

Title: Towards best practices for Measuring and Archiving Stable Isotopes in Seawater

Acronym: MASIS:

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Co-chairs:

Gilles Reverdin, LOCEAN, France
Email: Gilles.reverdin@locean.ipsl.fr

Antje Voelker, IPMA, Portugal
Email: antje.voelker@ipma.pt

Summary/abstract

The stable isotopic composition of seawater and the carbon isotopic composition of dissolved inorganic carbon are essential ocean tracers that have been widely measured since the 1960s. They are particularly important to measure well in times of wide-spread changes in the hydrological cycle, the bio-geochemical cycles, as well as the anthropogenic carbon penetration and induced acidification of the oceans, because they serve as a fingerprint of these ongoing changes. However, substantial issues of data collection, quality control, and compilation exist: common reference materials in seawater are not widely available, analysis methods have strongly diversified, regular intercomparison exercises are lacking, and as a result, large differences exist between different data sets. These differences currently prohibit the community from making full use of the potential of stable isotopes to identify climatic changes.

This working group is dedicated to remedying the current issues of data collection, quality control, and compilation of stable isotopes in seawater. First, we will assess the validation stage of the available stable isotopic datasets, as well as corresponding metadata. This effort will lead to a report of best practices from sample collection to measurement and quality control. Second, we will review current methods of bias adjustment in archives and make recommendations for the future to standardize these bias adjustments. Third, we will work towards complementing existing databases, with particular effort on surface ocean sampling data. In parallel with the aforementioned efforts, the working group will promote intercomparison exercises, and will actively carry out capacity-building.

1. Scientific background/rationale

Seawater stable isotopic composition (the $^{18}\text{O}/^{16}\text{O}$ and $^2\text{H}/^1\text{H}$ ratios expressed as $\delta^{18}\text{O}$ and $\delta^2\text{H}$ in ‰ versus VSMOW), and the carbon isotopic composition ($^{13}\text{C}/^{12}\text{C}$ expressed as $\delta^{13}\text{C}$ in ‰ versus VPDB) of dissolved inorganic carbon (DIC) have been widely measured since the 1960s, thanks to the use of mass spectrometry techniques that could be operated in well-equipped spectrometric laboratories, and required moderate volumes of water (on the order of 1-100 ml). These are the most commonly measured isotopic properties in seawater and its dissolved constituents, and both are classified as EOVC/ECVs (Essential Ocean/Climate Variables) by GOOS, CLIVAR, and IODE (UNESCO). There are important scientific reasons to first tackle those constituents, but we expect that the recommendations that will be made on the acquisition, quality control, and data assembly for these parameters will be relevant for a wider range of other isotopic measurements.

Stable seawater isotopes ($\delta^{18}\text{O}$ and $\delta^2\text{H}$) are used to investigate the water cycle, and to trace sources of freshwater (precipitation, evaporation, runoff, melting glaciers, sea ice formation and melting), both at the ocean surface and in the ocean interior (Schmidt et al., 2007; Hilaire-Marcel et al., 2021). Except for fractionation during phase changes, the water isotopic composition is nearly conservative in the ocean. Although there is limited global sampling - despite the GEOTRACES campaigns -, a major emphasis is on high latitude oceanography, where continental (or iceberg) glacial melt, formation or melt of sea ice, and high-latitude river inputs (for the Arctic) leave different imprints on the seawater isotopic composition. Seawater isotopes in the upper ocean at low latitudes are also vital for coral and paleoclimatic studies, as they are needed to calibrate proxies of past ocean variability in marine carbonate records such as corals and foraminifera (e.g., PAGES CoralHydro2k working group; Konecky et al., 2020). Seawater isotopes in the surface ocean can also be used to characterize evaporation rates and air-sea interactions (Benetti et al., 2017, Conroy et al., 2014, 2017). In contrast, there have been fewer studies on the isotopic signature in the deep ocean (e.g., Prasanna et al., 2015). Seawater isotopes are also important tracers in the coastal ocean, as different isotopic signatures are imprinted by evaporation, rain, or major river inputs (e.g., Amazon) (Karr and Showers, 2002). The isotopic signatures of these different sources are evolving in our warming world, which will imprint on the seawater isotopic composition (Oppo et al., 2007).

