledge is often not shared with the wider community. Hence, regular time-series workshops that discuss currently applied methodologies, achieve community consensus, and result in BP recommendations that are implemented accordingly in the here applied assessment, should take place regularly.

In the following, the results will briefly be presented for each assessed variable.

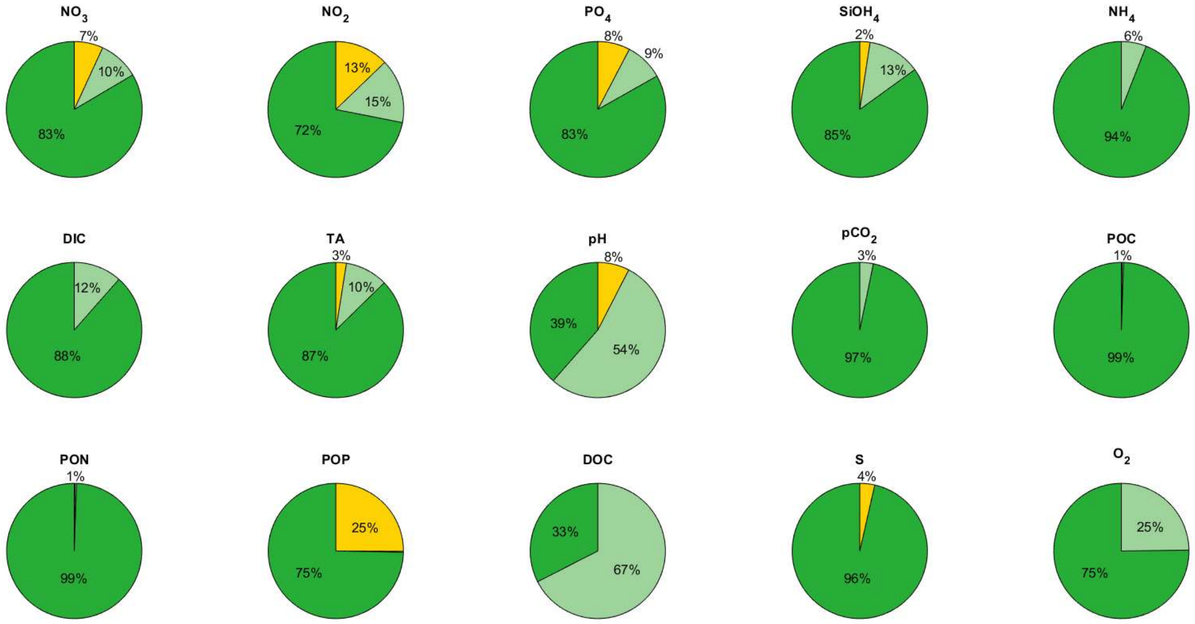

Figure 3: Overview of assigned BP flags. Percentages correspond to the number of samples in the combined dataset. Dark green colors indicate samples that have been measured according to all (incl. "desired") BP requirements, i.e. a BP flag 1 (Table 2). Light green colors indicate samples that have been measured meeting the "Required" BP requirements only, i.e. a BP flag 2. Orange colors indicate samples for which the methods do not meet the BP requirements, i.e. a BP flag 3. Variable synonyms correspond to the product header names (Table S8).

4.1.1. Salinity

For salinity, 96% of the bottle samples meet all BP criteria. DYFAMED, GIFT, Munida, and RADCOR only provided CTD salinity values and are not included in this statistic. The remaining 4% of bottle salinity samples with a BP flag 3 are a few cruises from ALOHA and CVOO. Salinity samples of the first 26 cruises of ALOHA were measured using an AGE Minisal 2100 salinometer. Also, the first 23 cruises of ALOHA used plastic bottles (instead of glass bottles) to sample salinity, which made them more prone to evaporation. Note that the data were corrected for it. Further, measurements taken on CVOO's research vessel "Islandia" used a Micro-Salinometer MS-310 (RBR Ltd., Canada) instead of a required AutoSal (Guideline Instruments, Canada).

4.1.2. Oxygen

Even though the overall statistics show that 75% of all bottle oxygen samples were measured according to the required BPs, 6 out of the 11 programs (Munida time-series program does not measure oxygen) did not regularly use certified reference KIO₃ (CSK, WAKO, OSIL) to assess the accuracy of the Winkler titration measurements. ALOHA, DYFAMED, GIFT, K2, KNOT, and RADCOR (as well as very few cruises from CVOO) used standard reference iodate. Further, note that during the first 10 HOT cruises, the in-situ temperature was used to calculate the mass, rather than the sample draw temperature, resulting in a slightly negative bias which is reflected in a BP Flag 2 of the concerned oxygen samples. The Winkler end-point detection method was either visual (starch) or computer-controlled potentiometric detection, both of which are accommodated in the applied BP assessment.

4.1.3. Nutrients

In most cases, all nutrient variables were measured simultaneously using one water sample (and/or with replicates at a single depth sampled), and the applied methods were identical. This is represented in similar BP flags of the nitrate, phosphate, and silicate samples. For these three variables, around 95% of the applied methods met either all BP requirements or the "required" requirements. The most restricting BP requirement is the comparison to reference materials, which, especially for older datasets, was not met. The remaining data with a BP flag 3 corresponds to 2% of the silicate, 7% of the nitrate, and up to 8% of the phosphate samples. These flags are linked to the preservation technique applied (poisoned instead of frozen for nitrate and phosphate) which particularly explains the lower fraction of silicate samples that do not fulfill the "required" criteria (DYFAMED, OWSM). Note that internal analyses at DYFAMED resulted in favoring poisoning nutrients for conservation over storing them frozen, and that DYFAMED reversed back to the former method in 2012, as reflected in the large percentage of BP flags 3. However, such insights were not integrated into this assessment and underpin the need for regular workshops discussing and updating BP recommendations for ship-based time-series. In this context, we want to mention the recently started Euro GO-SHIP project (https://eurogo-ship.eu/), and in particular the related comparability assessment of different nutrient measurement protocols.

Nitrite and ammonium samples show slightly different patterns because the number of measured samples deviates from the above-described nutrients, i.e. the influence of the ALOHA nutrient samples is smaller.

Differences in the type of autoanalyzer (rapid flow analyzer or continuous segmented flow), storage duration and temperature, defrost procedure, carrier solution ("in-house" artificial seawater that resembles the nutrient concentrations of the region, "in-house" low nutrient seawater or commercially available OSIL standard), reference material (WAKO, OSIL, KANSO) and sample filtering were not considered in the evaluation. Such differences can also occur in time within a time-series program, as shown for nitrate in Fig. 4. Note that the dependency of the CVOO time-series on research vessels of opportunity results in multiple small methodological changes – e.g., instrument, sample volume, and whether the sample is analyzed at sea or stored frozen.

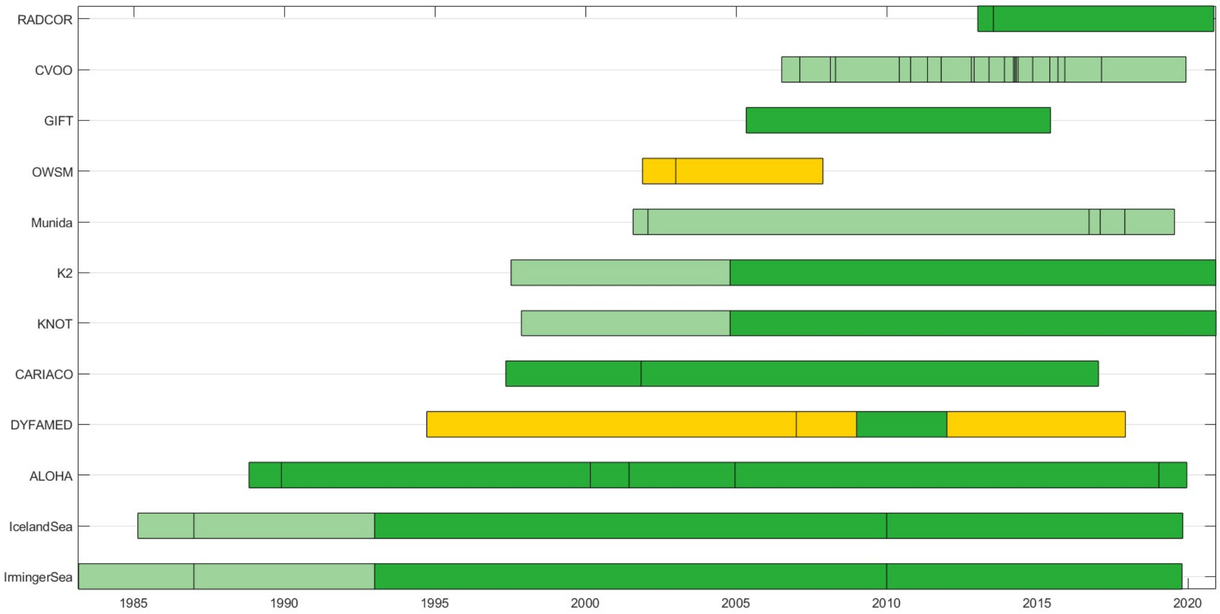

Figure 4: Time-dependency of assigned BP flag of each time-series program exemplarily shown for nitrate. Vertical black lines indicate method changes, captured and non-captured (e.g. instrument change) by the BP flags. The color scheme used, is identical to Fig. 3. Note that DYFAMED changed back to poisoning the samples for conservation based on internal analyses of conservation methods.

4.1.4. Dissolved Inorganic Carbon

For DIC, 88% of the samples were measured according to all BPs. DYFAMED is the only time-series program that measures DIC potentiometrically in a closed-cell. Even though DYFAMED made use of Dickson's CRMs since 1999, closed-cell potentiometric measurements of DIC alone have an offset (1-2% lower) (Bradshaw et al., 1981 and Millero et al., 1993), resulting in a BP flag 2. The remaining samples that do not meet the desired BP requirements are pre-1991 samples from ALOHA, IRM-TS, and IC-TS, for which certified reference material was unavailable, also resulting in a BP flag 2.

Differences in sample storage duration and coulometer calibration methods (gas loop calibration or sodium carbonate solutions) were not considered in the evaluation. Very few samples for DIC are taken on the RADCOR cruises.

4.1.5. Total Alkalinity

Total alkalinity is one of the few variables measured by all participating time-series programs. 87% of the samples met all BP requirements; 10% the "required" requirements only; and 3% did not meet the required BP. The latter correspond to cruises for which metadata on total alkalinity are not present (ALOHA cruises 1-22) and to cruises where total alkalinity was measured using a single-point titration (only few cruises at DYFAMED, K2 and KNOT) (Fig. 5). The BP flags of 2 are either linked to i) missing information on the indicator, cell type, and/or curve fitting method used, or ii) non-application of certified reference materials. Differences in storage duration, cell type, end-point, and curve fitting method (least-square or modified Gran functions) were not considered in the evaluation.

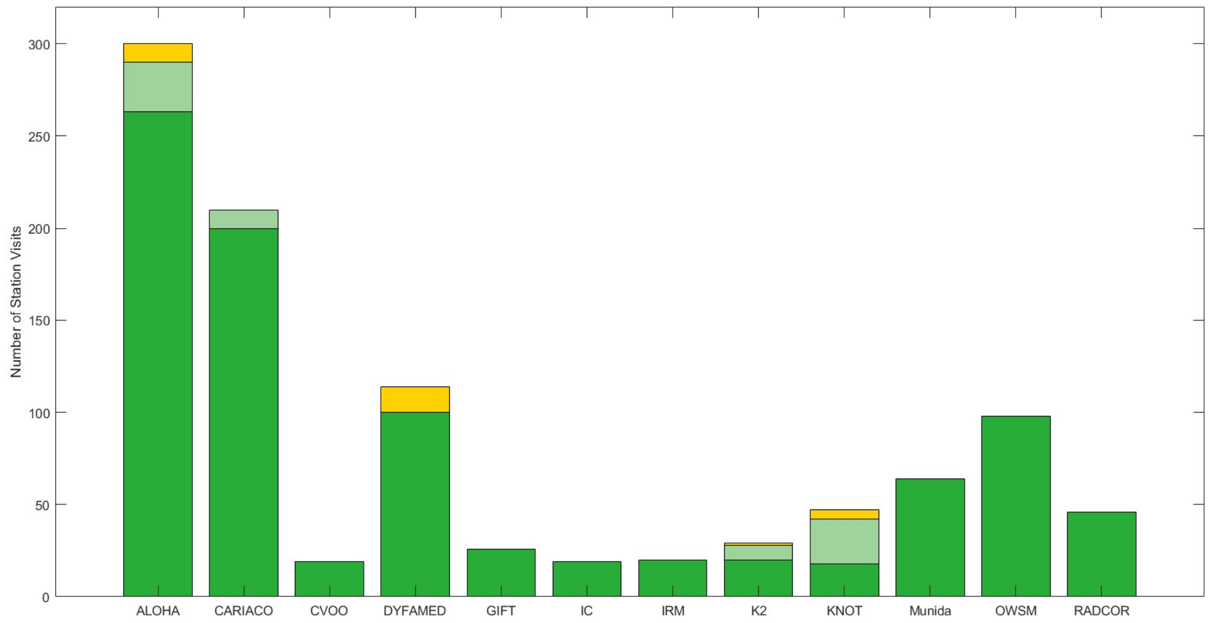

Figure 5: Assigned BP flags per station exemplarily shown for total alkalinity. Flags have been assigned on a cruise-per-cruise basis, i.e. per station visit. The color scheme used, is identical to Fig. 3.

