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## Ocean oxygen data: how to measure, how to manage?

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## Abstract

A global coordination and continuous synthesis of interoperable data related to biogeochemical Essential Ocean Variables (EOVs) is critically needed to enhance the creation of information products and services to sustainably manage the climate system and ocean health. Among the existing biogeochemical EOVs, data synthesis products—which demonstrate the immense value of data coordination—already exist for carbon-relevant data (e.g. SOCAT, Global Ocean Data Analysis Project), and for methane and nitrous oxide (MEMENTO). The roadmap for building a Global Ocean Oxygen Database and Atlas (GO<sub>2</sub>DAT) (Grégoire *et al* (2021 *Front. Mar. Sci.* **1638**)) provides the theoretical basis to increase the interoperability of ocean oxygen data sets, without creating yet another separate repository. The goal is now to advance from the idea of GO<sub>2</sub>DAT to its implementation, building a sustainable, interoperable, and inclusive digital ecosystem for all stakeholders who may use ocean oxygen data. Successful implementation will require (I) the provision of guidance on data acquisition/ocean oxygen measurements, (II) recommended practices for ocean oxygen data management, including metadata requirements, uncertainty and data quality control attribution, (III) development of the ocean oxygen data platform including data flow and application of the recommended practices introduced in I and II, as well as its deep integration with cross-domain data federations such as the Ocean Data and Information System. This document provides an outline of GO<sub>2</sub>DAT's objective and progress since 2021 and contributes to addressing these three requirements, synthesizing a series of global consultations on recommended practices for marine dissolved oxygen measurements, a working definition of ocean oxygen metadata, proposed data quality control levels and flags, a described novel mechanism for uncertainty attribution to allow the determination of data suitability for different scientific applications, and it concludes with an illustration of the data flow for implementation.

## List of acronyms

CMEMS	Copernicus Marine Environment Monitoring Service
EMODnet	European Marine Observation and Data Network
GLODAP	Global Ocean Data Analysis Project
GOOS	Global Ocean Observing System
IAP database	Institute of Atmospheric Physics database
IODE	International Oceanographic Data and Information Exchange
IOCCP	International Ocean Carbon Coordination Project
ODIS	Ocean Data and Information System
WOA	World Ocean Atlas
WOD	World Ocean Database

## 1. Introduction

Assessing and predicting ocean oxygen dynamics—particularly deoxygenation and its impacts on ocean health—are key priorities in the context of global warming and increasing nutrient pollution in the ocean. Dissolved oxygen is an Essential Ocean Variable (EOV; IOCCP 2017, Tanhua *et al* 2019), managed by the GOOS. Like humans, many marine organisms depend on oxygen to survive. 86% of the oxygen humans breathe (or six out of seven breaths we take) originated from the ocean over geological time scales (Grégoire *et al* 2023). However, the decline of ocean oxygen concentration (i.e. deoxygenation) in the coastal and open ocean over the past

60 years continues to increase (Breitburg *et al* 2018a). The primary drivers of this are: decades of increasing greenhouse gas emissions, resulting in ocean warming and increased stratification of the water column, and increasing nutrient loading in coastal waters. Relative to observational estimates, climate models currently underestimate oceanic oxygen loss by a factor of two to three, making rates of deoxygenation difficult to constrain (Oschlies *et al* 2018).

High quality data are needed for better management and mitigation strategies and to advance our understanding of extreme hypoxic events. The emergence of autonomous observation platforms equipped with oxygen sensors has dramatically increased the number of oxygen observations in the global ocean. The number of sensor-based oxygen (O<sub>2</sub>) measurements collected in the water column over the past decade alone from Argo floats and from O<sub>2</sub> sensor-based CTD data collected over decades of cruises is now comparable in quantity to all Winkler titration O<sub>2</sub> data collected since 1900 (Boyer *et al* 2018). It is expected that the number of sensor-based O<sub>2</sub> measurements will grow exponentially in the coming years with the increased deployment of moorings, gliders and biogeochemical Argo floats equipped with O<sub>2</sub> sensors. Efforts to use these measurements to further advance understanding of ocean deoxygenation and produce ocean oxygen data products would be greatly enhanced by federating all ocean oxygen data sources and supporting the creation of user-facing access points and services capable of discovering, filtering, and processing all available ocean oxygen data

sets. Such a federation can leverage the progress across Global Data Assembly Centers (GDACs), National Oceanographic Data Centers (NODCs), and regional hubs, while supporting them in co-developing collective data exchange norms and standard procedures.

It is therefore now urgent to (I) federate access to all oxygen data acquired from Eulerian and Lagrangian platforms in the coastal and open ocean in the past and present, (II) adopt and apply universal, globally actionable, and professional standards for metadata specification, sensor calibration, data quality checks and flagging. These standards must facilitate implementations of the FAIR and CARE data principles that, concretely, lead to increased interoperability among the data centers that manage ocean oxygen data, preparing them for interoperability with other ocean data systems. This will be the foundation for the development of the Global Ocean Oxygen Database and Atlas (GO<sub>2</sub>DAT).

GO<sub>2</sub>DAT was conceptualized in fall 2019, when members of the UNESCO-Intergovernmental Oceanographic Commission (IOC) GO<sub>2</sub>NE working group and other international experts met in Sopot, Poland, motivated by the fact that there was no common entry point to obtain all existing (or at least publicly available) ocean oxygen data provided by different observing platforms, with a common nomenclature, aligned quality controls and transparent adjustment procedures. GO<sub>2</sub>DAT is trying to fill this gap, forming an internationally coordinated effort towards the building of an open-access resource aligned with the FAIR and CARE Principles and their relevant global implementations, providing access to data from the coastal and open ocean, measured from Eulerian and Lagrangian platforms, adopting a widely interoperable metadata format with community-agreed content requirements, fully documented quality control, and flagging procedures. However, before being able to work on the implementation/development of such an online feature, the community needed to agree on the standards and recommended practices for GO<sub>2</sub>DAT: metadata requirements, quality control procedures, and the related quality flagging system. To do so, a GO<sub>2</sub>DAT steering committee was established, including representatives from the WOD, WOA, EMODnet, IOCCP, GLODAP, Argo, IAP database, and CMEMS.

The manuscript presented here collates (i) guidance on ocean oxygen data measurement, and access in section 2, (ii) a non-exhaustive summary of current practices for ocean oxygen metadata, data management, and quality control in sections 3 and 4, and (iii) a description of the development of the ocean oxygen data platform (the Database of GO<sub>2</sub>DAT) and its data flow in the context of these activities in section 4. Section 5 discusses the way forward for GO<sub>2</sub>DAT and future guidance on O<sub>2</sub> measurement as a template for other EOVs. The basis for this work

is a review of existing ocean oxygen recommended practices and a community survey, conducted from April to November 2023, collecting the input from the ocean oxygen community (via the GO<sub>2</sub>NE email list, GOOD Newsletter, ocean oxygen website and GO<sub>2</sub>NE Working Group). Recommended practices reviewed were sourced through the Ocean Best Practice repository, while the survey asked who is measuring oxygen in the ocean, how, what data treatment is applied and if the data are available freely. We conclude by outlining the roadmap to implement GO<sub>2</sub>DAT: data discovery and harmonization, data aggregation, and finally distribution, to be achieved under the ODIS, coordinated by the IODE, in full alignment with the developing IOC Data Architecture, comprising GOOS digital assets.

## 2. Recommended practices for dissolved oxygen measurement

A first step to enhance the quality of measurements and increase data availability is the documentation of high-quality methods and, where available, best practices for measurement and management of dissolved oxygen concentrations and data (Breitburg *et al* 2018a, 2018b, Kiel Declaration, Garçon *et al* 2019, IUCN Report 2019, Grégoire *et al* 2021, [www.ioccp.org/index.php/oxygen](http://www.ioccp.org/index.php/oxygen)). A method can be considered a best practice when it consistently produces superior results over other methods with the same objective (Simpson *et al* 2018, Pearlman *et al* 2019). Best practices inform the user of requirements for ocean observing systems or observations that may vary depending on the mission and the ocean environment. For example, best practices for high latitude measurements may not be applicable to the tropics, methodologies that excel in coastal areas may have little value in the deep ocean; and specific sensors and methodologies should be favored in oxygen deficient zones (Revsbech *et al* 2009, Larsen *et al* 2016, Garcia-Robledo *et al* 2021, Kwiecinski and Babbin 2021).