The isotopic composition of dissolved inorganic carbon (referred to as $\delta^{13}\text{C}$ -DIC) is measured to characterize biological processes associated with fractionation during biomass fixation, as well as remineralisation of organic matter (for those, these data are complementary to DIC, total alkalinity, inorganic nutrients). Modern ocean data is also used to ground truth isotopic signals in carbonate shelled organisms (e.g., benthic foraminifera shells; Schmittner et al., 2017). Finally, it is often measured to estimate the anthropogenic carbon penetration in the ocean, due to the $\delta^{13}\text{C}$ lowering related to anthropogenic carbon emissions (the so-called Suess effect) (Eide et al., 2017). This can yield an estimation of the ocean storage of anthropogenic carbon (Quay et al., 2003, 2017).

Earlier syntheses have been done such as the GISS Global Seawater Oxygen-18 Database for stable seawater isotopes (LeGrande and Schmidt, 2006), and the Global Ocean Data Analysis Project (GLODAP) (Olsen et al., 2016, 2020) for the biogeochemistry observations collected

during selected oceanographic research cruises. These syntheses have been used for validating modelling studies in which these parameters are explicit diagnostic variables (e.g., Roche and Caley, 2013; Schmittner et al., 2013, Kwon et al., 2022, Brady et al., 2019). A major update on a $\delta^{18}\text{O}$ ($\delta^2\text{H}$) seawater database is currently underway from the CoralHydro2k project, with a focus on the tropics and subtropics (35°N-35°S; deLong et al., 2022).

An optimal data accuracy on the order of 0.05 ‰ for $\delta^{18}\text{O}$ (0.25‰ for $\delta^2\text{H}$) and 0.03‰ for $\delta^{13}\text{C}$ is required to get the full benefit of these data sets. This accuracy is a demanding task, but not out of reach, as specific data studies suggest (for $\delta^{13}\text{C}$ -DIC, Humphreys et al., 2016; for water isotopes, Haumann et al., 2019).

However, in practice, this accuracy is currently not reached in many cases for three main reasons:

1: For both sets of variables, there are issues with internal standards and reference material (RM) used in the laboratories. For the seawater isotopes, a seawater RM is not available, and biases originating from sea salt are likely to happen, which depend on instrumentation and analysis methods. For $\delta^{13}\text{C}$ -DIC, there is no internationally-recognized liquid seawater RM. There have been attempts to run intercomparison studies with the same sample shared between different laboratories. For water isotopes, this is regularly organized by IAEA (WICO tests (Wassenaar et al., 2021), but with focus on fresh water samples), whereas, for $\delta^{13}\text{C}$ -DIC, it is not regularly done, although there has been a recent intercomparison exercise (Cheng et al., 2019). In both instances, the comparisons revealed a large spread of values between the different participants, suggesting systematic offsets between laboratories.

2: For both sets of variables, other analysis techniques than traditional mass spectrometry have recently spread, in particular cavity ring-down spectroscopy (CRDS) (Walker et al., 2016; Su et al., 2019). These new techniques, previously used for measurements in the atmosphere and in fresh water, are easy to implement in small laboratories, but present challenges, in particular due to the effect of salt deposits (for seawater isotopes), memory effects, and the stability and accuracy of the standards and RM. These instruments can also be used in a continuous way, for example on surface water during cruises, and there too, the accuracy of the data is not always precisely assessed (Friedrichs et al., 2010; Becker et al., 2012; Munksgaard et al., 2012; Bass et al., 2014). Because such instruments can be easily implemented with limited expertise, required documentation and metadata is not always available, limiting their use for comparisons and data-model integrations.

3: For both sets of variables, constructing earlier syntheses implied checking for biases, and adjusting subsets of data (Schmidt et al., 1999; Becker et al., 2016; Schmittner et al., 2017). However, this was not done comprehensively, and large biases/errors remain in subsets of the current databases, limiting their potential use. These databases are currently missing much of the data collected since the year 2000, and thousands of samples are now analysed each year in an increasing number of laboratories, with only a portion of the data making its way to GEOTRACES, GO-SHIP, GLODAP and other international archives. The new CoralHydro2k database illustrates the wide variety of archiving methods researchers now use to store their seawater isotope data, including publications, student theses, data repositories, cruise reports, and internal reports, each being associated with varying levels of metadata.