4.1.6. pH

Even though most programs which analyze pH follow the methodology of Clayton and Byrne (1993), pH has the lowest number of programs with methods meeting all the BP requirements. CARIACO's protocol is the only one which meets all pH BP requirements, as reflected in the overall percentage of samples with a BP flag of 1 being only 39%. ALOHA, GIFT, and RADCOR reported pH on the total scale at 25°C and 0 dbar and analyzed pH using unpurified m-cresol purple. But none of these programs corrected for the impurities of the dye (54% of the samples), thereby not meeting the BP flag 1 criteria. A few cruises of DYFAMED, K2 and KNOT measured pH, but pH was measured potentiometrically (less stable and accurate, Lorenzoni and Benway, 2013).

Differences in the storage duration, and more importantly whether an additional correction for pK* of the indicator dye m-cresol purple was applied (suggested by DelValls and Dickson, 1998), were not part of the BP flag evaluation. The latter correction has been applied by GIFT and CARIACO.

4.1.7. Partial Pressure of CO_2

The only two time-series programs that measure partial pressure of CO_2 (pCO_2) are the IRM-TS and IC-TS, both being measured by the same personnel using identical protocols. The presently applied protocol meets all BP requirements. Before mid-1993, the samples (3% of the total) were not poisoned for storage, but instead equilibrated gas was isolated and sealed in a 300 mL glass flask. Further temporal changes of the methodology are explained in Olafsson et al. (2010).

4.1.8. Particulate Matter

Particulate matter concentrations are only measured at ALOHA, CARIACO, and CVOO. ALOHA and CARIACO meet all BP requirements for particulate organic carbon and nitrogen, whereas CVOO (<1% of all samples) is missing information on standards used. ALOHA's particulate phosphorus measurements (75% of all samples) also meet all BP requirements, but CARIACO's metadata do not include details on the filter used for these measurements. CVOO also lacks detailed metadata for particulate phosphorus.

Differences in storage duration, and more importantly, filter sizes and types, heating temperature and duration, and leaching time were not part of the evaluation. According to ALOHA's protocols, differences in the latter resulted in large variations of the measured particulate phosphorus content. ALOHA particulate organic phosphorus samples pre-2012 are biased low. Also, note that ALOHA particulate matter includes inorganic components.

4.1.9. Dissolved Organic Carbon (DOC)

ALOHA, CARIACO, GIFT, and K2 have measured DOC, and the samples of CARIACO, GIFT and K2 have been filtered. Thus, 33% of the DOC samples have a BP flag 1, and all samples from ALOHA (67%) received a BP flag 2.

4.2. Minimum Variability

The layers with the lowest oxygen variability (0.7% - 3.4%) are all located below 1000 dbar and represent the bottom layer in the cases of ALOHA, DYFAMED, and the IRM-TS (Table 4). For CVOO, IC-TS, K2, and OWSM, the determined layers are "near-bottom" to intermediate layers, probably reflecting that oxygen concentrations at the bottom are more prone to boundary layer effects in these regions. At KNOT, we can link this layer to the continual influx of NPDW.

Salinity shows the lowest variability for all time-series stations ranging from 0.003% - 0.086%. The higher values indicate that natural variability likely had a strong influence on the calculated numbers. Silicate is generally the nutrient with the highest variability within and across the time-series programs, with the IRM-TS experiencing the highest variability (6.7%). Such a high coefficient of variation cannot solely be linked to large uncertainties in the measurements (silicate accuracies (V_{crm}) at the IRM-TS are around 3.5%). Hence, natural variabilities of the nutrients are very high in this region in the determined layer, which also corresponds with the upper end of the salinity variability. Nonetheless, silicate, having the highest of all nutrient variabilities, fits well to the assigned accuracy values and also to previous findings of rather high uncertainties in silicate concentrations (e.g., inter-laboratory studies described in Bakker et al., 2016) and experiences from the GLODAP quality control (Olsen et al., 2016). The coefficients of variation of DIC and total alkalinity are below 0.5% for all time-series stations with a maximum of 0.4% (around 9 μmol kg^{-1}) at DYFAMED and a minimum of 0.1% (around 2 μmol kg^{-1}) at ALOHA, K2, KNOT, and CVOO. The latter are within the provided accuracy estimates and indicate very constant DIC and total alkalinity data quality. Minimum pH variability could only be calculated for ALOHA (0.04%), which is in the range of the provided pH precision values at ALOHA. DOC variabilities could be calculated for ALOHA and K2. For the former, it is 8.5% and thus around twice as large as given accuracy and precision values. For the latter, it is 1.7% and fits very well with the provided precision values. For the IRM-TS and IC-TS pCO_2 data, the determined coefficients of variation are two to three times as large as the stated precision (Olafsson et al., 2010), which again can be linked to the rather high natural variability of all variables at these stations. No minimum consistencies could be calculated for particulate matter.

The obtained minimum variabilities can in some cases (e.g., ALOHA) be interpreted as an inter-consistency determination of the measurement quality. In these cases, low variability indicates a consistent level of data quality throughout the measurement period. A high variability then indicates a variable level of data quality. Here, the determined layers can also be used to detect suspicious samples. However, some sites (e.g., IRM-TS) are characterized by large natural variability on all depth surfaces (on several timescales), likely accompanied and recognizable by high salinity variability. For these stations, the high variability estimates should not be confused with a high variability in measurement quality.

Table 4: Minimum variability expressed as the coefficient of variation (%). The corresponding layer depth of the layer with the least oxygen variability (+/- 100 dbar) on which the variabilities have been calculated, is shown, too. The variable abbreviations are the same as in Table 1. The Rhombus denotes that CTD values have been used for the calculation.

	Layer	**S**	**O_2**	**NO_3**	**PO_4**	**$SiOH_4$**	**DIC**	**TA**	**pH**	**pCO$_2$**	**DOC**
ALOHA	4400 dbar	0.005	0.7	0.7	0.8	0.8	0.1	0.2	0.04	NA	8.5
CARIACO	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
CVOO	3000 dbar	0.008	0.8	2.2	2.8	2.5	0.2	0.1	NA	NA	NA
DYFAMED	2400 dbar	0.033$^{\#}$	1.8	3.3	4.3	5.1	0.4	0.3	NA	NA	NA
GIFT	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
IcelandSea	1200 dbar	0.017	1.4	3.4	4.9	5.1	0.2	0.3	NA	2	NA
IrmingerSea	1000 dbar	0.086	3.4	4.2	5.3	6.7	0.3	0.4	NA	3	NA
K2	5000 dbar	0.003	0.6	0.4	0.5	1.5	0.1	0.1	NA	NA	1.7
KNOT	3800 dbar	0.011	0.7	0.4	0.6	1.0	0.1	0.1	NA	NA	NA
Munida	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
OWSM	1200 dbar	0.009$^{\#}$	0.7	2.5	4.2	6.5	0.2	0.3	NA	NA	NA
RADCOR	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

4.3. Comparison to GLODAP

The relaxation of the crossover analysis (Sect. 3.4) enabled the determination of offsets between GLODAP and time-series stations of ALOHA, CVOO, IC-TS, IRM-TS, KNOT, K2, and OWSM (Table 5). Generally, the analysis indicates a very good fit between the SPOTS pilot and GLODAP at these sites. Significant offsets suggest the potential for bias in either the SPOTS pilot or GLODAP, but further analysis of both products is required to assess the source of bias. In the following, the results are presented for each time-series program individually.

Table 5: Mean offsets (rounded) of the SPOTS pilot against GLODAP core variables. The first number in parentheses shows the number of cruises from the time-series program compared to GLODAP. The second number in the parentheses shows the total number of cruises from GLODAP to which the time-series cruises are compared. The variable abbreviations are the same as in Table 1. The Asterix denotes whenever the crossover analyses have been performed on pressure surfaces. The Rhombus denotes that CTD values have been used for the calculation. NPDW stands for North Pacific Deep Water.

	S	**O_2**	**NO_3**	**PO_4**	**$SiOH_4$**	**DIC**	**TA**	**pH**	**Layer**
ALOHA	0.0019 (3;1)	0% (3;1)	NA	-2% (3;1)	-1% (3;1)	NA	NA	NA	2000 dbar – bottom
CARIACO	NA	NA	NA	NA	NA	NA	NA	NA	500 dbar – bottom
CVOO	0.0003 (6;9)	0% (8;9)	0% (6;9)	1% (6;9)	1% (4;5)	0 µmol kg^{-1} (2;4)	1 µmol kg^{-1} (2;4)	NA	1500 dbar – bottom
DYFAMED	NA	NA	NA	NA	NA	NA	NA	NA	NA
GIFT	NA	NA	NA	NA	NA	NA	NA	NA	NA
IcelandSea*	-0.0006 (5;4)	1% (3)	-2% (4;3)	-6% (4;3)	-4% (4;3)	-2 µmol kg^{-1} (2;2)	NA	NA	1000 dbar – bottom
IrmingerSea*	0.0068 (5;6)	-3% (1;3)	-4% (1;2)	-1% (1;2)	6% (1;1)	NA	NA	NA	500 dbar – bottom
KNOT	0.0002 (28;41)	0% (28;37)	0% (29;39)	0% (29;39)	-1% (27;35)	-2 µmol kg^{-1} (28;35)	-5 µmol kg^{-1} (30;37)	-0.005 (1;1)	NPDW
K2	0.0004 (15;17)	0% (16;18)	0% (15;17)	0% (16;18)	-1% (15;17)	0 µmol kg^{-1} (16;18)	-3 µmol kg^{-1} (14;16)	-0.005 (1;1)	NPDW
Munida	NA	NA	NA	NA	NA	NA	NA	NA	NA
OWSM*	0.0023$^{\#}$ (2;4)	0% (1;1)	-3% (1;1)	-3% (1;1)	-1% (1;1)	6 µmol kg^{-1} (2;4)	NA	NA	1000 dbar – bottom
RADCOR	NA	NA	NA	NA	NA	NA	NA	NA	NA

4.3.1. ALOHA

For ALOHA all calculated crossover offsets fall within the provided GLODAP consistencies (Lauvset et al., 2021), indicating a good fit between the two products. There are no crossover cruises for nitrate and carbon variables. Further, only three ALOHA cruises (HOT174 - HOT176) are compared against only one GLODAP cruise (49NZ20051031), as these are the only crossover pairs that meet the crossover criteria. Note that 49NZ20051031 has passed the full 2nd QC of GLODAP and that the individual crossover pairs offsets are similar. Nonetheless, the small amount of underlying data strongly reduces the confidence in the results.

4.3.2. CVOO

Crossover offsets could be calculated for all GLODAP core variables which were measured at CVOO. All analyzed variables fall clearly within the provided GLODAP consistencies, indicating a good fit between the two products at CVOO. The results are robust, given the number of CVOO cruises compared to GLODAP. Further, there is very good agreement between the individual crossovers, i.e. low standard deviations of the individual offset between one cruise and GLODAP, and consistency among all CVOO cruise offsets with no large outliers. Data from a few cruises are present in both products.

4.3.3. Iceland Sea

The crossover offsets of the IC-TS of salinity, oxygen, nitrate, and DIC against GLODAP are within the consistency limits of GLODAP, i.e. no significant offset is remarkable between the two products. For nitrate, the variability between the individual offsets is large, which reduces confidence in the analysis. For phosphate, the SPOTS pilot has 6% lower concentrations than GLODAP based upon four cruises from the IC-TS (B17-94, B9-96, B12-96, and B5-2002) and three GLODAP cruises (58JH19941028, 58JH19961030 and 316N20020530), which all passed GLODAP's 2nd QC. This large offset mainly originates from the 2002 cruise, while cruises from 1996 indicate a good fit. The same cruises show a -4% offset for silicate, and the underlying data show a similar pattern. However, the relatively large minimum variability of salinity (Sect. 4.2) demonstrates that the Iceland Sea is a dynamically active region with deep open ocean convection and complex seasonally varying currents; this high natural variability reduces confidence in the crossover analysis for the Iceland Sea region.