Benchmarking methods against one another—especially at a global scale—is a costly process, and thus discovering what is a true best practice is often not feasible in the short term. However, this does not mean that the tacit experience of the global oxygen observation community cannot be used to identify *recommended* practices, clearly identifying who recommends them and why. Following recommended practices allows the user to identify, meet, and communicate certain requirements for the quality of their data. For example, observing requirements for a so-called ‘weather quality’ would follow recommended practices leading to measurements of a quality sufficient to identify relative spatial patterns or short-term variation, whereas for ‘climate quality’ observations, recommended practices to

support detection of a long-term anthropogenically-driven trend over multi-decadal timescales would be required (Tilbrook *et al* 2019). The remainder of this section outlines elements foundational to establishing recommended practices—units and sensors, accurate determination of dissolved oxygen concentrations, and the ocean best practices project as a repository for recommended practices. It concludes with the results of a survey on the prevalence of ocean oxygen measurement practices with the ocean oxygen community.

#### UNITS

Dissolved oxygen comes in various units, e.g.  $\mu\text{mol O}_2 \text{ kg}^{-1}$ ,  $\mu\text{mol O}_2 \text{ l}^{-1}$ ,  $\text{mL}_{\text{STP}} \text{ O}_2 \text{ l}^{-1}$ ,  $\text{mg O}_2 \text{ l}^{-1}$ , hPa, or %  $\text{O}_2$  saturation, which all provide the amount of dissolved oxygen. This indeed can be a confusing aspect of dealing with oceanic  $\text{O}_2$  measurements. Oxygen can be expressed either as number of moles per unit mass (i.e. content) of solution (e.g.  $\mu\text{mol O}_2 \text{ kg}^{-1}$  gravimetric unit) or per unit volume (i.e. concentration) of solution (e.g.  $\mu\text{mol O}_2 \text{ l}^{-1}$ ,  $\text{mL}_{\text{STP}} \text{ O}_2 \text{ l}^{-1}$ ,  $\text{mg O}_2 \text{ l}^{-1}$ ). The unit  $\mu\text{mol O}_2 \text{ kg}^{-1}$  is recommended for oceanic applications because content is independent of temperature and pressure, both of which will change the concentration when expressed in a volumetric unit even without any production or consumption of oxygen.  $\text{O}_2$  content is used by large observing systems (see, e.g. Hood *et al* 2010, Thierry *et al* 2016). The standard reference method for  $\text{O}_2$  is a wet-chemical titration analysis (e.g. Winkler 1888, Carpenter 1965) that yields the amount of moles of  $\text{O}_2$  in a given sample volume (e.g.  $\mu\text{mol O}_2 \text{ l}^{-1}$ ).  $\text{O}_2$  concentration units per volume (e.g.  $\text{mL}_{\text{STP}} \text{ O}_2 \text{ l}^{-1}$ ,  $\text{mg O}_2 \text{ l}^{-1}$ ) are also commonly used for freshwater applications. Gravimetric and volumetric oxygen concentration can be converted by multiplying/dividing with the solution's density (mass per volume at a reference temperature, salinity, and pressure). When dealing with metabolic activities of marine organisms, the oxygen partial pressure  $p\text{O}_2$  (hPa, bar, mbar, atm) is the natural unit usually being used. Detailed conversions between these units are given in the SCOR Working Group 142's recommendations on  $\text{O}_2$  quantity conversions (Bittig *et al* 2018).

#### SENSORS

Two types of oxygen sensors are currently commercially available, both of which require unit conversions and corrections to report measurements per recommended practices. These sensors rely on two primary sensing principles. The first is an electrochemical method that uses a Clark-type polarographic cell (e.g. Clark *et al* 1953, Wei *et al* 2019). The second is an optical method based on dynamic luminescence quenching (e.g. Bittig *et al* 2018, 2019 for a review). Neither of these natively provides  $\text{O}_2$  data in units of  $\mu\text{mol O}_2 \text{ kg}^{-1}$ . As a consequence, whichever

sensor is considered, the data output must be corrected for temperature, salinity and pressure effects to convert the data to the standard  $\mu\text{mol O}_2 \text{ kg}^{-1}$ , along with prior corrections for the effects of temperature, salinity and pressure on the sensor response to oxygen concentration.

#### WINKLER TITRATION

The Winkler titration (Winkler 1888) is the standard reference method used to measure  $\text{O}_2$  and to calibrate and/or validate the data provided by  $\text{O}_2$  sensors. Winkler  $\text{O}_2$  determination during oceanographic cruises requires a discrete sample commonly collected from a Niskin bottle into a volume calibrated glass flask. The Winkler chemical titration is based on the oxidation of Mn-(II) by  $\text{O}_2$  in alkaline conditions and the reaction of the precipitated Mn-(III) with iodide in acidic conditions to form iodine and tri-iodine in a second step. The combined amount of iodine and tri-iodine is quantified by a titration with thiosulfate (Carpenter 1965, Langdon 2010) or spectrophotometrically (Labasque *et al* 2004) and from that, the concentration of  $\text{O}_2$  is calculated. Winkler  $\text{O}_2$  measurements conducted in a laboratory setting have an estimated accuracy of 0.1% using  $\text{O}_2$  saturated water at 1 total atmosphere (Carpenter 1965); equivalent to approximately  $\pm 0.25 \mu\text{mol kg}^{-1}$ . Emerson *et al* (1999) suggested an accuracy of  $\pm 0.1\%$  using  $\text{KIO}_3$  standards corrected for impurities. The estimated precision is approximately in the range of 0.15–0.87  $\mu\text{mol kg}^{-1}$  (Saunders 1986, Langdon 2010).

However, shipboard Winkler determinations have often not achieved such accuracy. The historical account of oxygen determinations at Woods Hole Oceanographic Institution (Warren 2008) is a good example of the systemic problems that have occurred over time. The need for cross-over corrections in oxygen data collected on cruises in the GLODAP data set (Olsen *et al* 2016, 2020) also shows that problems persist in even the highest quality data sets. In low oxygen areas, such as Oxygen Minimum Zones regions, it is recommended not to use Winkler determinations to correct *in situ* sensors in waters with  $\text{O}_2$  concentrations below 15–20  $\mu\text{mol kg}^{-1}$  due to the high interference of atmospheric contamination in anoxic and near anoxic water samples, producing values much higher than those found *in situ* (García-Robledo *et al* 2021). In such cases a zero-calibration is recommended.

#### CURRENT GUIDANCE AND RECOMMENDED PRACTICES—The Ocean Best Practices System

The Ocean Best Practices System (<https://search.oceanbestpractices.org>) collects and provides discovery functions for methodological documents, some of which are explicitly recommended by named organizations for the measurements of dissolved oxygen.

While not exhaustive or (currently) far ranging, the OBPS has attracted submissions from a selection of ocean communities who believe their methods are of high quality and candidates for best practices in their operational context. We thus used this resource to discover potential guidance in developing our recommendations. In total 75 documents are found with 56 being categorized as refereed (appendix 1, as of 7 March 2025). Among the 56 refereed, 13 were produced by the Alliance for Coastal Technologies (ACT), which serves as an unbiased, third-party testbed for evaluating coastal sensors and sensor platforms for use in coastal environments. A total of 15 are articles which were published in peer-reviewed journals. Ten documents are BGC-Argo guides and various updates of the Argo quality control manual for dissolved oxygen concentrations, the latest one by Bittig *et al* (2019) and a few articles related to air calibration of oxygen sensors on Argo profiling floats. IMOS (Integrated Marine Observing System), SOTS (Southern Ocean Time Series) and JERICHO-S3 (Joint European Research Infrastructure for Coastal Observatories-Science, Services, Sustainability) initiatives also contributed documents to this OBPS portal. The refereed documents comprise guidance on the various oxygen sensors from the following companies: RDO, Hach Hydrolab DS5X and HL4, Onset's HOBO U26, Aanderaa 3830/3930/3835, SeaBird SBE63, YSi Rapid Pulse, Greenspan Technology DO300/DO1200, XYLEM EXO2, SeaBird HydroCAT, Engineering miniDOT, *in situ* Troll 9000, and the Unisense STOX sensor.