Of the many new data sets that are now available, only a few have been carefully inter-calibrated, checked, and assessed, e.g., for seawater isotopes at LOCEAN (Reverdin et al., 2022) or the ACE archive (Haumann et al., 2019). The validation of the LOCEAN database covering more than two decades revealed issues of sample contamination during collection and storage. It also illustrated the difficulty of properly flagging and quality controlling such data, as well as assessing uncertainties (Reverdin et al., 2022). Issues were also identified due to long sample storage, and poor conservation of samples or internal water standards prior to analyses. Recommendations exist in that respect (Terzer-Wassmuth & Wassenaar, 2021; McNichol et al., 2010), although they might not be widely followed. It is imperative that proper metadata are collected to be able to assess these issues.

2. Terms of reference (ToR)

1. Assess the existing best practices and standard measurement procedures, including new techniques such as CRDS, and identify reference materials (liaise with IAEA for water isotopes and the Ocean Carbon & Biogeochemistry (OCB) working group for carbon isotopes in the ocean).
2. Assess which data and metadata on stable isotopes in seawater are stored, what is their status of validation/ qualification, and how and where they can be recovered and accessed. Establish a unified standard of data distribution (metadata and data) that allows an effective quality control to be shared between producers and scientific users.
3. Organise intercalibration exercises. Subdivide large volumes of deep and surface seawater from different programmed cruises into subsamples to be distributed to a large set of laboratories using different measurement techniques, and in different oceanic regions.
4. Assess methods (Quality Control/Quality Assessment) to evaluate the accuracy of already available data, such as comparing different data subsets in the same region, using derived properties such as d-excess, or the $\delta^{13}\text{C}$ -DIC relationship, and estimating the internal consistency of the global or regional databases.
5. Report on the results/outcome/perspectives at international conferences and in publications and actively promote capacity building through four workshops and exchange visits in order to widely disseminate the new international standards co-constructed in MASIS for producing and reporting high quality seawater isotope measurements (**Tor 1-4**). This is expected to lead to the merging of different data sets into a global database allowing for long awaited synthesis and modelling studies.

3. Working plan

During year 1 (2024), we will organize four online meetings to design a detailed action plan with a schedule and timeline for activities and deliverables, assign tasks and responsibilities to WG members, prepare workshops and venues to communicate with a wider community, and examine how capacity building can be reinforced. For this, we will establish four different sub-groups: (i) one on data production/acquisition, reference materials used, which will examine metadata available for the different datasets (**ToRs 1-2**), (ii) one on the intercalibration exercises (**ToR 3**), (iii) one on methods of qualification/validation of the data, including error assessments, and data distribution and archiving (**ToR 4**), (IV) one on communication and capacity building (**ToR 5**). At the start of the WG, we will set up an online communication forum to facilitate active interacting and sharing of data and validation tools. Most sub-groups will remain active till year 3 (Fig. 1).

A wide-ranging workshop could be run in parallel to an AGU fall meeting (2024) or OS (2025) in a hybrid mode (on site + remote) to facilitate the access to a wide user community, as well as to provide a continuation to the meeting organized by the US OCB-sponsored working group on ‘Carbon isotopes in the ocean’ (McNichol et al., 2021), and to the PAGES CoralHydro2k-piloted update of the seawater isotopes database. A similar workshop could be run in parallel to the EGU meeting (2024 or 2025, Vienna), with a link to IAEA. We will also organize two regional workshops (venues to be decided) in years 2 (2025) and 3 (2026), one in India (Bangalore) with focus on the South-Asian communities, and one in Brazil, to better interact with scientists in South America and South Africa, by potentially liaising with the All-Atlantic Alliance (AANChOR) which fosters collaboration between states neighbouring the Atlantic Ocean. The regional workshops are key for capacity building, and could also be ways to practically share some of the water samples of the intercomparison exercises.

In addition to organizing meetings and fostering shared activities with the wider research community, the working group will carry out the following tasks, with required interactions between the different sub-working groups that will be managed by online meetings.