4.3.4. Irminger Sea

All crossover offsets of the IRM-TS against GLODAP are above GLODAP's consistency limits except for phosphate. However, given i) that the minimum depth had to be set to only 500 m in a deep water formation area and ii) the relatively large minimum variability of salinity (Sect. 4.2), the larger offsets were expected and are likely attributable to the inherent natural variability of this region. Further, the relatively small number of crossovers does not allow for a more in-depth investigation of the offsets.

4.3.5. KNOT

Crossover offsets could be calculated for all GLODAP core variables. The calculations were performed on the NPDW, which has a residence time of about 500 years (Stuiver et al., 1983). Following the definition from Wakita et al. (2010), we used 27.69 σ (around 2000 dbar) and 27.77 σ (around 3500 dbar) as limits. All of the so-calculated offsets of KNOT against GLODAP are clearly within the consistency limits except for total alkalinity (-5 µmol kg^{-1}). Confidence in the analysis is provided through a large number of crossover cruises and consistency of calculated offsets. Data from a few cruises are present in both products.

4.3.6. K2

Crossover offsets could be calculated for all GLODAP core variables. The calculations were again performed on the NPDW using the identical limits as those of KNOT. All of the so-calculated offsets of K2 against GLODAP are clearly within the consistency limits. Confidence in the analysis is provided through a large number of crossover cruises and consistency of calculated offsets, as exemplarily shown for nitrate (Fig. 6). Data from a few cruises are present in both products.

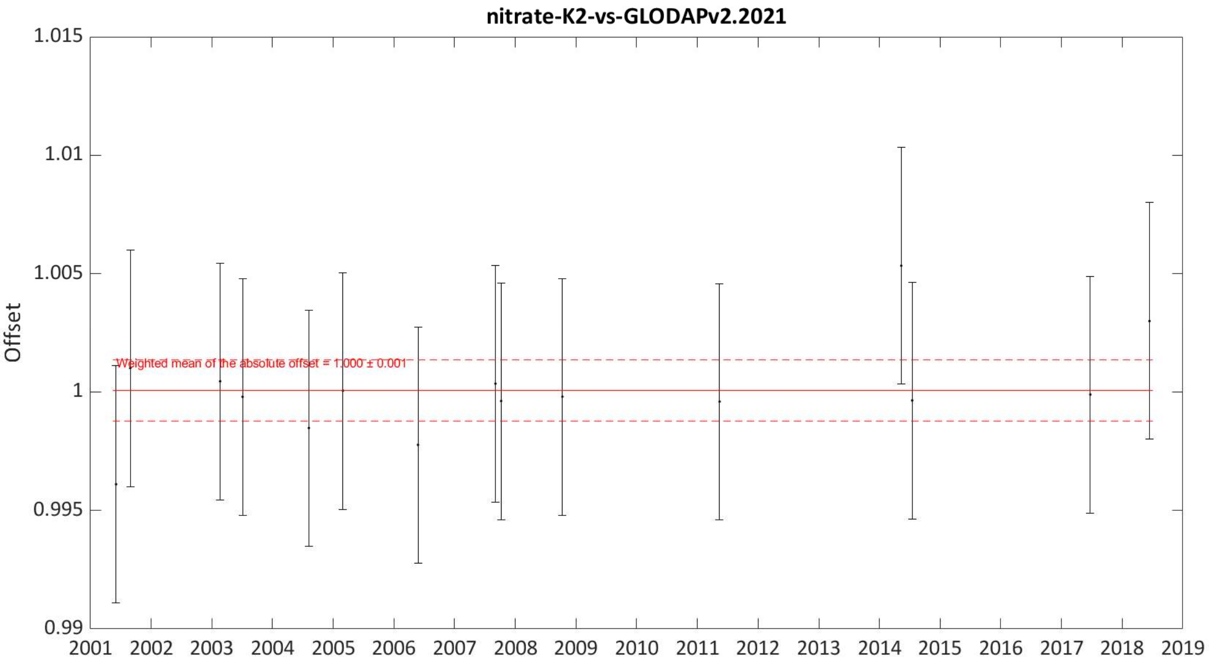

Figure 6: Total weighted offset of the SPOTS pilot nitrate data against GLODAPv2.2021 at station K2 in the North Pacific Deep Water (NPDW) layer. The total weighted offset is multiplicative and illustrated by the red line. The dashed red lines are

the corresponding standard deviation. The black dots display the weighted offsets of individual K2 cruises against GLODAP cruises with the corresponding error bars displaying their standard deviation. If the calculated standard deviation of the individual cruises is lower than GLODAP's nitrate consistency limit (2%) it is set to the latter. The summary figure indicates a very good fit between the SPOTS pilot product and GLODAP at the K2 station for nitrate with a total weighted offset of 0.0%.

4.3.7. OWSM

Crossover offsets at OWSM indicate slight mismatches between the nitrate, phosphate, and DIC concentrations of the SPOTS pilot vs. GLODAP. The total weighted mean offsets are -3%, -3%, and 6 µmol kg^{-1}, respectively. The former two offsets are only based upon a comparison between the OWSM cruise from 20020415 (no CRUISE ID present) and 316N20020530. Three more recent OWSM cruises from 2019 are additionally checked against 58JH20190515. Both GLODAP cruises passed GLODAP's 2nd QC. However, the DIC offsets are very dependent on the crossover pair and the final offset should be treated with caution. The small number of crossovers does not allow for a more in-depth investigation of the relatively small offsets.

5. Product File Description

The product file variable names are described in Table S8. Each fixed-location time-series station is identified by the entry under “TimeSeriesSite”, and individual cruises are identified by “CRUISE”. Station, cast, and bottle numbers are linked to the original cruise campaign numbering (if provided). In some cases, station number duplicates within the same time-series program exist as the data originates from different research vessels of opportunity (Table 1). Nitrate values can contain nitrite concentrations (Table S4). Similarly, ALOHA’s particulate organic matter includes particulate inorganic components. Since all pH values were reported on the total scale at 25°C, no additional pH temperature entry is provided. Conversely, for $p\mathrm{CO}_2$ corresponding temperature measurements are given. In addition to the WOCE flags, each bottle variable is further accompanied by the assigned BP Flag (Sect. 4.1) and by the provided precision and accuracy estimates (Sect. 3.4). The last column lists the digital object identifier (DOI) of the original dataset. All missing entries are indicated by -999.

A total of 108,332 water samples are included in the product. Bottle salinity with 75,654 measurements is the variable with the most abundant data (Table 6). The number of bottle salinity samples is about twice the number of bottle oxygen and nutrient (excluding ammonium and nitrite) samples and almost five times the number of included DIC and total alkalinity samples. pH and nitrite have around 10,000 samples and the product includes between 4,900 and 7,600 samples of particulate matter, DOC, and ammonium. With 1,898 samples from the IRM-TS and the IC-TS, $p\mathrm{CO}_2$ is the variable with the fewest measurements. Silicate, nitrate, and total alkalinity are the only variables measured at all sites. Around 56% of all bottle data values originate from ALOHA (Table 6) and 14% from CARIACO. The remaining 25% are distributed rather equally across the different programs. ALOHA’s large percentage can be explained by measurements at ALOHA i) having taken place consistently on a monthly basis for ≥30 years; ii) including up to 30 hydrocasts per station visit; and iii) including all but two of the product’s bottle variables. The dominance of ALOHA’s measurements is most pronounced for salinity, particulate phosphate (inorganic and organic), and DOC (around 70% - 80% of the samples are measured at ALOHA). For oxygen and nutrients, ALOHA’s samples represent around 52% of all samples, and for the inorganic carbon variables (DIC, total alkalinity, and pH) between 32% - 42%.

Table 6: Summary statistics showing the total number of samples per variable included in the SPOTS pilot of each time-series site. Percentages in brackets show fractions in comparison to the total number per variable except for the last column. Percentages are rounded; thus, the sum is not always equal to exactly 100%. Variable abbreviations are identical to Table 1.

	S	O_2	NO_3	NO_2	PO_4	$SiOH_4$	NH_4	DIC	TA	pH	$p\mathrm{CO}_2$	POC	PON	POP	DOC	Total
ALOHA	63334 (84%)	21937 (57%)	18130 (52%)	750 (6%)	17648 (53%)	17656 (52%)	0	5911 (35%)	5780 (32%)	4124 (42%)	0	3659 (48%)	3637 (49%)	3675 (75%)	4778 (67%)	171019 (56%)
CARIACO	4026 (5%)	3528 (9%)	3705 (11%)	3768 (32%)	3724 (11%)	3691 (11%)	3680 (69%)	0	3687 (21%)	3760 (39%)	0	3870 (51%)	3804 (51%)	1221 (25%)	975 (14%)	43439 (14%)
CVOO	345 (<1%)	534 (1%)	451 (1%)	507 (4%)	451 (1%)	411 (1%)	73 (1%)	346 (2%)	304 (2%)	0	0	39 (1%)	39 (1%)	24 (<1%)	0	3524 (1%)
DYFAMED	0	2328 (6%)	1525 (4%)	1670 (14%)	1611 (5%)	1482 (4%)	0	1086 (6%)	1114 (6%)	56 (1%)	0	0	0	0	0	10872 (4%)
GIFT	0	480 (1%)	479 (1%)	0	0	477 (1%)	0	0	470 (3%)	463 (5%)	0	0	0	0	199 (3%)	2568 (1%)
IcelandSea	2214 (3%)	2111 (5%)	2070 (6%)	0	2087 (6%)	2101 (6%)	0	1824 (11%)	280 (2%)	0	1101 (58%)	0	0	0	0	13788 (4%)
IrmingerSea	1901 (3%)	1792 (5%)	1774 (5%)	0	1767 (5%)	1784 (5%)	0	1477 (9%)	209 (1%)	0	797 (42%)	0	0	0	0	11501 (4%)
K2	1921 (3%)	1904 (5%)	1996 (6%)	1997 (17%)	1994 (6%)	1983 (6%)	1188 (22%)	1897 (11%)	1805 (10%)	509 (5%)	0	0	0	0	1129 (16%)	18323 (6%)
KNOT	1864 (2%)	1997 (5%)	1859 (5%)	1893 (16%)	1851 (6%)	1862 (5%)	376 (7%)	1821 (11%)	1802 (10%)	174 (2%)	0	0	0	0	0	15445 (5%)
Munida	0	0	285 (1%)	0	285 (1%)	280 (1%)	0	220 (1%)	298 (2%)	0	0	0	0	0	0	1368 (<1%)
OWSM	49 (<1%)	905 (2%)	1004 (3%)	0	911 (3%)	1004 (3%)	0	2053 (12%)	1320 (7%)	0	0	0	0	0	0	7246 (2%)
RADCOR	0	1215 (3%)	1270 (4%)	1279 (11%)	1268 (4%)	1284 (4%)	0	190 (1%)	739 (4%)	678 (7%)	0	0	0	0	0	7923 (3%)
Total	75654	38731	34548	11810	33597	34015	5317	16825	17808	9764	1898	7568	7480	4920	7081	307016

6. Stakeholders

The main stakeholder groups of SPOTS are the data providers on the upstream-end, i.e. the individual time-series programs (Sect. 2), and users of time-series data on the downstream-end. Regarding the latter, the SPOTS pilot is intended to be applied in different ocean BGC fields: evaluations of ocean BGC, neural networks such as CANYON-B (Bittig et al., 2018), CANYON-MED (Fourrier et al. 2020), or ESPER (Carter et al., 2021), regional ocean BGC models, (e.g., models participating in RECCAP such as Ishii et al., 2015), 1D model applications (e.g., Mamnun et al., 2022 using REcoM2), global ocean BGC models participating in model intercomparison projects (e.g., Coupled Model Intercomparison Project - Orr et al., 2016); evaluations of autonomous BGC observing networks such as BGC Argo (Bittig et al., 2019); global scientific assessments such as the Global Carbon Budget (Friedlingstein et al., 2022); or multi time-series studies and analyses (e.g., Bates et al., 2014; O'Brien et al., 2017). These time-series can also contribute ocean carbonate chemistry data to the United Nations Sustainable Development Goals, especially target 14.3 to minimize and address the impacts of ocean acidification.

6.1. Benefits

The main goal of SPOTS is that both stakeholder groups benefit from the product. Through a use-case, the benefits for the users are implicitly demonstrated in Sect. 6.2.