When restricting the search to only documents being refereed and endorsed, three documents appear. Two endorsed by the GOOS, the OceanGliders Oxygen Standard Operating Procedures (SOP) v1.0.0. by López-García *et al* (2022) and the [OOI Biogeochemical Sensor Data Best Practices and User Guide. Version 1.1.1. by Palevsky \*et al\* \(2023\)](#). The third one is the International Organization for Standardization (1983) ISO 5813:1983. Water quality—Determination of dissolved oxygen—Iodometric method Edition 1. Manual being reviewed in 2023 (see: [www.iso.org/standard/11959.html](http://www.iso.org/standard/11959.html)). The two first documents and the publications on BGC-ARGO by Bittig *et al* (2018), Bittig *et al* (2019)) and Thierry *et al* (2021a, 2021b) constitute the seminal documentation for O<sub>2</sub> measurement recommended practices, with either electrochemical or optical sensors, including all platforms: ship-based, biogeochemical Argo profilers, gliders, moorings, benthic platforms, and underway systems. In addition, for the Winkler titration (Winkler 1888), the commonly used reference to calibrate the data provided by O<sub>2</sub> sensors, one may refer to the ISO

5813:1983 (1983), last reviewed and confirmed in 2023. One may add those listed in appendix 1 for ultra-low oxygen concentrations SOP (Revsbech *et al* 2009, Larsen *et al* 2016).

In addition to the SOP archived in the OBPS repository (appendix 1 as of 7 March 2025), appendix 2 provides additional SOP as an update to ARGO user's manual (Carval *et al* 2022) and Garcia-Robledo *et al* (2021) for an accurate determination of *in situ* O<sub>2</sub> concentrations in anoxic or near-anoxic waters.

RECOMMENDED PRACTICES USED—Responses from the ocean oxygen community

Box 1 presents the survey questions and answers that were sent to the GO<sub>2</sub>NE, GOOD, and UNESCO-IOC networks from April to November 2023 to collect knowledge on oxygen measurements, standard operating procedures and recommended practices within the community. A total of 92 experts from 36 countries all over the world answered with the majority of responses from government affiliated agencies and research laboratories. Responses indicate that coastal waters are the regions most sampled for oxygen as compared to the open ocean. The Atlantic (North and South) is best observed followed by the Pacific (North and South), the Indian Ocean and then the high latitudes (Arctic and Southern Ocean). Many oxygen data are also obtained in semi-enclosed seas such as the Mediterranean Sea, Baltic Sea, Black Sea and Caribbean Sea. CTD oxygen sensors along with classical Winkler titrations of samples from Niskin bottles remain the most frequently reported methods of acquiring oxygen data. Fixed moorings (surface, water column, benthic) represent the second most frequent method before Lagrangian platforms (Argo floats and gliders).

The most used SOP by respondents is the Winkler titration method, via the GO-SHIP Repeat Hydrography user Manual from Langdon (2010) with 40 submissions, then factory sensor calibration (15), the Argo manual (5), and other sources (Box 1). With respect to oxygen data storage, 35 answers indicate that data are stored in databases/data centers with full open access, 16 indicate that data are stored but not freely accessible, and 21 partly accessible. Overall, 45 answers point to the fact that many oxygen data are not complying with the FAIR principles. The survey is planned to be repeated every two years.

### 3. Recommended practices for metadata, data formats, and vocabularies

This section describes published recommended practices for O<sub>2</sub> metadata, data formats and vocabularies. We started searching on **Ocean Best Practices** for the *Dissolved oxygen metadata* and it yielded more than one thousand results over the 1972–2025

### Box 1- Survey list of questions and answers about oxygen measurements SOP and best practices

Name First name Affiliation Country email

Are you currently measuring dissolved oxygen in open ocean and/or coastal waters? Please select the ocean basin(s) and seas you are measuring dissolved oxygen in?

Which kind of platform are you using to measure dissolved oxygen?

Please provide the Standard Operating Procedure, Best Practices Reference describing the methodology you use for ocean oxygen measurements?

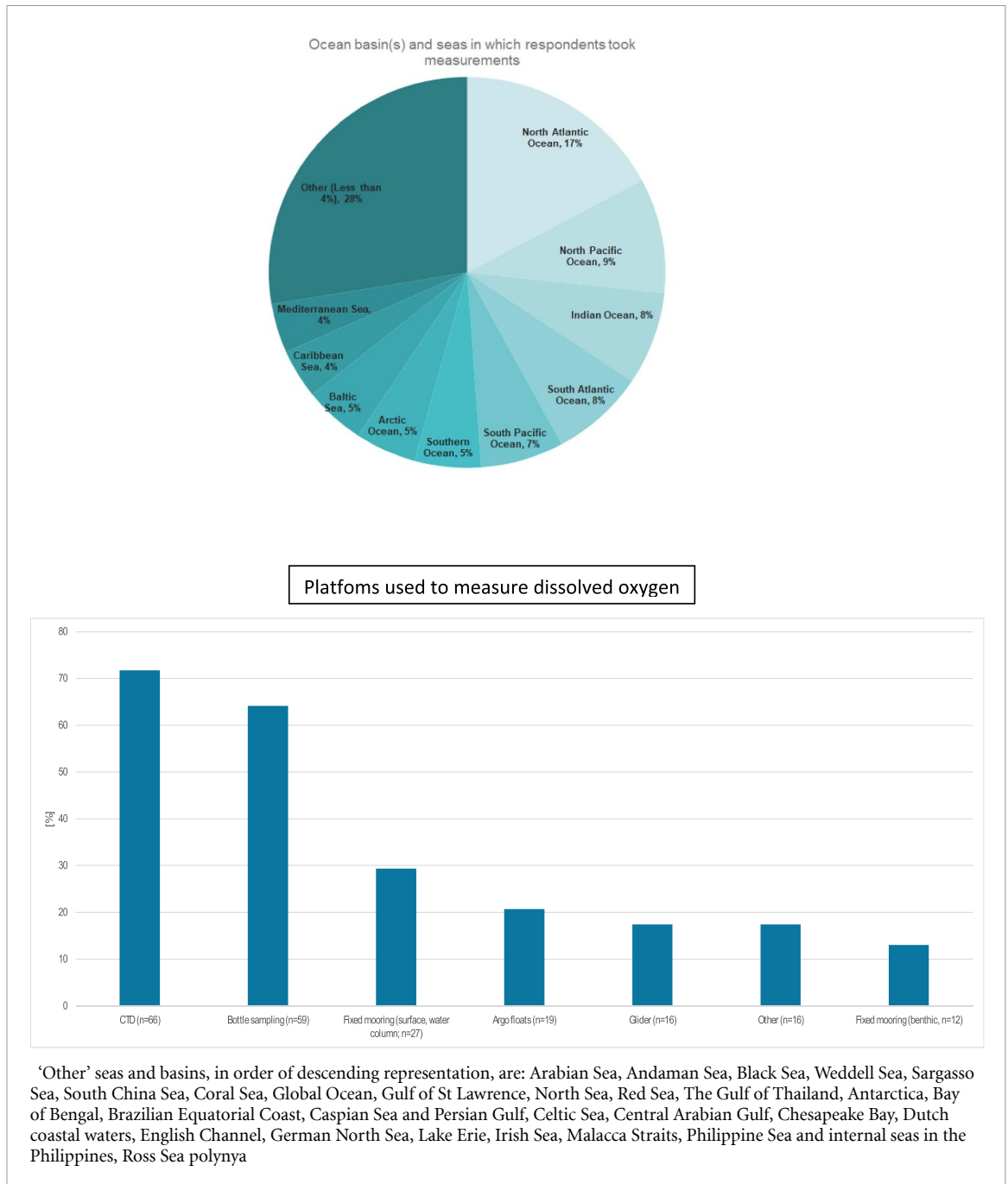
Are your ocean oxygen data stored in an institutional data base, National Oceanographic Data Centre, international or regional data centre? If you answered yes or partly to the question above, please provide the URL(s) to the respective data centre(s).