ToR 1, year 1: Review the existing best practices and standard operating procedures, and liaise with IAEA and OCB working group on carbon isotopes in the ocean.

ToR 1, years 2-3: Work on a white paper and companion publication on data production, validation/qualification, and data distribution (list best practises and Standard Operating Procedures). We will adopt the Ocean Best Practices platform (OBP, <https://www.oceanbestpractices.org/>; cf also <https://exchange-format.readthedocs.io/en/latest/>) as the repository for these.

ToR 2, years 1- 3. Investigate datasets or metadata that would complement the current databases, both for water stable isotopes and $\delta^{13}\text{C}$ -DIC. The largest effort will be for the period since 2000, and for continuously acquired measurements. Special attention will be devoted to measurements from surface monitoring projects, noting for example that for $\delta^{13}\text{C}$ -DIC, their data are currently not included in GLODAP, and that for water isotopes, some metadata are still lacking in the CoralHydro2k database. We will thus establish an inventory of what is available, where, and whether the metadata are complete or can be complemented. We will also define quality flags to be attributed to the different datasets or different versions of the same data set (we will for example investigate whether GEOTRACES

flags can be adopted; also see <https://exchange-format.readthedocs.io/en/latest/>). The inventory will be shared with groups producing the databases/sets.

ToR 3, year 1-2: Intercalibration exercises. Collect a large volume of seawater from different programmed cruises (e.g., GO-SHIP) to be subdivided into several subsamples to be distributed to different laboratories using the different methods. Those samples will be from the 'deep' ocean, but also from the surface ocean to provide a range of values. This intercomparison could be done regionally, to lessen logistical issues, but also with a few core institutions that will participate in all regional intercomparisons. Samples will be distributed during meetings and/or shipped to participants, who will fund the respective analyses themselves. A limited exercise has already been initiated in 2022 with 9 participants, in order to better evaluate the challenges of the intercomparison effort.

ToR 3, year 3: Analyse and report results of the intercalibration experiments (including all the metadata) and produce a statistical summary of these.

ToR 4, years 1-2: Review and test existing statistical techniques to identify biases or errors, and estimate required adjustments in the databases. For example, two datasets that partially overlap in time and geographical coverage (e.g., surface Atlantic Ocean) have been identified as test cases to check methods. Identify what is required to link validation and quality flagging of data sets already archived in data centres, such as PANGAEA, or as part of data products such as GLODAPv2 (Olsen et al., 2020) with the original data/metadata. Define which other measured (auxiliary) parameters are required for the validation. Estimate whether the stable isotopic data are correctly cross-referenced with the other relevant data set/databases; this will thus require to liaise with efforts done for the UN Ocean Decade, e.g. the World Ocean Database Programme (WODP) and in particular IODE (cf. <https://catalogue.odis.org>), GEOTRACES, and potentially with the European Marine Observation and Data Network (EMODnet), NCEI and other regional/national centres for Chemistry and/or Physics.

ToR 4, years 2-3: An outcome of this effort might be to propose a unified standard of data distribution (metadata and data), and propose ways to implement the validation methods to check internal consistency of updated or newly produced data sets.

ToR 5, year 1 to 3: Starting in the 2nd semester of year 1, we will present our results and perspectives at international conferences and workshops. Reports and publications arising from the different ToRs (see deliverables, Fig. 1) will be finalized during years 2-3. Furthermore, as detailed in Section 5, we will organize lectures, workshops and procure funding to enable other capacity building activities, in particular for early career scientists.

Figure 1: Timelines for ToR and some related deliverables

ToR#	ToR related tasks	YEAR 1 - 2024			YEAR 2 - 2025			YEAR 3 - 2026			Deliverables
		1	2	3	1	2	3	1	2	3	
1	A) Assess the existing best practices and standard measurement procedures	█									
1	B) White paper and referred publication										Publication reporting on best practices
2	Assess metadata availability and Establish a unified standard of data distribution										doi referenced publication and data set
3	A) Intercalibration exercises (sample collection and analyses)										doi referenced data set
3	B) Statistical analysis and reporting of the intercalibration experiment results										Publication on outcomes of intercalibration exercises
4	Quality Control/Quality Assessment to evaluate the data accuracy and databases										Paper with recommendations on error and bias detection
5	A) Communication of working group outcomes										Webpage, conference presentations, and publications
5	B) Capacity Building										Lectures, specified workshop, potentially exchange visits