On the upstream end, data providers benefit from the product in several ways. First of all, the product increases the impact of individual ship-based time-series programs. For smaller and less well-known time-series programs, the impact is particularly improved by increasing their visibility and discoverability. Here, two "pull factors" contribute: i) the popularity and success of the included larger time-series programs and ii) being exposed on the Ocean Data and Information System (ODIS) catalog (https://book.oceaninfohub.org) in a schema.org-friendly way (Sect. 7.2). The larger sites also benefit from the latter, but the impact of larger time-series programs is in particular increased through enhanced usability of their data. Here, the proverb "the whole is greater than the sum of its parts" perfectly describes the benefits of SPOTS. The envisioned (non-exhaustive) list of users underscores the idea that consistent and inter-comparable data from multiple time-series programs (i.e. the "whole") leads to an extended range of applications relative to those of a single time-series program. The data being automatically uploaded to ERDDAP, which increases the accessibility, interoperability, and machine-readability (Sect. 7.2), also becomes important in broadening users and applications of data from these time-series programs.

Further, participating time-series programs benefit from optional data management support for formatting, QC, and data archival. This support aims at reducing the data management workload of individual programs and being directly ascribed to the FAIR data practices. Regarding guidelines and BPs, the participating time-series programs also benefit from the product fostering collaborations across several programs, which is especially relevant for emerging time-series programs.

Ship-based time-series programs represent one of our most powerful tools for monitoring marine ecosystem changes. The product contributes to the development of a sustained, globally distributed network of time-series observatories that sample a core set of biogeochemical and ecological variables guided by common best practices (methodological, FAIR data, etc.). These are required attributes of a GOOS observing network, and achieving this status would ultimately help position ship-based time-series programs for expansion under the United Nations Decade of Ocean Science umbrella. In addition, the product links individual time-series efforts to larger policy directives such as the Marine Strategy Directive Framework in Europe with respect to e.g., ocean monitoring indicators.

6.2. Use-Case

As an example to demonstrate both the utility and potential misuses of the SPOTS pilot, we applied the recently developed Trends of Ocean Acidification Time Series software (TOATS, https://github.com/NOAA-PMEL/TOATS) to the mixed layer total alkalinity data included in the product (Fig. 7). The TOATS software is a supplement to the recently published best practices for assessing trends of ocean acidification time-series and provides a python based Jupyter Notebook to compare trends across different (BGC) time-series data sets (Sutton et al., 2022). It was developed based on several published trend analysis techniques to standardize estimating and reporting trends from ocean carbon time-series data sets. Following a strict sequence of approaches[8], TOATS

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[8] 1. assess data gaps in the time-series; 2. remove periodic signals (i.e. normally occurring variations due to predictable cycles) from the time-series;3. assess a linear fit to the data with the periodic signal(s) removed; 4. estimate whether a statistically significant trend can be detected from the time-series; 5. consider uncertainty in the measurements and reported trends; and 6. present trend analysis results in the context of natural variability and uncertainty.

estimates i) the linear trend, ii) its uncertainties, and iii) the trend detection time of the assessed time-series data. The latter indicates the minimum observational period needed to statistically distinguish between natural variability (noise) and anthropogenic forcing. This method requires time-series with sub-seasonal sampling frequency to constrain seasonal variability of surface ocean carbonate chemistry; however, for the purpose of this example, we assessed all time-series programs rather than restricting the assessment to time-series datasets with regular monthly measurements. The only non-trivial calculation step we applied before running TOATS was to calculate the surface mixed layer depth for each cruise (defined using a 0.3 potential density anomaly criteria following de Boyer Montégut et al. (2004)) and to average total alkalinity concentrations within the estimated mixed layers. The results of our use-case (Fig. 7) show trends in alkalinity for all time-series (seven of them with significant trends).

The ease of use in applying TOATS to multiple time-series demonstrates the main benefits and potential misuse of the SPOTS pilot at the same time. Concerning the benefits, the combination of the SPOTS pilot and TOATS enables any user to perform joint time-series studies that follow published BPs without requiring any in-depth programming knowledge. The need to, a priori, know about existing time-series program data and to subsequently mine, format, and QC the data, becomes redundant for all time-series datasets included in SPOTS. The required input format of TOATS is also readily available by accessing the time-series product data through ERDDAP (Sect. 7.2). Further, detailed information on methods and their changes over time will become even more accessible once the ODIS user interface is online. This will enable a sophisticated information-driven data selection of (subsets of) time-series data to analyze the effects of method changes on detected trends without having to study multiple cruise reports. A similar advantage is provided through the possibility of selecting subsets of data based on the assigned BP flags (Sect. 4.1). Lastly, the estimates of precision and accuracy included in the SPOTS pilot (Sect. 3.4) additionally enable confident uncertainty estimations of the trend analyses (uncertainties of the observations being a mandatory input in TOATS).

Regarding the potential misuse of the SPOTS pilot, caution must be applied in interpreting the results, particularly because the use-case analysis includes values accompanied by BP flags 2 and 3. Simply assuming that the determined trends (Fig. 7) are valid and interpreting differences across time-series programs could lead to false conclusions. Robust trend analysis also requires the user to acknowledge the impact of large data gaps in time-series that inhibit the ability to constrain seasonal variability in many of the included datasets (e.g. CVOO), and make it impossible to remove periodic signals with confidence (second step of TOATS trend analysis). Following TOATS guidelines, we recommend applying TOATS to surface ocean biogeochemical data with at least regular seasonal measurements or to restrict the trend analysis to specific seasons. Increasing the number of samples using additional interpolation and computational techniques could relax this restriction (e.g., multivariate linear regression (MLR); Vance et al., 2022), but computations accompanied by large uncertainties might also harm the robustness of the trend analyses. Note that in the case of interpolating concentrations of single variables vertically, we recommend using a quasi-Hermetian piecewise polynomial (Key et al., 2010). And if techniques to increase the data coverage involve using CO2SYS (van Heuven et al., 2011), we recommend using the carbonate dissociation constants of Lueker et al. (2000), the bisulfate dissociation constant of Dickson (1990), and the borate-to-salinity ratio of Uppström (1974).

Another large pitfall is neglecting the provided metadata and assuming that restricting the analyses to time-series data with a BP flag 1 erases all artifacts in the trend analyses. Such a restriction would increase the robustness of the analysis, but unaccounted differences within the BP flag 1 (Sect. 4.1) would still bias the results. For example, ALOHA particulate phosphorus samples analyzed before 2012 are biased low but still fulfill all assessed BP requirements (Sect. 4.1). Similarly, some standardizations of the product resulted in the neglect of valuable time-series details (e.g., information on ventilation events provided through the unique QC flags of CARIACO (Sect. 3.2)). We included all information in the additional metadata, made it easily accessible, and encourage users consult it, particularly to check for any correlations of the trend analyses to method changes (Table S6) and/or specific time-series events.

Even though this example highlights a multiple time-series study use-case, it depicts the benefits and especially the potential misuses for other applications of the SPOTS pilot. If the limitations of the product (e.g., data gaps and varying baselines) are acknowledged, quality descriptors are utilized, and the data are used in conjunction with the supporting metadata, multiple applications can benefit from this time-series product.

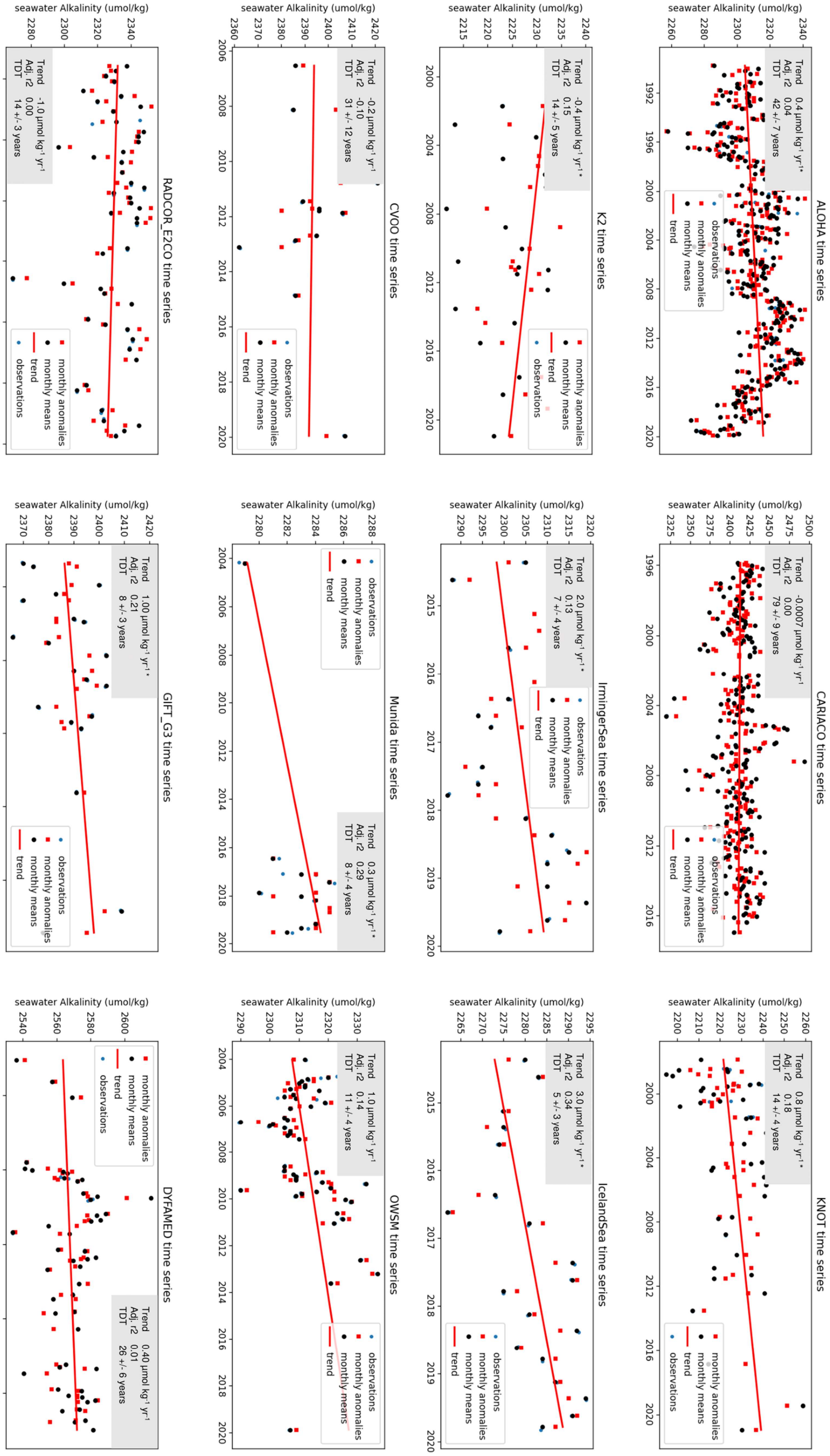

Figure 7: Trend analysis of total alkalinity in the mixed layer using TOATS. Data symbols show the original time-series observations (blue circles), the time series of monthly means (black circles), the de-seasoned monthly means (red squares), and the trend of the de-seasoned monthly means (red line) (From Sutton et al., 2022). The monthly anomalies (red squares) that are used for the trend analyses are shown as de-seasoned monthly means. The grey boxes include the yearly trend, adjusted R2 and the minimum trend detection time (TDT). An Asterix next to the yearly trend number indicates that the result is significant (two-sided t-test p-value < 0.05). Note that x- and y-axis are not in synch among the different time series subplots.

6.3. Recommended Standard Operating Procedures (SOPs) for Ship-Based Time-Series Programs

The process of generating the SPOTS pilot resulted in the formulation and recommendation of SOPs regarding metadata documentation, internal QC, and uncertainty estimation. These are directed at the data providers, i.e. those who help run the ship-based time-series programs. The proposed SOPs are briefly presented here, the full guidelines can be accessed at https://www2.whoi.edu/site/mets-rcn/.