'Other' locations are: Cameroon, Italy, Mexico, Namibia, Norway, Peru, Portugal, Republic of Tanzania, Sweden, Thailand, Algeria, Argentina, Brazil, Bulgaria, Colombia, Georgia, Greece, Indonesia, Iran, Ireland, Malaysia, Morocco, Netherlands, Panama, Philippines, Qatar, Saudi Arabia, Uganda

(as of 29 May 2025) period. Restricting the search to 'refereed and endorsed' documents, the number of documents decreased but navigating the different metadata requirements in these repository documents remained still difficult. So in terms of content requirements, we constructed a set of properties that were inspired by the requirements of the Sustainable Development Goal (SDG) Indicator 14.3.1, for ocean acidification. As an SDG Indicator, this specification reflects the needs of the key, global consumer of ocean data for multilateral action. We thus adapted the 14.3.1 metadata sheet to ocean oxygen data for the proposed GO<sub>2</sub>DAT metadata requirements. This is indispensable for transparent quality controls (see <https://book.odis.org/thematics/variables/index.html> and figure 1). Further, the GO<sub>2</sub>DAT metadata content specification takes into account requirements from the Argo program, the WOD and EMODnet, described below.

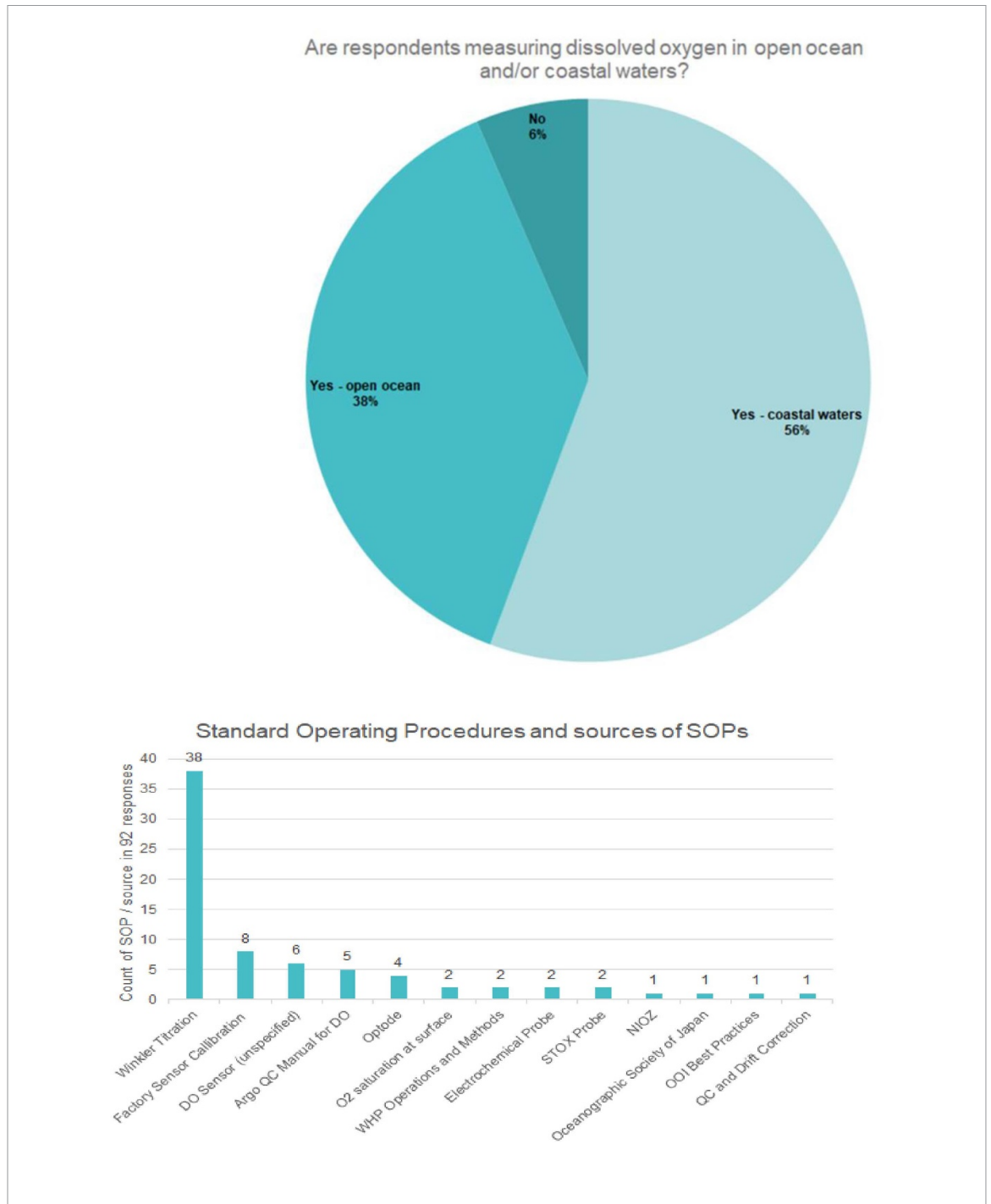
- The **BGC Argo community** provides a full set of documentation, encompassing recommended practices and metadata specifications. It is recommended to store any data transmitted by the O<sub>2</sub> sensor with meaningful names (in the form XXX\_DOXY), whatever the unit of the sensor output is, to account for later changes that may occur in the calibration/conversion equations used to convert the sensor output. The dissolved oxygen value in  $\mu\text{mol kg}^{-1}$  estimated from the telemetered variables and corrected for any pressure, salinity or temperature effects should also be stored in DOXY. Configurations for the calculation of DOXY are a function of the sensor model, sensor serial number, the set of calibration coefficients, and intermediate parameters. The recommended configurations (e.g. salinity compensation of MOLAR\_DOXY, correction for pressure on quenching, temperature compensation)



and thus the required metadata are available in the Processing Argo oxygen data at the national data center (DAC) level (Thierry *et al* 2021b) (<https://archimer.ifremer.fr/doc/00287/39795>), as recently updated in the Argo User’s Manual version 3.41.1 (Carval *et al* 2022). The accuracy and the resolution of the sensors are provided as partial pressure in units of hPa as suggested by Bittig *et al* (2018). Accuracy depends primarily on the individual calibration of the sensors, and on the proximity of calibration or reference data to the deployment. To allow the scientific use of DOXY data, an *in-situ* adjustment of DOXY (in real time (RT) or delayed mode) is crucial in order to correct O<sub>2</sub> sensitivity

drift (which can be in the order of several % per year when not deployed, Bittig *et al* (2018)). Data delivered and transmitted by the oxygen sensor have different units. The unit of the transmitted data that is directly related to the oxygen concentration is given in the SENSOR\_UNIT field (Thierry *et al* 2021b).

- **Ocean gliders** oxygen SOP (López-García *et al* 2022) should align with metadata requirements described in the documentation ‘Processing Argo oxygen data at the DAC level’ (Thierry *et al* 2021b, <https://archimer.ifremer.fr/doc/00287/39795>). Prior to deployment, all the required metadata should be sent ahead of the mission to the GDAC.



Before deployment, the glider should be well configured and intermediate parameters (phase measurements) should be sent in RT as well. This will allow first to check if dissolved oxygen values computed inside the glider are appropriate and allows the dissolved oxygen concentration to be recomputed using any updated method associated with the sensor model, intermediate parameters and calibration coefficients.

- **Moored Oxygen Optodes** recommended practices have been described by Miller *et al* (2024). Recommendations include conducting cal-dip casts with optodes attached to shipboard CTD

frame, as well as calibration casts with Winkler titrations after deployment and before recovery. Time and pressure dependent reversible drift is expected during deployment. An absolute accuracy of 1% or better can be achieved including in dynamic deep ocean environments such as the sub-polar North Atlantic only if rigorous best practices for calibration are conducted.