4. Deliverables

1. A publication summarizing the best practices, from sample collection to analysis and data qualification/validation (**ToR 1**).
2. A doi-referenced data paper identifying orphan stable isotopic datasets, corresponding metadata and dissemination requirements (**ToR 2**) and issuing recommendations on how 'orphan' isotopic data can be distributed (e.g., surface $\delta^{13}\text{C}$ -DIC data sets).
3. A publication reporting the data and statistical analyses of the intercomparison exercises (water isotopes and $\delta^{13}\text{C}$ -DIC) (**ToR 3**).
4. A methodological paper with recommendations on error and bias detection as well as on the adjustments that could be proposed to databases (**ToR 4**).
5. An assessment report of new data products, examining sources of data errors and proposed adjustments to be applied (**ToR 4**). The data products will not be produced by the working group, but the proposed adjustments will be communicated to the managers of the data products, as well as through proper identification to the originators of the data to update the associated metadata in repositories. This is not designed to be exhaustive, but hopefully will help dimension long-term validation effort to be carried out.
6. Archiving the data collected and validated within the working group (**ToR 2, 3**), together with metadata/quality flags, in the respective databases (e.g., GLODAP).
7. Contribute to capacity building (**ToR 5**) by developing lectures on the use of seawater stable isotopes and MASIS outcomes/recommendations to reach the wider scientific community and organizing a workshop to explain best practices to early career scientists.

5. Capacity building

It will be key to integrate stakeholders who will outlast the working group, and to promote the transfer of analytical techniques/expertise to other teams and countries than the traditional data providers (until 2000, largely in Europe/North America/Japan/Australia). In addition to the important role that the members of the working group will play in their own countries, we have also established informal contacts in Chile. We expect that the regional meetings will be opportunities to establish contacts and promote the use of seawater isotopes for environmental monitoring and marine science in countries outside the 'member countries'. Contacts shall be established by inviting scientists from the country hosting a regional meeting and from neighbouring countries, benefiting from networks in Africa and South America established under AANChOR activities and focusing on early career scientists. In Brazil, the recent introduction of state-of-the-art small research vessels holds great potential for fostering knowledge acquisition in the oceanographic community, creating a favorable environment for international cooperation. In Columbia, the scientists executing the annual monitoring along sections in the Caribbean Sea and Pacific Ocean are interested

in adding stable water isotope and/or $\delta^{13}\text{C}$ -DIC to the parameters to be analyzed. We, therefore, plan to conduct at least one dedicated workshop in South America (in Brazil), with the hope to better liaise regionally with the different stakeholders.

Other workshop opportunities, such as in southern or eastern Asia are also being considered. As discussed last year, future AANChOR activities should include exchanges of scientists from south to north and south to south (in the Atlantic Ocean realm) and we hope to exploit such funding possibilities to train early career scientists. We will also explore national funding options, e.g., DAAD exchange grants in Germany, or JSPS Invitational Fellowships for Research in Japan, and approach philanthropies interested in ocean-related research (e.g., Minderoo Foundation, Waitt Foundation, Rev Ocean) and ask if they would be willing to financially support such capacity building efforts, in particular exchange visits.

In addition, we aim to give lectures to disseminate the aims of SCOR, the use of seawater isotopes in general and the outcome of the working group either in person or through video conferencing, in order to reach university groups, institutes etc. on a more global scale. One or more working group members becoming SCOR visiting scholars would be the ideal option to allow for in person presentations in South (and Latin) America and in Africa or other countries. In addition, public lectures to the wider scientific community in the country hosting the regional MASIS WG workshop (e.g., India and Brazil) will be given by 1-2 working group members, concurrent with the workshop. We, furthermore, aim to hold a training course on sampling techniques and isotope analysis in conjunction with the regional workshops or one of the large meetings/conferences. For instance, the Regional Graduation Network in Oceanography in Namibia offers a good framework to contribute a course block on stable isotope analysis to a summer school. Finally, we will explore the possibility to provide talks given during such capacity building opportunities as lectures to the e-learning platform of the Ocean Teacher Global Academy (<https://classroom.oceanteacher.org/>), making use of the different languages spoken by working group members.