1. **Metadata documentation**: The first SOP is the recommended metadata template (Table S2), which provides a structure for time-series programs to uniformly document the applied methodologies, thereby ensuring that relevant information, including differences between individual cruises, is recorded. It should be filled out for each cruise individually. The metadata enables detailed method comparisons of ship-based BGC EOV data such as the BP assessment of the participating sites of the data product. We recommend that the metadata template be updated as the community re-determines, expands, and specifies the BPs for BGC EOV ship-based time-series data.
2. **Consistent QC routine:** The second SOP recommendation involves the use of a consistent routine to QC time-series data. The main goal is that scientists follow consistent criteria to flag single samples. Different characteristics of time-series programs - e.g., location (depth and seasonal influence), funding opportunities (duration and frequency of visits), and scientific goals (variables measured) - preclude a "one-size-fits-all" QC method. Thus, a decision tree approach guides the user in choosing the appropriate type of QC for their dataset. All suggested semi-automated checks make particular use of comparisons with historical time-series data. To evaluate the flagging results, the SOP is accompanied by a comparison to the well-established HOT QC results.
3. **Calculating uncertainty:** The third SOP has been developed by the Oslo and Paris Conventions Commission (OSPAR), Hazardous Substances & Eutrophication Committee (OSPAR, 2011) and was originally intended for assessments of contaminants in biota and sediment done in OSPAR areas. It can also be applied to BGC EOV ship-based data. It provides detailed recommendations for a consistent estimation of one total measure of uncertainty, including exact formulas that combine the information obtained through duplicate measurements (precision) and comparisons to reference material (accuracy).

7. Data Access and Availability

7.1. METS-RCN Website

All information regarding the SPOTS pilot and the collaborative NSF EarthCube funded Marine Ecological Time Series Research Coordination Network (METS-RCN) can be accessed at https://www2.whoi.edu/site/mets-rcn/. The SPOTS web page (https://www2.whoi.edu/site/mets-rcn/ts-data-product/) includes detailed information on the participating time-series programs, including:

- contact person(s)
- time-series website URL
- relevant data repositories
- cruise reports and papers
- detailed metadata on the BGC EOVs measured
- recommended SOPs (Sect. 6.3) and in-depth information on the assigned BP flags
- links to AtlantOS QC software and crossover toolbox used

The website also provides several options for users to download the SPOTS pilot (DOI: 10.26008/1912/bco-dmo.896862.1), including:

- Comma-separated value (CVS) format (directly from the website)
- Link to the BCO-DMO repository (https://www.bco-dmo.org/dataset/896862, Lange et al., 2023)
- GOOS-relevant ERDDAP server (https://data.pmel.noaa.gov/generic/erddap/tabledap/bgc_ts_product.html)

7.2. Environmental Research Division's Data Access Program (ERDDAP)

Providing the data through ERDDAP enables FAIR-compliant data access services and gives users significantly enhanced capabilities rather than just downloading the dataset directly from the website. Optional constraints within the ERDDAP dataset enable downloading subsets of the dataset. The constraint options include amongst others variable-, station- and time selections. ERDDAP also enables downloading the dataset in several formats, such as tab-separated or netCDF. The latter format also entails additional metadata attributes, including alternative variable names (NERC P01 or following the recommendations from Liqing et al. (2022)). On the ERDDAP server, users find a link "Make a graph" (https://data.pmel.noaa.gov/generic/erddap/tabledap/bgc_ts_product.graph), which enables plotting the data using the web-based ERDDAP tool. In addition to giving the users more degrees of freedom, hosting the dataset on the ERDDAP server has two important benefits. First, the dataset is machine-readable, enabling an automated transfer to other repositories and higher-level infrastructures (e.g., SeaDataNet, Copernicus Marine Environment Monitoring Service). Second, ERDDAP data managers are working to provide direct access to metadata information stored in the ODIS catalog, which, once achieved, will significantly improve metadata interoperability.

7.3. ODIS catalog

Through collaborating with ODIS, we developed two json-ld templates to publish time-series program metadata in a schema.org-friendly way (inspired by Science on Schema; Shepherd et al., 2022) and to enable FAIR metadata. The first template (***EventSeries***) is designed to capture the general information about the time-series programs (e.g., location, time, principal investigators, funding, and related datasets). A "sub-events" section is used for more details about the individual cruise's location, time, personnel, and vessel. That section also includes details about the applied measurement methodologies for each cruise and provides links to cruise reports. The second json-ld template (***Dataset***) is designed to describe the metadata of the related BGC discrete bottle datasets. Here, the included variables and in particular, the applied semantics of the dataset are described. By using and linking these templates for each of the participating sites, we could include the metadata of the time-series sites and related datasets in the ODIS catalog. Here, the time-series programs are exposed on the web and machine-readable (interoperable) access to the metadata is guaranteed. Presently, these json-ld files are hosted by the METS-RCN GitHub repository (https://github.com/earthcube/METS-RCN). Eventually, the individual time-series program's data centers can host (and update) these files and assign unique identifiers. The metadata of the SPOTS pilot itself (***Dataset***) are also stored in the ODIS catalog, clearly linking all related metadata to the data synthesis product.

7.4. Fair Data Usage Agreement

While the SPOTS pilot is made available without any restrictions (Creative Commons Attribution 4.0.), users of the data should adhere to fair data use principles: For investigations that rely on data from a particular time-series program, principal investigators should be contacted to explore opportunities for collaboration and co-authorship and if there are any uncertainties regarding methodological details or interpretation of datasets. The original dataset DOI and any articles where the data are described should be cited. Contacting principal investigators comes with the additional benefit of expert insight into the specific site under investigation. This paper should be cited in any scientific publications that result from the usage of the SPOTS pilot.

8. Conclusion

The SPOTS pilot synthesized data from 12 ship-based ocean time-series programs, each representative of a unique marine environment. Time-series data and metadata were compiled and assessed to provide an internally consistent data product. As a pilot study, for feasibility, the focus of this initial ship-based time-series data product was BGC EOV data, which served as a use-case for the METS RCN and provided a template for a sustained living data product for ocean time-series.

Through an external qualitative assessment of the applied methodologies, flags were assigned that reflect the degree to which BPs were followed, which determines the comparability of the data. The most recently applied methods typically met the required BPs, but measurements of oxygen and pH still show room for improvement. Though the methods are adequately documented by many time-series programs, several others need to document their methods more thoroughly. The assessment also revealed the need to determine the level of granularity of both required documentation and required BPs for fully comparable data. The importance of inter-laboratory studies (e.g., QUASIMEME) must be highlighted in this context. In addition to the included precision and accuracy estimates, quantitative assessments yielded additional indicators that describe the consistency within- and across the time-series programs. For time-series stations dominated by water masses that contribute negligible natural variability, the calculated minimum variabilities demonstrate a high continuity in measurement quality. Reasonable fits between GLODAP and the majority of the time-series programs further increase the confidence in the data quality.

By making BGC EOV datasets from multiple sources consistent and ready to use, the SPOTS pilot facilitates an improved understanding of the variability and trends of ocean biogeochemistry. It represents an important and necessary step forward in broadening our view of a changing ocean and maximizing the return on our continued investment in ship-based ocean time-series programs. It also enhances data readiness (Lindstrom et al., 2012) by implementing FAIR data practices for all included data. In particular, the implementation of ERDDAP and ODIS (Sect. 7.2) enables easy data integration into e.g., OceanOPS and Copernicus Marine Environment Monitoring Service. On a higher level, this effort facilitates the consolidation of the international ship-based time-series network by collaborating closely with the participating time-series programs, developing, and recommending SOPs, and supporting the network to become more fit-for-purpose.

9. Outlook

We envision the SPOTS pilot to be the basis for a sustained living data product of time-series data that supports the timely delivery of scientific information on ocean biogeochemistry trends and variability across the main bio-eco domains of the world ocean. A product that complements SOCAT, GLODAP, and MEMENTO, together forming the primary source of EOV data for global marine BGC research and assessment. Three related near-term goals would be to i) regularly update the data of the already included sites to extend the data coverage in time; ii) extend the product by attracting further ship-based time-series programs measuring BGC EOVs, linking to the plus 340 sites identified by IGMETS and particularly closing the gap in the Indian and Southern Ocean to extend the data coverage in space; and iii) promote further development and adoption of BPs and the proposed SOPs by the ship-based ocean time-series community. In the long term, the product could extend the pilot's scope beyond BGC EOV data and include biological EOVs, as well as measurements from moorings. Work towards a "bio use-case", initiated by METS RCN, has already started, and leveraged from the knowledge and methods developed by this pilot effort. Including time-series data from moorings is far beyond current capabilities though. More generally, we hope that this effort contributes to increasing the recognition of the utility and value of ship-based BGC time-series data. A (ship-based) time-series BGC observing network that collaborates with the observing programs Surface Ocean CO_2 Reference Observing Network (SOCONET) and GO-SHIP and that complies with the requirements of an ocean observing network, as articulated by the GOOS Observations Coordination Group, needs to be established accordingly. This network should govern the product using an integrated approach with the existing BGC data synthesis products SOCAT and GLODAP.

Author contributions

NL, TT, and BF led the team that produced the SPOTS pilot. ABC, AW, BF, DRR, EH, FMK, FP, IS, KC, LC, MA, MH, MW, NL, SF, and SRO compiled and/or provided original datasets and metadata. FMK, DRR, KC, NL, SL, and TT developed the BGC EOV metadata template. NL, TT, and BF developed the recommended QC guidelines for BGC EOV time-series programs. NL conducted additional QC analyses on a few original datasets, executed the assessments (method evaluation, minimum variability, GLODAP offset), merged the SPOTS pilot and applied the TOATS notebook to the data. PLB and NL generated machine-readable metadata (ODIS) for all time-series programs and the SPOTS pilot itself. PLB manages the inclusion of the data product and individual time-series programs into the ODIS catalog and ODIS user interface. KOB uploaded the data product to ERDDAP and implemented all related functionalities. HB coordinates METS RCN and related activities (website, workshops). All authors contributed to the manuscript.

Competing interests

The authors declare that they have no conflict of interest.

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7

Synthesis

7 Synthesis

The overarching goal of this thesis was to improve the BGC data landscape through the manifestation of BGC synthesis products as an integral part in the BGC ocean observing system. This overarching goal was addressed by working towards four individual objectives. In this section, the main contributions from this thesis for each objective are presented. Eventually, the limitations of the presented work are discussed.

7.1 Individual Research Goals

For the overarching goal, the following four objectives were identified at the onset of this thesis (Section 1.2):

O1. Evaluating BGC EOV synthesis products in support of the elimination of any weaknesses

O2. Continuously updating existing living BGC EOV synthesis products with new data

O3. Developing and implementing improvements

O4. Expanding the BGC EOV synthesis product landscape to previously overlooked observations

As outlined in Section 1.2, each publication addressed, in particular, one objective. In the following, the main results of each publication are set into the context of the corresponding objective, and the contributions are briefly summarized and discussed. Additional results of this thesis that go beyond the individual publications, but are relevant for these objectives, are also included. However, parallel efforts that this thesis did not support, but which also relate to these objectives are not presented, e.g. the annual updates of SOCAT (Bakker et al., 2023).

7.1.1 Evaluating BGC EOV synthesis products in support of the elimination of any weaknesses

In the larger context, the FOO readiness of an (BGC) ocean observing system depends on the maturity of all its components, input, processes, and output (Section 1.3.1, Lindstrom et al., 2012). However, for “Data and Information Products”, i.e. the output of the FOO engineering approach to ocean observations, and more particularly its sub-category “Data Products”, assessments of the maturity are missing (IOCCP 2017a-h). Aiming at closing this gap, and supporting the work towards more sophisticated methods to determine the maturity of ocean observing systems designed to capture BGC phenomena, an objective assessment of BGC data synthesis products with a clear scoring system was developed (Section 3).