- Metadata being used in the **World Ocean Database (WOD)** can be found in Garcia *et al* (2024a). The World Ocean Atlas 2023 (WOA23) released in January 2024 (Garcia *et al* 2024b and <https://doi.org/10.25923/z885-h264>) includes oxygen,

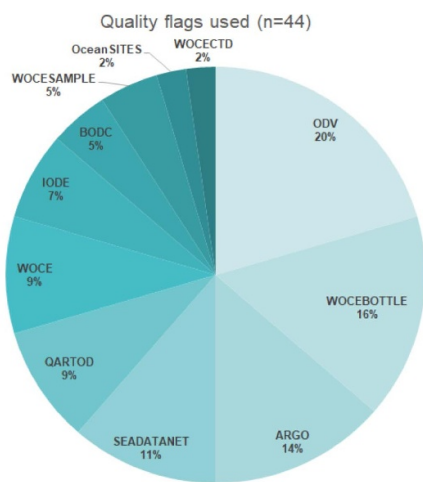
**Box 2 Survey answers on Quality control checks and flags specification**

**Do you conduct any quality checks before submitting the data to a data centre?**

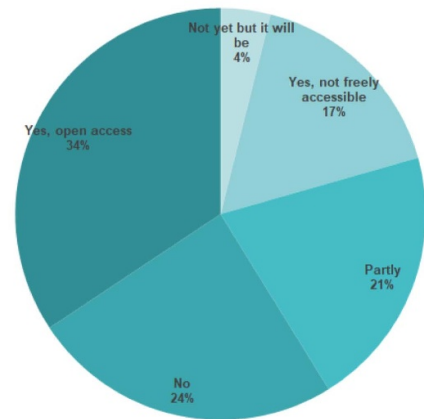
**If you answered yes to the previous question which quality checks do you conduct?**

**Please provide the reference(s) for the applied quality checks.**

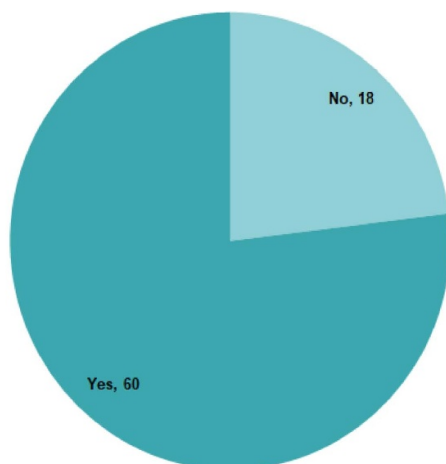
**In case relevant please let us know which type of quality flags do you use?**



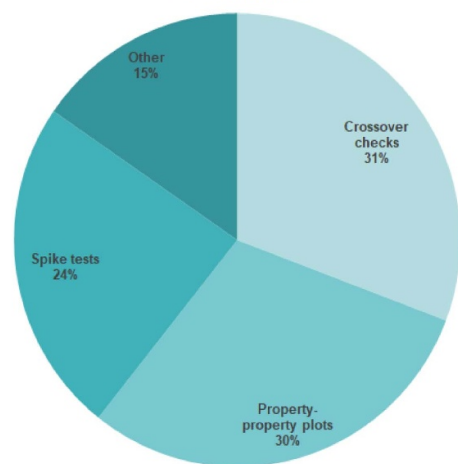
**Are respondents' data stored in an institutional data base, National Oceanographic Data Centre, international or regional data centre?**



**Are quality checks conducted before submitting the data to a data centre?**



**QC Conducted**



nutrients, density, conductivity, mixed layer depth, and bottom temperature, in addition to the temperature and salinity climatological fields. WOA23 includes approximately 2.4 million new oceanographic casts added to the WOD since WOA18's release, as well as renewed and updated quality control.

- The **Ocean Observatories Initiative (OOI) Biogeochemical (BGC) Sensor Data Best Practices and User Guide** available at <https://repository.oceanbestpractices.org/handle/11329/2112.2> also provides metadata specifications for both the Fast Response Dissolved oxygen (DOFST, contraction of DO FAST) instrument

manufactured by Sea-Bird Electronics, used to measure dissolved oxygen concentration usually on shallow coastal profilers through strong oxygen gradients, and the Stable Dissolved oxygen (DOSTA, contraction of DO STABLE) instrument manufactured by Aanderaa, used on mobile assets, deep profilers, and at fixed-depths on moorings. OOI has been focused on implementing the Gross Range and Climatology tests from Quality Assurance of Real Time Ocean Data (QARTOD) for all sensors. All of OOI data quality control procedures were designed with the goal of meeting the U.S. Integrated Ocean Observing System QARTOD quality control standards. As of March 2023, these tests have been implemented for CTD, pH, and pCO<sub>2</sub> sensors, with tests for dissolved oxygen and fluorometric chlorophyll sensors in process.

- **EMODnet Chemistry** (<https://emodnet.europa.eu/en/chemistry>) offers access to dissolved oxygen concentration data within its eutrophication portfolio covering six major European sea regions: the Arctic Ocean (Norwegian Sea including Barents Sea), Baltic Sea, Northeast Atlantic Ocean (Celtic Sea, Iberian coast and Bay of Biscay, and Macaronesia), North Sea, Black Sea, and Mediterranean Sea. EMODnet Chemistry uses SeaDataNet (SDN) infrastructure ([www.seadatanet.org/](http://www.seadatanet.org/)) for its technical set-up and adopts SDN standards for metadata (Partescano *et al* 2024, <https://doi.org/10.6092/e25b219f-b17d-411e-a0ee-e12db5685e23>) and common Vocabularies (i.e. standardized terms that cover a broad spectrum of disciplines) to allow consistency and interoperability ([www.seadatanet.org/Standards/Common-Vocabularies](http://www.seadatanet.org/Standards/Common-Vocabularies)).
- The **British Oceanographic Data Center** manages and updates all vocabularies used by EMODnet Chemistry (<https://vocab.seadatanet.org/search>). Lipizer *et al* (2022) in the EMODnet Phase V Updated guidelines for SDN ODV production Eutrophication & Contaminants give general recommendations for metadata and dataset preparation for all chemical variables including oxygen. They recommend the use of software (MIKADO, NEMO, OCTOPUS developed within SDN; ODV) to produce and check metadata and datasets which guarantee harmonization, standardization and interoperability of datasets ([www.seadatanet.org/Software](http://www.seadatanet.org/Software)).
- The **Institute of Atmospheric Physics** (IAP, Chinese Academy of Sciences) (Gourteski *et al* 2024) ([www.ocean.iap.ac.cn/](http://www.ocean.iap.ac.cn/)) provides global ocean temperature, salinity and oxygen *in situ* data before and after quality-control and bias-corrections. The data are sourced from WOD and other private data providers. The gridded analysis and time series for climate indicators are

also available. IAP dataset includes a set of oxygen metadata (location, date and time, type of sensor, model, adjustment/calibration, country, institute, platform (ID for instrument, ship name), and T/S if possible, which align well with those we adopted from the SDG 14.3.1 metadata sheet.

#### 4. Data quality control of oxygen observations and assessment, including flagging system

The discussion among in-person and online participants during the last GO<sub>2</sub>DAT workshop at UNESCO-IOC Headquarters in March 2023 clearly highlighted that GO<sub>2</sub>DAT does not start in a vacuum. Many efforts and experiences among the Steering Committee members of GO<sub>2</sub>DAT emphasized current good quality control practices for ocean oxygen data. We members of the GO<sub>2</sub>DAT SC highlighted the transparent QC/QF procedures and data accessibility efforts of the Argo and OceanGlider communities, as well as the IAP AutoQC system (Gourteski *et al* 2024) and IQuOD project and its associated testing of temperature and salinity data (Good *et al* 2023).