Organizing meeting sessions associated to, or shouldering large international meetings (e.g., the 15th International Conference on Paleoceanography in Bangalore (India) in 2025), is a way to enhance the outreach of the working group into user communities. Connections will be established with users of different communities a) the paleoclimate community (such as the PAGES 2k network; those working on the hydrological cycle using speleothems (e.g., PAGES SISAL working group), or stable isotopes in biomarkers) and b) the modeling community (especially groups working on the carbon cycle/biogeochemistry and the hydrological cycle). Both Arctic and Antarctic Ocean researchers often include stable isotopes in seawater as tools, in a very inter-disciplinary context, with observations both in the ocean, the sea ice or on the continents. We will also seek connections with these communities. For this task, and for more general advice and help in promoting the working group, we have established a list of other experts in the field, that will be contacted. As such the already started intercalibration exercise (funded by the participating scientists/labs), includes researchers that, for reasons of SCOR working group member number limitations, cannot be official members of the MASIS working group, but will contribute to the outcomes of the group.

Although meetings are expected to structure the activity and provide a good means to reach the main goals of the capacity building, it is hoped that other means can help too, such as a discussion forum and/or an interactive website. In addition, spreading the word on the outcome of the working group will be done by publishing short articles in the PAGES newsletter and in EOS.

To further promote the best practices, we will explore the possibilities to promote them on national levels, such as updating laboratory's web information with links to best practices and laboratory protocols, as well as recommendation to users on how they should report their datasets (e.g., with which metadata). In addition, we will investigate how to promote the existence of a single community information and communication platform, which could become an active and lively evolving site.

Finally, the results of ToR1 and the future capacity to produce marine data of high quality is dependent on the availability of relevant primary standard and reference materials. The group will actively promote the production of such materials.

6. Working Group composition

Full Members

Name	Gender	Place of work	Expertise relevant to proposal
Gilles Reverdin (co-Chair)	M	LOCEAN, Paris, France gilles.reverdin@locean.ipsl.fr	Physical oceanographer, interested in recent climate variability, the hydrological cycle, air-sea exchanges, oceanic carbon. Long-time involvement in the observation of the ocean, with experience in stable isotopes research (both sea water stable isotopes and $\delta^{13}\text{C-DIC}$).
Antje Voelker (co-Chair)	F	IPMA, Lisbon, Portugal antje.voelker@ipma.pt	Paleoclimatologist with interest in proxies of past and recent climate variability. Study of stable isotopes in seawater to trace water masses and circulation changes, and to calibrate paleo-climate proxies.
F. Alexander Haumann	M	AWI, Bremerhaven, Germany alexander.haumann@awi.de Early career scientist	Oceanographer with research on air-sea-ice interactions, in particular in the Southern Ocean, and their impact on ocean circulation and water mass changes. Experience in qualification/validation stable sea water isotopes (ACE expedition).
Andre Luiz Belem	M	UFF, Rio de Janeiro, Brasil andrebelem@id.uff.br	Physical oceanography, with analysis of exchanges between the coastal regions with the deep

			ocean. Use of stable isotopes as tracers of water masses and ocean processes.
Alyssa Atwood	F	Florida State University, Tallahassee, USA aatwood@fsu.edu	Tropical paleo-climatologist spanning the fields of oceanography, atmospheric science, and geochemistry. Use of geochemical data and climate models. Co-lead of the CoralHydro2k $\delta^{18}\text{O}$ ($\delta^2\text{H}$) Database Project and organizing committee member of PAGES 2k Phase 4.
Eun Young Kwon	F	Pusan University, Pusan, South Korea ekwon957@pusan.ac.kr	Expert on ocean variability at interannual to interdecadal time scales, with foci on water masses, penetration of ocean carbon, data assimilation and modeling. Interest in stable isotopes in seawater.
Fajin Chen	M	Guangdong Ocean University, Zhanjiang, China fjchen@gdou.edu.cn	Expertise on coastal oceanography and on river inputs to the coastal ocean. Experienced in $\delta^{13}\text{C}$ -DIC and water stable isotope measurements.
Juan Muglia	M	Centro para el Estudio de los Sistemas Marinos, CONICET, Argentina jmuglia@cenpat- conicet.gob.ar Early career scientist	Modelling $\delta^{13}\text{C}$ in the modern and past ocean to infer circulation changes. Experience in data base building.
Supriya Karapurkar	F	NIO, Goa, India supriya@nio.org	Strong experience in IRMS measurements of seawater samples and on seawater isotope data from the Indian Ocean.
Helen Bostock	F	Univ. Queensland, Australia h.bostock@uq.edu.au	Oceanography and paleo-oceanography with focus on ocean circulation. Use of water stable isotopes and participating in ongoing intercalibration exercise.