Accordingly, for the evaluation of BCG synthesis products, an objective scoring scheme was developed, utilizing a criteria catalog that has been created based on the FOO readiness level concept. The novel scoring scheme thus introduced and applied the FOO readiness concept to the evaluation and guidance of synthesis data products, and for the first time provides an objective measure of a synthesis products maturity. Four BGC EOV data synthesis products, SOCAT (Bakker et al., 2016), GLODAP (Lauvset et al., 2022), MEMENTO (Kock and Bange, 2015), and GO$_2$DAT (Grégoire et al., 2021), were selected to which this new evaluation scheme was applied. The four synthesis products represent the entire spectrum of BGC EOV data synthesis products, spanning different stages of development (maturity), focusing on different EOVs (Inorganic Carbon, Nitrous Oxide, and Oxygen), and implementing an EOV-based, and a platform-based synthesis approach. The evaluation showed that of these four products, SOCAT is the most mature one reaching a “Mature” status, followed by GLODAP being in the “Pilot” phase, and MEMENTO and GO$_2$DAT both being in the “Concept” phase. The reliability of the ranking and hence the developed evaluation system was further proven by the product’s identified impact, as approximated through the number of publications citing a product. Overall, the results underline the

importance of further improving synthesis data products (and thereby the maturity of “Data and Information Product”), as for multiple BGC EOVs, e.g. oxygen, and associated BGC phenomena, the output of the ocean observing systems and in particular the sub-category “Data Products” appears to be a weak link in the ocean observing value chain (Section 1.3.1, Section 3, IOCCP 2017a-h).
During the development and application of the evaluation, several critical features of BGC synthesis data products were identified that should guide new and existing BGC data synthesis products to realize their full potential, above all:

- Theme-oriented concept
- Achieving FAIR (Wilkinson et al., 2016) data (original data and synthesis product) with, in particular
    - the recognition and attribution of original (meta)data
    - the adaptation of common community standards
    - the implementation of Interoperable (meta)data
- Incorporating an automated data flow as much as possible
- Implementing a (customized) QC that is traceable
- Feeding back to requirements (FOO)
- Obtaining sustainable project-independent funding

7.1.2 Continuously updating existing living BGC EOV synthesis products with new data

A successful synthesis product involves the continuous inclusion of newly obtained data, i.e. it is a “living synthesis”. As an integral part of this thesis annual updates of GLODAP could be realized, releasing v2.2019 (Olsen et al., 2019), v2.2020 (Olsen et al., 2020), v2.2021 (Lauvset et al., 2021), and v2.2022 (Lauvset et al., 2022), with v2.2023 on the horizon. The updates harmonized, QC’ed, archived, and added a total of 361 new cruises[21] to GLODAPv2 (Olsen et al., 2016), averaging about 90 new cruises per update. v2.2022 now includes inorganic carbon-relevant bottle data from a total of 1085 cruises. The total amount of samples has increased from 999,448 samples to 1,381,248 (Table 8 in Lauvset et al., 2022), and the coverage in time has been extended from 1972 until 2013 (v2) to 1972 until 2021 (v2.2022). Most of the newly added cruises cover repeat hydrographic sections in the Pacific Ocean (about 51%), particularly the North West Pacific. However, a large amount of newly added data can also be attributed to the inclusion of selected cruises from CODAP-NA (Jiang et al., 2022) and the GEOTRACES intermediate data product (GEOTRACES, 2021), the addition of Davies Strait cruise data, Line-P cruise data, as well as the extension of Weather Station M in the Norwegian Sea (Skjelvan et al., 2008; 2022) with an additional 10 years of data. Even though not many cruises from the Indian Ocean could be added, the few that were, have proven to be of significant importance, e.g. global anthropogenic carbon inventory estimates (Müller et al., 2023). Most of the data can be attributed to cruises being younger than 2014 (58%), but also newly (re-) discovered old datasets, e.g. from cruises taking place in 1982, were added during those updates. The upper 100 m remain the best-sampled part throughout all updates, and the number of observations steadily declines with depth until 1,000 m, caused by the reduction of ocean volume towards greater depth (Figure 11 in Lauvset et al., 2022).

During the course of this thesis, a few changes have been applied to the product. Since v2.2020 GLODAP includes discrete fCO_2 samples, which led to the adaption of the calculation scheme for “missing” inorganic carbon sub-variables using CO2SYS (Olsen et al., 2020). Also, since v2.2020, no internal consistency evaluation procedures of the inorganic carbon system were used to assess or correct sub-variables of the inorganic carbon system. This change followed studies demonstrating that such evaluations are prone to “[…] errors owing to incomplete understanding of the thermodynamic constants, major ion concentrations, measurement biases, and potential contribution of organic

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[21] v2.2019: 116 new cruises; v2.2020: 106 new cruises; v2.2021: 43 cruises; v2.2022: 96 new cruises

compounds or other unknown protolytes to alkalinity (Takeshita et al., 2020) […]" (Olsen et al., 2020, p. 3661) leading to pH-dependent offsets in calculated pH (Álvarez et al., 2020; Carter et al., 2018). On the other hand, comparisons to calculated data from neural networks (CANYON-B and CONTENT), which are trained using GLODAPv2 (Bittig et al., 2018), were used more extensively in both (external) 1st QC and 2nd QC for all core variables. Since v2.2022, also SF_6 undergoes the full 2nd QC process of GLODAP extending the number of "core variables" to 13 (Section 4). Hence, the 2nd QC methods applied have been adapted slightly, however, the crossover analysis remained the main method throughout all updates. Most importantly, adjustments were only applied when detected offsets to the earlier data product release were not attributed to natural variability or anthropogenic trends. Often, the thorough 2nd QC detected incomplete applied QA and 1st QC and instead of applying depth-independent bias corrections, the data generators could resolve the problem once supported by the QC results, e.g. by correcting wrongly applied unit conversions, or by correcting towards measured CRMs.

Generally, the trend towards detecting fewer biases for more recent measurements remained (Figure 8 in Lauvset et al., 2022), reflecting the improvements in data quality due to the widespread adaption of standardized sampling- and analyzing practices, and the implementation of thorough QA, in particular the usage of CRMs. Furthermore, by applying the formula for the propagation of uncertainty[22] to the global consistencies of all releases since v2, (e.g. Table 7 in Lauvset et al., 2022), the overall improvement in consistency due to the (2nd) QC of data (and the corresponding corrections of detected systematic offsets), is evident (Table 5). The improvements were strongest for v2, however, the corrections of each annual release improved the consistency of newly added cruises to the previous release for all variables. In particular, $SiOH_4$ adjustments applied to analyses using different standards (North Pacific, Section 4) stand out when only considering the updates. Note that the shown consistencies and corresponding improvements can vary strongly regionally and that pH consistencies are not shown as the corresponding data were not estimated for v2.

Table 5: Evolution of GLODAP consistency estimates and overall improvements. Overall improvements were calculated using the law of uncertainty propagation.

	v2		**v2.2019**		**v2.2020**		**v2.2021**		**v2.2022**		**Overall**	
	unadj.	*adj.*	*unadj.*	*adj.*	*unadj.*	*adj.*	*unadj.*	*adj.*	*unadj.*	*adj.*	*unadj.*	*adj.*
Sal (x1000)	4.1	3.1	3.5	3.5	2.4	2.4	2.9	2.9	1.3	1.3	3.7	3.0
O_2 (%)	1.7	0.9	1.0	0.8	0.5	0.5	1.0	1.0	0.5	0.4	1.5	0.8
NO_3 (%)	1.7	1.2	0.8	0.8	0.5	0.5	1.5	1.1	0.4	0.4	1.5	1.1
$SiOH_4$ (%)	2.8	1.7	1.3	1.1	1.0	0.8	1.7	1.2	1.4	0.6	2.4	1.5
PO_4 (%)	2.2	1.3	1.0	0.9	0.8	0.8	2.2	1.8	0.7	0.7	1.9	1.2
DIC (μmol kg^{-1})	4.4	2.6	4.2	4.0	2.2	1.9	2.6	2.4	2.4	2.4	4.0	2.7
TA (μmol kg^{-1})	5.8	2.8	3.3	2.7	2.4	2.1	3.2	3.0	1.9	1.8	5.0	2.7

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[22] $\sqrt{}(w_{v2}*\sigma^2_{v2} + w_{v2}*\sigma^2_{v2.2019} + w_{v2}*\sigma^2_{v2.2020} + w_{v2}*\sigma^2_{v2.2021} + w_{v2}*\sigma^2_{v2.2022})$,
with w=number of cruises of version/ total number of cruises; σ=consistency estimate of version

7.1.3 Developing and implementing improvements

Over the last decade, GLODAP has matured with a set of well-documented protocols and development of dedicated software (Section 5). With the onset of this thesis and the annual GLODAP updates several further improvements to GLODAP itself (besides adding data) and to the underlying data flow were made. These improvements can mainly be linked to four software developments (Table 6). The corresponding advancements and implications for the data flow of GLODAP are discussed below.

Table 6: Crucial software developments for GLODAP during the course of this thesis. Note that the consultation efforts focused on the aspects pertaining to the applicability to GLODAP, rather than the coding.

New Software	Application in GLODAP	Status	Thesis' Contribution
AtlantOS QC	1st QC	Finished	Consultation
Python-based Crossover Tool	2nd QC	Ongoing	Consultation
Python-based "Make Ocean" Routine	Merging	Finished	Co-development
Digital Earth Viewer	Visualization	Finished	Consultation

To begin with, the development of AtlantOS QC for the 1st QC of hydrographic data (Velo et al., 2021; Section 2.5.3) was embedded in the data flow of GLODAP since v2.2019. Its utilization improved the QC of the data itself, enabled a transparent and traceable flagging of data, and also directly addresses F2 of FAIR (Section 1.3.2). Regarding the 2nd QC of GLODAP, developments of a Python-based crossover tool are still ongoing. The existing beta version already shows significant improvements in computational speeds, and user-friendliness, and provides much more flexibility in the crossover analysis (e.g. manually excluding questionable crossover-pairs for calculating total mean offsets). Further progress is initiated by working towards a direct connection between the Python-based crossover tool and the GLODAP adjustment table[23] implementing a more automated, streamlined, and interoperable data flow. In this context, the currently applied merging Python routine (Section 2.6) that harmonizes, applies flag changes, applies adjustments, assigns QC flags, interpolates, estimates missing variables, and produces the regional and global GLODAP datasets, also represents a major improvement resulting from this thesis. The routine generally follows the "rules" set out in Key et al. (2004) and Olsen et al. (2016). However, apart from erasing detected "bugs" in the product (e.g. wrongly assigned flags) and/or code and adding extra columns to the data product (DOI, expocodes, SF_6 2nd QC flags), several important improvements have been implemented in the merging routine since the release of GLODAPv2.2019:

- Approximating bottom depth using ETOPO1 (Amante and Eakins, 2009) instead of the Terrain Base (National Geophysical Data Center/NESDIS/NOAA/U.S. Department of Commerce, 1995)
- Adaption of calculation scheme for missing carbon system variables due to the inclusion of fCO_2
- Inclusion of conversion routine to calculate fCO_2 from pCO_2 values
- Calculating neutral density following Jackett and McDougall (1997) instead of using the polynomial approximation of Sérazin (2011)

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[23] https://glodapv2-2022.geomar.de/

The last major software development of GLODAP is the utilization of the DigitalEarthViewer[24] for visualizing GLODAP. The viewer enables a 4D presentation of all data included in the bias-corrected products, as well as of the mapped GLODAP climatology. Moreover, the development of the DigitalEarthViewer in combination with the individual files generated by the merging routine, makes an interactive and flexible extraction system that enables customized sub-setting, as well as the provision of synthesized unadjusted data, more feasible. All of these software developments further follow the guideline to use open-source software. Besides these software developments, it is also important to mention the development and dissemination of an official GLODAP cruise submission requirement document that includes clearly articulated mandatory and optional requirements for inclusion into GLODAP.

For the future, GLODAP developed a clear vision that builds upon these recent developments: "[the] GLODAP team now strive for advancements on two fronts towards a semi-automated system that reduces the work intensity and associated errors. Firstly, implementing a uniform, semi-automatic, and standards-compliant data ingestion system that will facilitate the data submission and quality control (QC) procedures. […] Secondly, upgrading to a modern and versatile data extraction system that provide users more flexibility and options […] "(Tanhua et al., 2021). The overall vision is to reduce existent bottlenecks, manual work intensity, and associated errors, and implement fully FAIR data.

7.1.4 Expanding the BGC EOV synthesis product landscape to previously overlooked observations

Even though the spatial footprint of fixed time-series stations is still limited (10% - 15% of the global ocean, Henson et al., 2016), time-series programs represent one of the most powerful vehicles for monitoring marine ecosystem changes. During the past decade, several studies underlined their collective value regarding our understanding of BGC phenomena, e.g. of ocean acidification (e.g. Bates et al., 2014, O'Brien et al., 2017). However, the BGC ship-based time-series community is as of now neither an official GOOS network nor had the community clearly articulated community standards for data management. Collaborating closely with the recently established METS-RCN and generating the pilot of SPOTS (Section 6), addressed these shortcomings and followed the mandate to work towards fit-for-purpose ocean BGC time-series data (Benway et al., 2020, Telszewski and Palacz, 2022).

For the generated pilot the focus was set on BGC ship-based time-series programs that measure BGC EOVs, the latter focus links to the general concept of FOO for GOOS (Section 1.3.1). In total, 108,332 water samples of 12 ship-based time-series programs, representative for different marine environments, and different program structures, were included. Besides the collection, and harmonization of data and metadata, the synthesis included optional 1st QC, and archiving, as well as the implementation of a set of 2nd QC methods. Both 1st QC and 2nd QC were developed with BGC ship-based time-series in mind. The 2nd QC constituted of three complementing approaches, all aiming at comparable data (Section 6):

1. A qualitative assessment of the applied methodologies: This entailed the development of community-agreed method recommendations, and particularly resulted in significant improvements in metadata documentation of individual time-series programs. Overall, “the most recently applied methods typically met the required BPs, but measurements of oxygen and pH still show room for improvement”.
2. Comparisons to GLODAP: For the comparisons the crossover routine was adapted and employed. Generally, a good consistency between SPOTS and GLODAP could be identified even though robust comparisons were limited.