In the set of resources evaluated, WOD and EMODnet were identified as the primary archives/databases of interest here due to their large volumes of hosted data, and as being mandated or administered by the European Commission and the National Oceanic and Atmospheric Administration (NOAA) respectively. However, data quality control and flagging procedures differ across databases. Table 1 maps the flagging systems of WOD to those of EMODnet and Argo. This shows, for instance, that a QF of 0 is associated with passing all QC tests applied in WOD and with no quality control in EMODnet and Argo. QF of 1 and 2 are associated respectively with good data and probably good data in EMODnet and Argo and with questionable data in the WOD. WOD QC flags do not qualify data values as good or erroneous, they represent pass/fail of a quantifiable metric test or SME assessment (table 2). An ‘accepted’ cast/value means that it passed all tests. The observed data always reproduce the same originator data except for any unit conversion when necessary. All of the original data added to WOD are archived at NOAA NCEI enabling reproducibility of WOD. In addition to the WOD QC flags, WOD data retains the QC flags from the data originator if made available so the data user can select which data flags to use and/or to conduct their own QC assessment. In EMODnet the flagging is not exclusively linked to the objective criteria but regional expert judgment is also used.

These heterogeneous approaches and schemes to communicate QC are somewhat inevitable as systems developed independently, however it impedes the building of a consistent, interoperable oxygen data

**Table 1.** Comparison of the flagging system used in EMODnet, WOD and Argo ([https://odv.awi.de/fileadmin/user\\_upload/odv/docs/ODV\\_quality\\_flag\\_sets.pdf](https://odv.awi.de/fileadmin/user_upload/odv/docs/ODV_quality_flag_sets.pdf)). Numbers here only indicate the respective quality flag definitions of these three widely used oceanographic flagging schemes.

Flag description (EMODnet)	EMODnet	WOD	ARGO
No quality control	0	0	0
Good value	1	0	1
Probably good value	2	0	2
Probably bad value	3	4	3
Bad value	4	4	4
Changed value	5	0	5
Value below detection	6	0	0
Interpolated value	8	0	8
Missing value	9	0	9
Value phenomenon uncertain	A	0	0
Nominal value	B	0	0
Value below limit of quantification	Q	0	0
Flag description (WOD)	WOD	EMODnet	ARGO
Accepted value	0	1	1
Range outlier (outside of broad range check)	1	3	3
Failed inversion check	2	3	3
Failed gradient check	3	3	3
Observed level ‘bullseye’ flag and zero gradient check	4	3	3
Combined gradient and inversion checks	5	3	3
Failed range and inversion checks	6	4	4
Failed range and gradient checks	7	4	4
Failed range and questionable data checks	8	4	4
Failed range and combined gradient and inversion checks	9	4	4

**Table 2.** Definition of the WOD quality control flags. Reproduced from Garcia *et al* (2024a). CC BY 1.0. Public domain.

Flags on individual observations Depth flags	
Accepted value	0
Duplicates or inversions in recorded depth (same or less than previous depth)	1
Density inversion	2
Flags on individual observations Observed level flags	
Accepted value	0
Range outlier (outside of broad range check)	1
Failed inversion check	2
Failed gradient check	3
Observed level ‘bullseye’ flag and zero gradient check	4
Combined gradient and inversion checks	5
Failed range and inversion checks	6
Failed range and gradient checks	7
Failed range and questionable data checks	8
Failed range and combined gradient and inversion checks	9

system. However, this also shows the need for mediation functions within GO<sub>2</sub>DAT: as a community- and domain-specific system, GO<sub>2</sub>DAT’s partners can collaboratively develop mapping and conversion functions to generate generic quality metadata. Organizationally, GO<sub>2</sub>DAT can help the global ocean oxygen community coordinate with ODIS and other broader data federations to ensure this collective metadata is interoperable across other domains and communities.

GO<sub>2</sub>DAT aims to provide information on data uncertainty and, based on this, guidance on its appropriateness for a certain application. Uncertainty

may be derived from instrument precision, cross-over consistencies, or replicate measurements. The source of the uncertainty has to be provided in the metadata (figure 1) to fully inform the users about the data quality.

For the development of GO<sub>2</sub>DAT, the quality control system adopted by IAP (table 3) which refines the automated checks could serve as a base for implementing the GO<sub>2</sub>DAT QC/QF standards:

1. *Automated checks/tests*—based on the established ones. For instance, each test of the IAP AutoQC system is attributed a 0 (passed) or a 1 (failed) (0

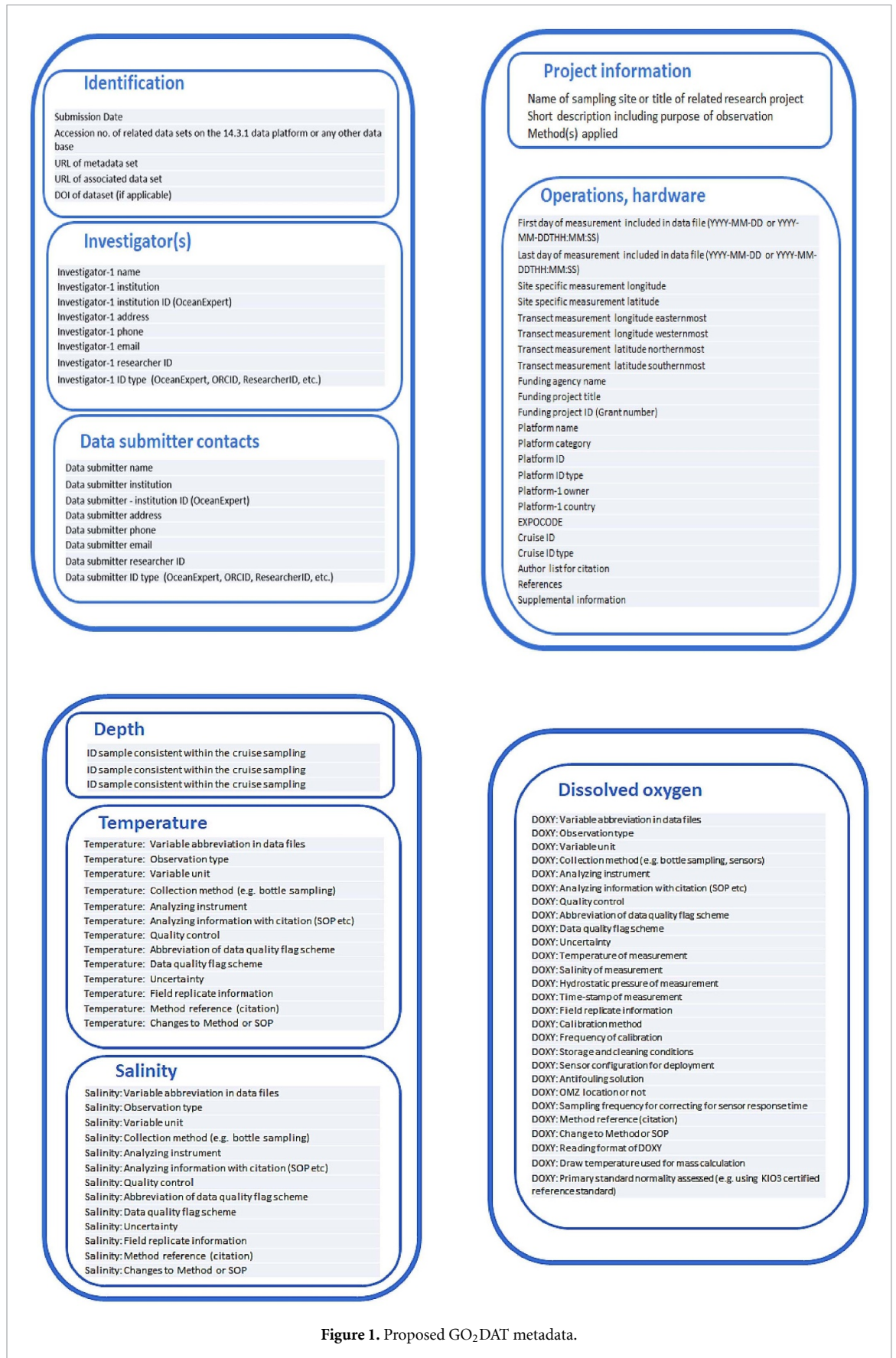


Figure 1. Proposed GO<sub>2</sub>DAT metadata.

**Table 3.** List of quality control checks adopted in the IAP dataset (Gourteski *et al* 2024). In the sequence of 9 checks, each test will be attributed a 0 (passed) or a 1 (failed) (0 and 1 are the quality flags). Reproduced from (Gourteski *et al* 2024). CC BY 4.0.