Associate Member

Name	Gender	Place of work	Expertise relevant to proposal
Ulysses Ninnemann	M	UiB, Bjerkness Center, Bergen, Norway ulysses.ninnemann@uib.no	Interest in climate variability past and present, including investigation of water isotopes. Works with mass spectrometers and IRMS spectrometers, and participates in ongoing intercalibration exercise.

Douglas Wallace	M	Dalhousie University, Nova Scotia, Canada douglas.wallace@dal.ca	Ocean chemistry and geochemistry, with particular North Atlantic and transient tracers focuses. Extensive experience with CRDS measurements and inter-comparison exercises, both for stable water isotopes and $\delta^{13}\text{C}$ -DIC.
Anita Flohr	F	NOC, Southampton, United Kingdom anita.flohr@noc.ac.uk Early career scientist	Biogeochemist with interest in ocean carbon and ocean $\delta^{13}\text{C}$ -DIC. Experienced in CRDS measurements.
Leonard I. Wassenaar	M	Danube University Krems, Austria len.wassenaar@wcl.ac.at	Large experience at IAEA in inter-comparison exercises, IRMS, CRDS measurements of water isotopes, and influence of seawater composition on the measurements.
Liping Zhou	M	Peking University, China lpzhou@pku.edu.cn	Specialist of past and present climate variability, using water isotopes in the present climate for calibration of proxies and to trace water masses. PAGES, GEOTRACES member; participating in ongoing intercalibration exercise.
Luisa Espinosa	F	INVEMAR, Colombia Luisa.Espinosa@invemar.org.co	Chemistry of coastal sea waters, in charge of tropical Atlantic and Pacific Colombian coastal waters monitoring. Aiming to incorporate seawater isotopes into the monitoring.
Prosenjit Ghosh	M	IISC, Bangalore, India pghosh@iisc.ac.in	Geochemist with ocean, atmosphere and land experience, with an oceanic focus on the Bay of Bengal and Southern Ocean (carbon cycling and relationship with the hydrological cycle). Link with the 'Future earth' program.
Sarah Fawcett	F	Univ Cape Town, South Africa sarah.fawcett@uct.ac.za	Biogeochemical oceanographer, interested in stable isotopes in the ocean, particularly in nitrogen, and recently also including water stable isotopes. Liaise with the Southern Ocean Observing System (SOOS) committee

Roberta Hansman	F	NOSAMS, WHOI, USA rhansman@whoi.edu	Mass spectrometry. Biogeochemist, with interest in tracing carbon in the ocean (both using radio-isotopes and stable isotopes).
Shigeru Aoki	M	Hokudai University, Sapporo, Japan shigeru@lowtem.hokudai.ac.jp	Oceanography expert in ocean variability in particular in the Southern Ocean, air-sea-ice interaction and water mass changes. Experienced in IRMS and CRDS measurements of stable water isotopes.

7. Working Group contributions

Gilles Reverdin is producing water stable isotope and $\delta^{13}\text{C}$ -DIC data from the global ocean for more than two decades and has participated in previous small-scale intercalibration exercises. He is very much aware of essential metadata missing in existing isotope data bases that hamper quality-based comparisons between data themselves and data and model outputs.

Antje Voelker studies the distribution of water stable isotopes and $\delta^{13}\text{C}$ -DIC in North Atlantic waters since 2010 and spearheads the intercalibration exercise started in 2022, besides her paleoceanographic research interests. She contributes to GEOTRACES and PAGES working group efforts and provided input to the All Atlantic Data Space (AA-DATA2030) Road Map document (AANCHOR pilot action).