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[24] https://www.digitalearthviewer-glodap.geomar.de/

3. Estimating the minimum variability on the most consistent depth layer: Low variabilities could in some cases be linked to internally high continuity in measurement quality.

Besides reaching more comparable data, the pilot of SPOTS resulted in more FAIR data for each included time-series program. This is most notably through the provision of enhanced metadata (Section 6) to the ODIS catalog and the implementation of ERDDAP services, of which the former addresses the FAIR principles F1-3, I1-3, as well as R1.1 and R1.13, and the latter I1-2 and A1 (Section 1.3.2). Furthermore, the pilot effort contributed to the consolidation of the international ship-based time-series network, led to community-proposed recommendations (metadata documentation, QC, uncertainty estimations,) and created a template for a sustained living SPOTS (Section 6). On a higher level, the pilot helped to position ship-based time-series programs for expansion under the United Nations Decade of Ocean Science umbrella, linking individual time-series efforts to larger policy directives such as the Marine Strategy Directive Framework in Europe. This is further evidenced by the network recently obtaining the status of an “Ocean Coordination Group potential new emerging network” (Benway, 2023).

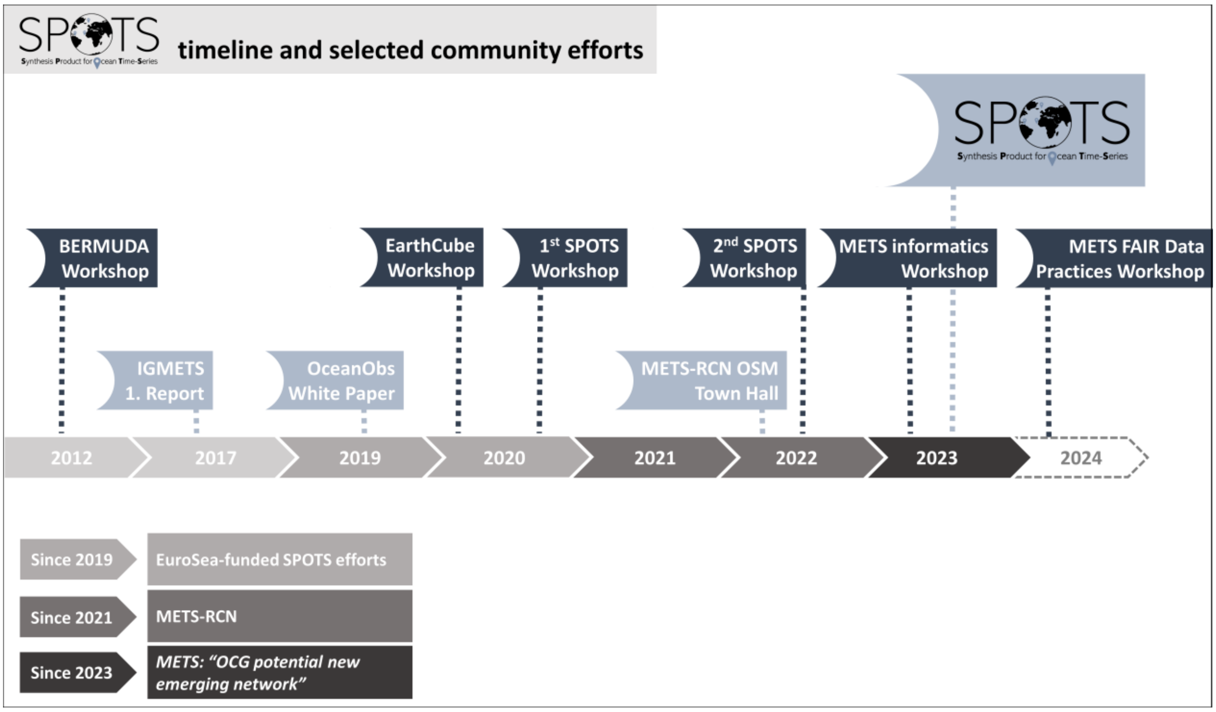

Figure 14: Timeline of SPOTS with selected events highlighted.

7.2 Limitations

This section highlights the methodological and conceptual constraints associated with this thesis at large, the reached objectives O1 – O4 (Section 7.1), and respective publications (Section 3 - 6). First, the general limitations of this thesis regarding the role of synthesis products in the BGC data landscape are discussed. Subsequently, specific limitations addressing the developed evaluation method for synthesis products (O1), as well as specific limitations regarding GLODAP and SPOTS (O2 – O4) are outlined.

Setting this thesis in the wider context of the BGC data landscape, it must be recognized that the achievements can only represent a part of the solution towards manifesting BGC data synthesis products. More specifically, while the pilot of SPOTS addresses the data synthesis gap for ship-based BGC time-series data and the updates of GLODAP continue to cover carbon-relevant hydrographic cruise data, their general limitation to ship-based data must be highlighted. Even if one acknowledges the complementing (existing and planned) BGC EOV data synthesis products, SOCAT, MEMENTO, and GO$_2$DAT, not all FOO-targeted BGC phenomena (Figure 6) are captured. In particular, if one considers that to capture these phenomena appropriately multiple time- and spatial scales must be covered (Telszewski et al., 2018). The complementing nature of the five mentioned BGC EOV data synthesis products is presently further constrained by their comparability amongst each other. This links to missing full uncertainty analyses of the BGC EOV data synthesis products (Section 7.1.1). Moreover, the focus on EOVs excludes further established BGC synthesis products focusing on other BGC variables, e.g. GEOTRACES (Schlitzer et al., 2017) or HalOcAT[25]. I.e., the FOO-motivated EOV approach in itself is limiting, disregarding the potential contributions of non-EOV BGC data synthesis products to the overarching goal of this thesis to improve the BGC data landscape. Thus, presently this thesis' achievements are limited in terms of covered EOVs, observing platforms, and hence BGC phenomena.

It is also crucial to understand that the general concept of synthesis products, i.e. displaying delayed mode data with rather high latencies, restricts their impact to climate-related studies. Other data management efforts that work alongside data synthesis products will, thus, always be needed for full coverage of BGC EOV observations. In this context, Global Data Assembly Centers, such as the GDAC Argo (BGC)[26], or SeaDataNet[27] are important complementing data efforts. Similarly, the importance of repositories is striking, facilitating the archival of all modes of (meta)data (real-time and delayed mode). Thus, given their constraints, synthesis products should not be seen in isolation. Considering the results of the synthesis product evaluation, a very important finding and present limitation is the fact that fully FAIR data have not been reached, yet (Section 3). That also holds for SPOTS. Clearly, all the BGC EOV synthesis products have enhanced the FAIRness of their data, however, not all FAIR principles are fully complied with. For GLODAP, for example, many of the (1,085) synthesized datasets, were submitted with inferior metadata ignoring existing metadata submission forms, e.g. the OCADS inorganic carbon metadata submission template. Specifically, method-relevant information (e.g. application of CRMs) is often missing, and even if provided, it is not available in the form of structured metadata (OCADS uses MD Metadata ISO 19115). Often users' only option to obtain detailed information about methods is to search for the information manually in related cruise reports. Thus, GLODAP's metadata handling doesn't fully comply with the FAIR principles F2, A1, I3, and R1. To give two examples for SPOTS: Some included datasets do not, yet, have their own persistent identifier which relates to the FAIR principles F1, F3, A1, and R1; Some of the header names used (e.g. TimeSeriesSite) are not defined in common and defined ontologies (I1, and I2).

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[25] https://halocat.geomar.de/
[26] ftp://ftp.ifremer.fr/ifremer/argo
[27] https://www.seadatanet.org/

Last but not least, funding, and in particular sustained funding, is a major limitation for the survival of living data products, for new developments, expansions, and maturing (Section 3, Section 5, Bakker et al., 2023). Also, for both GLODAP and SPOTS only few core personnel did receive funding for the data management of the syntheses. However, all supporting efforts by the community, e.g. the active engagement of experts in the GLODAP reference group or the metadata retrieval and provision from participating time-series programs for SPOTS was dependent on volunteering for the greater goal. This is even more evident by looking at other BGC data synthesis efforts, as MEMENTO did not update its product since 2017, and SOCAT experienced a dramatic decline in its data collection since 2017. Recently, SOCAT further warned about being "[…] at immediate risk upon losing its European data management team, while facing persistent funding shortfalls" (Bakker et al., 2023).

In the following more specific limitations about i) the evaluation scheme, ii) GLODAP, and iii) SPOTS are briefly presented (O1 – O4).

Considering the development of the novel evaluation scheme, it is above all important to acknowledge that the scoring system and criteria catalog display a first objective basis for assessing the readiness of synthesis products (Section 7.1.1). As such further refinement by the community is expected. It is however not expected that these refinements strongly alter the assessed maturities at large, but rather put more weight on some aspects than others (e.g. archival of data vs. free data). Nevertheless, it is important to understand that at this stage the developed scoring system and criteria catalog do not represent a "mature" and widely adopted scheme.

Specific important (non-FAIR related) limitations of GLODAPv2.2022 (Lauvset et al., 2022):

1. Limitations of the applied 2nd QC, more specifically the crossover-analysis:
    a. It is constrained to cruises with "deep" data and well-observed regions, i.e. regions with multiple crossovers. This is also reflected in the ratios of measurements not being 2nd QC'ed, ranging from 11% for salinity to 66% for pH measurements.
    b. It is not suited to detect non-linear, i.e. concentration-dependent, biases.
2. The consistency estimates are still too high to meet the requirements of the GOA-ON climate goals (e.g. 2 $\mu mol\ kg^{-1}$ for TA; Newton et al., 2015).
3. The relation between accuracy and consistency became more diffuse with the increasing number of new cruises being adjusted towards GLODAPv2. Strictly speaking, the determination of offsets can only be correlated to accuracy when an inversion is performed in addition to offset determinations. This extra inversion step is needed to minimize the offsets between all cruises, i.e. to generate an empirical truth, and to, thus, link consistency to accuracy. Nevertheless, if the number of new cruises is neglectable in relation to the reference dataset, their contribution to the inversion results can also be neglected in terms of the empirical truth. However, with the fourth GLODAPv2 update, almost a third of all cruises are "new" cruises, in some regions the ratio is even above 50% (northwestern Pacific). This had led to some adjustment decisions in favor of consistency rather than accuracy, e.g. silicate from JMA post-2018 (Section 4).

Specific important (non-FAIR related) limitations of SPOTS (Section 6):

1. The combined "spatial footprint" of the included stations is limited (following Henson et al., 2016). Nevertheless, note that 12 included time-series programs are a reasonable amount for a pilot, especially as the selected time-series programs are representing a wide range of marine environments.

2. The irregularity of the sampling frequency of some included time-series programs (e.g. K2, CVOO) limits their applicability for advanced trend analysis techniques (e.g. Sutton et al., 2022).
3. Some ODIS-related services, such as an interface (for humans), are not provided. Consequently, as of now, services that allow users to easily obtain information on (alternating) applied methodologies within a time-series, or services that enable automated (granular) metadata integration into ERDDAP-generated netCDF files, are withheld. Nevertheless, note that the generated structured metadata display a crucial step towards more interoperable (FAIR) metadata.
4. For the "BP assessment," it is expected that the underlying requirements will continuously be redefined. In particular, as the level of granularity of requirements displays a difficult balance between simplicity and feasibility on one side and enough attention to detail on the other. Expected insights into specific consequences for measurement comparability from upcoming laboratory intercomparison exercises and workshops thus likely lead to regular updates in the requirements, and hence the assigned BP flags. A typical example here would be whether exact freezing procedure requirements for the preservation of nutrient samples are needed for a thorough assessment or whether the present requirement "If stored: Frozen upright" is sufficient.
5. A sound error propagation into e.g. models is limited, as the different applied methods to estimate the accuracy based on (certified) reference material measurements prevented the calculation of a "total uncertainty", combining precision and accuracy estimates.

While it is crucial to recognize all of the above-described limitations, it is equally important to acknowledge the significant progress made through this thesis, through general advancements in the BGC EOV data synthesis community, and beyond.

8

Conclusion

8 Conclusion

In this Section, the results of the individual objectives are brought together, emphasizing the added collective value of this thesis, and more generally the value of synthesis products in the broader BGC data landscape (Figure 3). Subsequently, the main conclusions based upon this thesis' achievements are summarized. Eventually, an updated outlook on relevant future research opportunities regarding the continuing manifestation and improvement of BGC data synthesis products is presented.