List of quality checks	
Automatic checking	1
Geographical location: position, platform, sensor, units, date.	
Format	
Duplicates	
Automatic checking	2
Range check (gross range 0–500 mol kg <sup>-1</sup> )	
Removal of any blunders	
Automatic checking	3
Crude range check (temperature/oxygen, oxygen/pressure)	
Removal of any blunders	
Automatic checking	4
Maximum solubility check	
Automatic checking	5
Stucked value check	
Automatic checking	6
Spike check	
Automatic checking	7
Multiple extrema checks (profile shape check)	
Automatic checking	8
Oxygen vertical gradient check	
Automatic checking	9
Local climatological range	

and 1 are the quality flags). They are carried out sequentially and if a test fails then an overall QC flag 1 is assigned but still the individual test results are visible to the data user.

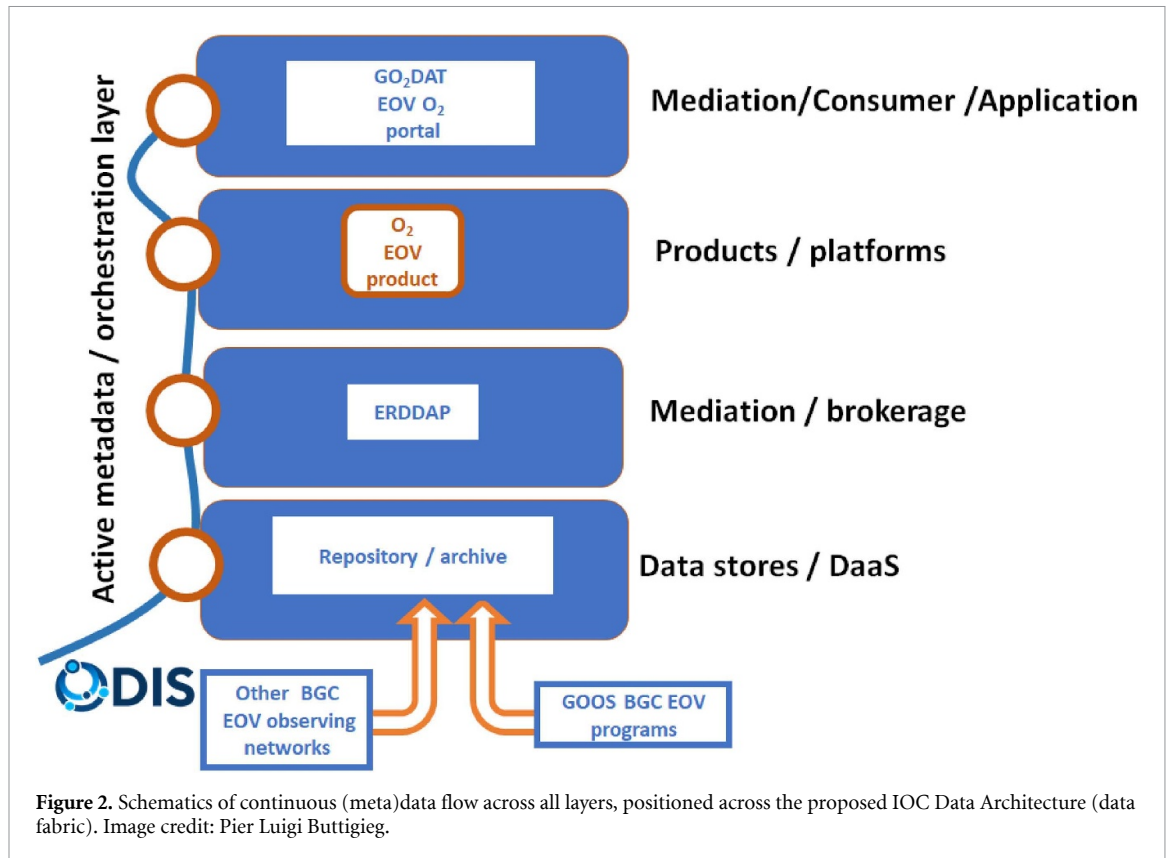
- [Expertized *Manual QC*]<sup>39</sup>. This should be highly recommended in impacted, heterogeneous coastal areas, as well as regional-scale analyses.
- Bias/Crossover checks*—based on Gourteski *et al* (2024).
- Uncertainty attribution*. This will be performed following the OSPAR's Joint Assessment & Monitoring Programme (JAMP OSPAR, JAMP 2011) guidelines for estimation of a measure for uncertainty in OSPAR monitoring. Uncertainties based either upon instrument precision, crossover consistencies, or replicate measurements, are not comparable. It will be crucial to collect precise information on precision (based on replicate measurements, indicated by the relative variability  $V_{dup}$  (JAMP OSPAR, 2011)) and on accuracy (based on fit with golden standard which could be e.g. GO-SHIP cruises). Note that the Argo program provides an uncertainty estimate for all real-time and delayed mode adjusted oxygen data

in the Argo database. These uncertainty estimates are updated based on standardized protocols based on calibration method, frequency of *in situ* calibration, and time lag, since data were inspected by human operators (Thierry, Bittig and the Argo-BGC team 2021a).

The following steps are envisioned (figure 2):

- Agree on a common minimum metadata requirements form for all oxygen observations.
- Translate the common metadata file into JSON-LD/[schema.org](https://schema.org) format which will be used to access and index all oxygen resources in ODIS and ODIS nodes—facilitated by the ODIS Team and the Clean and Healthy Ocean Integrated Programme (CHO-IP) to be recruited data engineer.
- Encourage a common process of each data provider/aggregator adding a JSON-LD snippet to the individual resource webpages—to be done by data managers with ODIS support. All resources are accessible centrally at the GO<sub>2</sub>DAT EOVS O<sub>2</sub> portal or the participating data centers. The data provenance and provider should stay visible throughout the process. The data submission system has to be sustainable, thus the decision was taken to collect the bulk of data via established data nodes (NODCs, ADUs, GDACs).

<sup>39</sup> Probably not applied due to high dependence on human and financial commitments.



4. A GO<sub>2</sub>DAT community is formed inside ODIS as a coalition of the willing from among those who agree to connect existing databases. The GO<sub>2</sub>DAT Steering Committee is playing that role. This could include mutual archival of resources, creating regional DACs with healthy redundancy.
5. QC/QF—This is proposed in section 4 above and will be part of the common metadata requirements sheet. ERDDAP<sup>TM</sup> can be used to get all data in the same format, but not for e.g. unit conversions, flag mapping so the final data harmonization service is still missing. Implementation of structured metadata, controlled vocabulary, and utilization of ERDDAP<sup>TM</sup> does not always equal harmonized data. Writing codes/programs that can automatically provide that harmonization service is needed.
6. Once all oxygen resources can be pulled together through ODIS, the visualization, Atlas, can be implemented. This will be achieved within the EU BioGeoSea proposal (2025–2028).

Following data discovery and data harmonization, the next step is data aggregation and distribution, achievable through the GOOS ERDDAP<sup>TM</sup> and ERDDAP<sup>TM</sup> from other observing networks from individual/corporate end-users. It will be mandatory to give feedback to the data providers regarding quality issues and to ensure that known uncertainties accompany each observation.

## 5. Discussion and conclusion

GO<sub>2</sub>DAT will transform our understanding of the oxygen cycle by: (1) making ocean oxygen data of known quality accessible to all scientists and thereby, (2) greatly increasing the use of ocean oxygen data to understand the connection between oxygen loss, climate change, and ocean and human health, (3) provisioning high quality and consistent information for all stakeholders and decision makers to inform and take action on limiting dead zones and open ocean deoxygenation (4) opening new avenues to use the ocean sustainably, contributing to a sustainable economy by expanding practices of co-design with stakeholders to better monitor and protect the ocean.