8.1 Collective Value: Synthesis Products in the BGC data landscape

By means of the first research question of this thesis the individual objectives, the goal, and BGC EOV synthesis products are placed into the broader context of the BGC data landscape and the ocean observing system at large:

Why are BGC EOV data synthesis products important for the BGC data landscape, more specifically if all data would be FAIR, will synthesis products become redundant?

Regarding the first component of the question, all thesis achievements (referring to O1 – O4) indicate that the importance of BGC EOV data synthesis products is primarily linked to their main concept: Having a theme-oriented data approach. More precisely, the data synthesis products' approach of organizing the continuously growing "jungle of BGC data" into (EOV) theme-oriented, readily available, FAIR, and consistent data products. It was shown that by applying advanced QC methods (Section 2.5), synthesis efforts generate high-quality data tailored towards specific types of (theme-oriented) applications. Both data synthesis products, which have been updated and generated by means of this thesis, GLODAPv2.2022 (O2) and SPOTS (O4), respectively, demonstrate this. GLODAP is tailored towards climate research of interior ocean carbon storage, whereas SPOTS addresses the differentiation of natural and anthropogenic variability. Further, the applicability of GLODAPv2.2022 and SPOTS highlights that synthesis efforts enable scientists to focus on their actual research rather than to spend time for (meta)data retrieval, formatting, harmonization, and QC. It can be concluded that synthesis efforts correlate to superior reproducibility and comparability of scientific results as their standardized data flow (following community-agreed methods; O3) prevents the (repetitive and error-prone) application of different individual schemes to QC and merge data from multiple sources. Furthermore, the reached objectives underline that BGC EOV data synthesis products are important tools for community-supported implementation of FAIR data and FAIR data solutions. Especially, since a lot of the BGC data landscape is still far from complying with all FAIR principles (Section 7.2). Hence, this thesis emphasizes that BGC EOV data synthesis products occupy a unique position in the data landscape, in between data repositories (data enhancing) and further down-stream (data provision) services (Table 1 and Figure 2), complementing other data management efforts with less focused scopes (Section 1.1), e.g. World Ocean Database (Boyer et al., 2018), and GDACs.

The second component of the research question addresses the value of BGC EOV synthesis products in a theoretical world with fully FAIR data. Regarding this idealized "thought experiment", all thesis achievements demonstrate that the synthesis products' uniqueness is synonymous with increasing the efficiency and utility of marine BGC EOV data and advances beyond FAIR data (e.g. Boeckhout et al., 2018). This is particularly reflected in the developed evaluation scheme (O1), under which a fully mature BGC EOV data synthesis product is required to (in addition to FAIR data) provide open, free, and above all, comparable data. The applied evaluations under O1 demonstrate that the community-driven nature of synthesis products enables a holistic view on the observing system and directly links to the FOO feedback loop. Consequently, a BGC EOV synthesis product that "only" achieves fully FAIR data would not be 100% mature neither sustainable nor fit-for-purpose. The increased consistency of data through the application of GLODAP adjustments (O2), or SPOTS' categories (O4, which are inspired by SOCAT's accuracy categories; Bakker et al., 2016), highlights the value of the implemented QC methods in this context. Furthermore, the evaluations under O1 revealed that all assessed synthesis products (as well as SPOTS) are designed, accordingly. Hence, the great benefit of BGC EOV data synthesis products for the BGC data landscape can be described by the products' unique implementation of the notion "the whole is greater than the sum of its parts" (Aristotle, 350BCE/2016) that is still warranted in a fully FAIR world. In conclusion, the thesis highlighted that BGC EOV data synthesis products represent an important component in the ocean observing system, striving for FAIR, highly efficient, and utile observations. Accordingly, the continuous expansion and development of BGC data synthesis products is vital for the BGC data landscape and a sustained ocean observing system.

The second research question connects the individual objectives more directly to the overarching goal by addressing the key aspects required to manifest (the unique position of) BGC EOV data synthesis products in the BGC data landscape and the ocean observing system:

What are the key aspects for the sustainable success of BGC EOV data synthesis products?

The past and future success of BGC EOV data synthesis products roots in being community-driven efforts. The FOO evaluation scheme (O1) links the critical features of this bottom-up approach (community consensus, expert review, FOO feedback loop) to the main stages of the products' readiness ("Concept", "Pilot", "Mature"). In that context, the timeline of SPOTS (O4, Figure 14) illustrates the importance of international collaborations. Nevertheless, considering that the uniqueness of data synthesis products is closely linked to their focus on particular scientific applications (themes), tailored QC methods, as developed and applied for updating and generating GLODAP (O2) and SPOTS (O4), respectively, are equally important. Thus, their implementation in BGC EOV synthesis data flows will continue to be crucial for their success, as well. Further, all the objectives of this thesis, in various capacities, relate to the FAIR principles. This includes their incorporation throughout i) the readiness level evaluation scheme (O1), ii) the improvements of GLODAP (O2 and O3), and iii) the design of SPOTS (O4). Even though FAIR-related aspects could already be improved through synthesis products (e.g. FAIR I1: Common semantics), several limitations remain (Section 7.2). Hence, the progression and advancements towards FAIRer data, e.g. employing schema.org structured metadata (Section 2.4), is another key aspect for the sustainable success of BGC EOV data synthesis products. Moreover, the results related to O3 highlight that developments towards a more streamlined automated data flow, e.g. GLODAP's envisioned ingestion system or SOCAT's planned automation of metadata, are vital for the continuous success of BGC EOV data synthesis products, especially in view of the era of "marine big data".

More generally, a successful synthesis product involves the continuous inclusion of newly obtained data, i.e. for sustained success, data synthesis products must be "living" data products. The importance of updates is highlighted by the four most recent annual updates of GLODAP, adding 361 cruises with a total of 381,800 water samples representing almost 30% of all GLODAPv2.2022 available water samples. Outside of the scope of this thesis, during the same time (2019 – 2023) SOCAT released four annual updates, as well, with SOCATv2023 including 35.6 million surface fCO_2 observations covering the period from 1957 to 2022 (Bakker et al., 2023). SOCAT thereby expanded its data coverage by about 10 million observations and included three additional years to the dataset (SOCATv2019: 25.7 million observations from 1957-2019, Bakker et al., 2019). However, since 2017 the yearly amount of new fCO_2 samples drastically decreased (Bakker et al., 2023). Moreover, for MEMENTO, no updates were made during that time period. These points relate to the most fundamental aspect of a sustained success of synthesis products, their sustained funding. Without sustained funding, there is an ongoing risk that synthesis efforts will diminish or disappear independent of their unique value and importance for the ocean observing system.

Essentially, the following six key aspects were identified for sustained success of BGC EOV data synthesis products:

- Bottom-up approach
- Customized QC
- Implementation of FAIR
- Automation and stream-lining of data handling
- Continuous update of the product(s)
- Sustained Funding

In conclusion, through the work of this thesis, an evaluation system to assess the FOO readiness of BGC data synthesis products was developed and successfully applied. Annual GLODAPv2 updates were achieved and improvements to the data flow of GLODAP were developed and implemented. Furthermore, the BGC EOV data synthesis landscape was successfully expanded by the previously overlooked ship-based time-series programs, which supported the marine ecological time-series network in obtaining the status of “Ocean Coordination Group potential new emerging network”. Moreover, the work of this thesis and BGC EOV synthesis efforts in general were set in context with the BGC data landscape and the ocean observing system at large. Its unique value was shown and key aspects for continuous and sustainable success were elaborated on. Altogether, through the work in this thesis, important steps towards the overarching goal of **improving the BGC data landscape through the manifestation of BGC synthesis products as an integral part in the BGC ocean observing system** were realized. However, as the discussed limitations highlight, more work needs to be done to fully reach this vital goal.

8.2 Outlook

Several pending and envisioned efforts that are likely to contribute to the overall goal of manifesting BGC EOV data synthesis products are outlined in the following. These efforts cover different outstanding issues. The anticipated resources to implement them range from a few person-months over years of team efforts to pure futuristic visions. The different efforts and visions are presented following the order of the thesis objectives.

Presently, the GLODAP team is awaiting the approval of the FAIR-impact[28] support action "FAIRness assessment challenge". In case of approval, the support action would be focused on assessing the FAIRness of GLODAP, and would thus complement and correlate to the applied FOO readiness evaluation of GLODAP. Ideally, anticipated insights could be incorporated into the developed readiness evaluation scheme and thereby follow the call of refining the FOO evaluation scheme and criteria catalog.

The largest pending effort relates to the generation of GLODAPv3 as part of the Horizon Europe project OceanICU Improving Carbon[29]. Above all, GLODAPv3 will include a full inversion and will thereby address the discussed limitations of steadily increasing new cruise data being adjusted towards GLODAPv2. Accordingly, the correlation between the consistency and accuracy of GLODAPv3 will be improved, and a new reference dataset for another decade of carbon-relevant hydrographic cruise data will be available. Many further developments are linked to this effort, amongst others the synchronization of all original datasets with the synthesis product, the inclusion of (at least) fCO_2 in the 2nd QC, and the implementation of further model data into the 2nd QC (e.g. ESPER; Carter et al., 2021). Work towards GLODAv3 is planned to start in October 2023, with an anticipated release planned for late 2025. Before the kick-off of GLODAPv3, GLODAPv2.2023 will be released. In addition to GLODAPv3 (and v2.2023), the GLODAP team envisions the development and implementation of a "[…} uniform, semi-automatic, and standards-compliant data ingestion system that will facilitate the data submission and quality control procedures" (Tanhua et al., 2021, p. 3), as well as a more advanced data extraction system. This could also entail leveraging from the developed schema.org structured metadata template for ship-based BGC time-series data (Section 2.4.3) to enhance the FAIRness of the metadata archival of the original cruise data. However, no funding for enhancing the data flow of GLODAP could, yet, be obtained.

As outlined in Section 6, SPOTS aims at becoming a sustained living data product with regular releases. In addition to that SPOTS aims at attracting and including more ship-based time-series programs with BGC EOV data. Considering future prospects, the inclusion of mooring data, as well as the inclusion of biological variables, is envisioned. The upcoming METS FAIR data practices workshop[30] (Bermuda, January 2024) represents the first step toward these goals.

Considering the wider BGC EOV synthesis landscape: Despite their chronicle shortcoming of funding, SOCAT continues to pursue annual updates. Moreover, it strives for the automation of metadata, the widespread adaption of QuinCe amongst its data generators, and the inclusion of further variables such as atmospheric CO_2 (Section 3). Regarding GO_2DAT and MEMENTO, no specifics are known. However, evidently, the BGC data landscape would strongly benefit from the implementation of GO_2DAT's roadmap (Grégoire et al., 2021) and the revitalization of MEMENTO. Additionally, a new joint research group on Southern Ocean climate interactions (Alfred-Wegener-Institute, Ludwig-Maximilians-University) plans to produce a data synthesis product for the oxygen isotopic composition

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[28] https://fair-impact.eu/
[29] https://ocean-icu.eu/
[30] https://us14.campaign-archive.com/?u=be293460fdcca7c7856fb3819&id=c111d1c475

of the seawater in the Southern Ocean. This synthesis product would further expand the BGC EOV data synthesis product landscape. Besides, the CARIMED (Sanleón-Bartolomé et al., 2017) focusing on carbon-relevant data from hydrographic cruises in the Mediterranean Sea, is still under construction.
On a higher level, the vision of an all-encompassing BGC EOV data synthesis product displays the most ambitious and equally important goal. This “[…] integrated BGC data product could combine all the different synthesis products and provide intercomparable and FAIR cross-platform and cross BGC EOV data to scientists and down-the-line services. Here, the interoperability and comparability of the different products will be enhanced to the full extent” (Lange et al., 2023, p. 11). Clearly, this displays a rather futuristic vision. Nevertheless, it is important to realize that to fully address all GOOS-targeted BGC phenomena, only all available observations combined (platforms, BGC EOVs) approach a comprehensive coverage of the related time- and space domains.

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...Für dich, Mama…

Erklärung

Hiermit erkläre ich an Eides Statt, dass ich die vorliegende Dissertation, abgesehen von der Beratung durch meinen Betreuer Prof. Dr. Arne Körtzinger, selbstständig und ohne fremde Hilfe angefertigt, keine anderen als die angegebenen Quellen und Hilfsmittel benutzt und die den benutzten Quellen wörtlich oder inhaltlich entnommenen Stellen als solche kenntlich gemacht habe. Diese Arbeit hat in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegen. Sie ist unter Einhaltung der Regeln guter wissenschaftlicher Praxis der Deutschen Forschungsgemeinschaft entstanden. Mir, Nico-Maurice Dennis Lange, wurde bis zum jetzigen Zeitpunkt noch kein akademischer Grad entzogen.

Kiel, 07.07.2023

(Nico-Maurice Dennis Lange)