The development of GO<sub>2</sub>DAT requires human resources and engagement from the community of scientists, data managers, data providers and data users, and also a clear roadmap for guaranteeing the sustainability of GO<sub>2</sub>DAT. The GO<sub>2</sub>DAT Steering Committee draws on the expertise of this community to define and implement GO<sub>2</sub>DAT standards, and recommended practices for achieving these standards, to guide the sustainable measurement and management of ocean oxygen data. These standards include: standard operating procedures and recommended practices for sampling and calibration, guidance on fit-for-purpose metadata specification, quality control, and assignment of quality flags. Based on these recommendations, metadata requirements for

ocean oxygen data for GO<sub>2</sub>DAT will then be determined and any uncertainties in sampling or recording attributed, allowing data users to make informed decisions on what data to include in the course of their work, e.g. where data may be used for warning of coastal hypoxia vs climatological use.

Data will be made available via the development of the GO<sub>2</sub>DAT EOVS O<sub>2</sub> portal and visualized in the Atlas (to be described separately). The development of this digital hub will include tasks such as advancing and developing tools and procedures to facilitate data ingestion, database interoperability, and procedures to standardize metadata definition and quality control. These tasks will be facilitated by emplacing GO<sub>2</sub>DAT as an ODIS node under the OceanData2030 framework, a catalyst for maturing the ocean digital ecosystem.

The objective here is not to establish a new database but rather a federated system within the new IOC data fabric architecture. ODIS will link all oxygen data nodes through a JSON-LD + schema.org based, decentralized, interoperable architecture. The ultimate goal is to collaborate with existing database providers to ensure the reproducibility of ocean oxygen content in the ocean and to minimize the current underestimation of deoxygenation in the ocean by models assessed by the IPCC.

We conducted a survey to globally map the methods/platforms/oceanic areas sampled/data QC/QF procedures being used for oxygen measurements on a routine basis. The accuracy of a questionnaire depends on the quality of questions chosen and distributed to the respondents, namely, structured versus open questions, instructions with the survey questionnaire, short and concise questions, unbiased questions, responses to pilot testing, limitations of both response and non-response bias, unbiased and representative sampling of the respondent population from a statistical point of view, and assessment of the clarity and transparency of the reporting of the survey results. We have tried in our approach to comply as much as possible with the previously cited protocols.

The results of the survey indicated the following. Coastal waters are those most commonly observed, Eulerian platforms are most commonly used, with CTD-O<sub>2</sub> sensors and/or classical Winkler titration performed on samples from Niskin bottles, and from fixed moorings. The Winkler titration method, with the GO-SHIP Repeat Hydrography user Manual (Langdon 2010) (see section 2) constitutes the most commonly used SOP. With respect to oxygen data storage, only a third of respondents indicated that data are stored in databases/centers with full open access. A large majority of respondents conduct quality checks before submitting oxygen data to

a data center with classical QC such as crossover checks, property/property plots, and spike tests (see section 4).

This analysis showed clearly the crucial need for making all ocean oxygen data fully accessible to achieve the OceanData2030 objectives. This confirms results by Garçon *et al* (2019) which showed that Eastern Boundary Systems, typically exhibit a highly heterogeneous, often as yet insufficient, level of readiness concerning data management and information, as assessed following the 3rd pillar of the Framework for Ocean Observing (FOO, 2012).

Open ocean observations such as those collected by Argo profiling floats usually obey the FAIR principles whereas measurements performed in the coastal ocean comply less often with these principles. The lack of clear community-adopted standard procedures and recommended practices for data methods and QC might be a barrier to releasing and integrating data for many coastal regions. The recently approved Global Environment Facility CHO-IP on hypoxia and eutrophication will only be successful in supporting countries to develop monitoring capacities and contribute to global ocean oxygen observations if clear guidance on recommended practices for oxygen measurement and related data management is given to reinforce their communities as data providers and users.

Our international approach, although it nicely fits within the IOC digital infrastructure development efforts, might probably suffer from a few limitations stemming from methodological, technical and logistical constraints. One first constraint is data accessibility. Indeed several coastal low oxygen zones are found in EEZ waters of a few countries and it is critical to include oxygen data collected in these EEZs. Presently, some countries are reluctant in sharing data collected within their EEZs. Our initiative has been endorsed by the Member states at the 2025 IOC Assembly so hopefully awareness of the importance of EEZ data sharing should alleviate the restrictions imposed by national authorities in order to comply with the FAIR principles (Accessible). Getting all ODIS nodes agree on metadata, QC/QF, and uncertainty attribution on data observations remains a challenge. Again the international approach will facilitate this task. Technically, the developing efforts progress rapidly and our approach will be performed in full synergy with the VLIZ team engaged in the building of this IOC digital infrastructure. The GO<sub>2</sub>DAT steering committee includes representatives from the WOD, WOA, EMODnet, IOCCP, GLODAP, Argo, IAP database, and CMEMS, and it will, according to its Terms of Reference, alleviate the constraints of alignment on metadata, QC/QF, and uncertainty attribution.


## Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

## Acknowledgments

We thank the Global Ocean Oxygen Network (GO<sub>2</sub>NE) expert working group of the Intergovernmental Oceanographic Commission of UNESCO (IOC-UNESCO) and its secretariat for supporting this work. IOCCP has also been instrumental in supporting this action under the Global Ocean Observing System (GOOS). The authors acknowledge funding from the United States National Science Foundation (Grant No. OCE-2513154) to the Scientific Committee on Oceanic Research (SCOR, United States) for the International Ocean Carbon Coordination Project (IOCCP). VG, MT, TT and MG are supported by the BioGeoSea project funded from the European Union's Horizon Europe research and innovation programme under Grant Agreement No. 101216427.

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## List of appendices

Appendix 1: List of ‘EOV Oxygen’ documents from OBPS repository (as of 7 March 2025)

Appendix 2: List of ‘EOV Oxygen’ best practices documents not referenced in the OBPS repository (as of 7 March 2025)

### Appendix 1: List of ‘EOV Oxygen’ documents from OBPS repository (as of 7 March 2025)

‘Refereed’ according to OBPS are indicated in bold italics

**Orange color** indicates the NOAA-funded Alliance for Coastal Technologies (ACT) documents

**Red color** indicates documents produced by oceanographic consortia such as Argo, OceanGliders, SOTS, IMDOS, JERICHO-S3

**Blue color** indicates peer-reviewed articles in journals

Black color indicates all other sorts of documents

\*\* indicates being refereed and GOOS endorsed according to OBPS

The two refereed and GOOS endorsed documents (Lopez-Garcia *et al* 2022 and Palevsky *et al* 2023) and the publications on BGC-ARGO by Bittig *et al*

(2018), (2019) and Thierry *et al* (2018a), (2018b) would constitute the seminal documentation for O<sub>2</sub> measurement best practices, with either electrochemical or optical sensors, including all different platforms: ship-based, biogeochemical Argo profilers, gliders, moorings, benthic platforms, and underway systems. They are highlighted by an orange rectangle. For measurements of ultra-low oxygen concentrations, one may refer to Revsbech *et al* (2009) and Larsen *et al* (2016), also highlighted by an orange rectangle. In addition, for the Winkler titration (Winkler 1888), the commonly used reference to calibrate the data provided by O<sub>2</sub> sensors, one may refer to the International Organization for Standardization (1983) ISO 5813:1983, last reviewed and confirmed in 2023.

### Alphabetical order per color category.

Aanderaa Data Instruments AS (2018) Aanderaa Oxygen Optodes: Best Practices for Maintaining High Data Quality. Bergen, Norway, Aanderaa Data Instruments AS, 28pp. DOI: <http://dx.doi.org/10.25607/OBP-868>

CalCOFI (2014) Dissolved oxygen. LaJolla, CA, California Cooperative Oceanic Fisheries Investigation, 5pp. DOI: <http://dx.doi.org/10.25607/OBP-1593>

Cervantes, D. (2020) Rosette water sampling R/V Dr. Fridtjof Nansen. Bergen, Norway, institute of Marine Research, 11pp. DOI: <http://dx.doi.org/10.25607/OBP-1752>

Cervantes, D. (2020) R/V Dr. Fridtjof Nansen Video Series: Collecting dissolved oxygen samples from a CTD rosette water sampler. Bergen, Norway, Institute of Marine Research for the EAF-Nansen Programme of the FAO, 4.23 mins (Video mp4). DOI: <http://dx.doi.org/10.25607/OBP-1788>

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