F. Alexander Haumann, who is building a unified isotope database for the Southern Ocean, was recently awarded an ERC Starting Grant, the VERTEXSO project, which will study vertical transport processes in observations and model simulations, including for carbon exchange.

Andre L. Belem combines modern ocean stable isotope work with paleoceanographic studies, which provide some of the “end user” subjects for the working group outcomes. He aims to use a Python software and updated $\delta^{18}\text{O}$ data bases to calculate calcification depths for the interpretation of planktonic foraminifera $\delta^{18}\text{O}$ data.

Alyssa Atwood leads the CoralHydro2k effort to release an updated and greatly expanded seawater $\delta^{18}\text{O}$ database in 2023 and provides her insights gained from that exercise to the group. She studies the role of the tropics in the global climate system in the past and present, pairing reconstructions with modern observations and climate model simulations.

Eun Young Kwon is both a biogeochemist, and oceanographer and a climatologist with data analysis and modelling skills, which will offer a perspective on what are the requirements on data sets accuracy, homogeneity, as well as respective coverage in the coastal and open ocean.

Fajin Chen, a coastal oceanographer, has expertise in complex environments with river inputs characterised by often large sedimentary load and dissolved and particulate organic matter, presenting specific challenges.

Juan Muglia, an ocean paleo-climatologist, has large modelling expertise on $\delta^{13}\text{C}$ -DIC in the modern and past ocean to infer ocean circulation changes. He was a member of the PAGES OC3 working group and build the recently published database on $\delta^{13}\text{C}$ data of the last 23 thousand years.

Supriya Karapurkar, who has lots of experience in different techniques of IRMS analysis, is responsible for the IRMS facility in the Chemical Oceanography department at CSIR-NIO and is performing the water isotope analyses for the northern Indian Ocean samples collected by her colleagues and her. Thus, she provides knowledge in the IRMS methods and in Indian Ocean stable isotope distribution to the working group.

Helen Bostock recently established a laboratory to analyse stable isotopes in seawater samples, bringing that type of analyses back to Australia. She studies present and past changes in ocean chemistry to reconstruct ocean circulation and its relationship to global climate, with focus on the southwest Pacific and Southern Ocean.

8. Relationship to other international programs and SCOR Working groups

The general approach and some objectives of the MASIS working group (WG) are similar to the ones of past SCOR WG 147 “Towards comparability of global oceanic nutrient data (COMPONUT)”. The seawater stable isotope data to be tackled by the MASIS WG are classified as EOJ/ECVs by international programs such as GOOS, GO-SHIP, CLIVAR, and IODE (UNESCO). They are complementary to DIC, total alkalinity, inorganic nutrients, which is reflected in the inclusion of $\delta^{13}\text{C}$ -DIC data in the GLODAP products and the planned inclusion of stable isotope data in the biogeochemistry section of the IMBeR-OFI Marine Data Hub (IMBeR is a SCOR project). They are also listed among the parameters that should be measured along GEOTRACES (SCOR project) transects, although this has happened only for a few transects. Besides their linkage to nutrient cycling, a topic of SOLAS Core Theme 1, $\delta^{13}\text{C}$ -DIC data can be used to trace the intrusion of anthropogenic carbon into the deeper ocean, providing a link to ocean acidification studies. Thus, the outcomes from MASIS regarding quality control, essential metadata and statistical error margins arising from the intercalibration exercise shall be highly relevant for the Integrated Ocean Carbon Research (IOC-R) programme, an Intergovernmental Oceanographic Commission WG with links to IMBeR and SOLAS. On more regional scales, providing such information for all three stable isotopes will also be helpful for studies done under the umbrella of the ‘Southern Ocean Action Plan 2021-2030’ (defined with contributions of IMBeR’s ICED regional programme). MASIS outcomes and recommendations will also be highly relevant, if analysing seawater isotope data and $\delta^{13}\text{C}$ -DIC were included in future monitoring efforts, such as within IMBeR’s regional program on Sustained Indian Ocean Biogeochemistry and Ecosystem Research (SIBER), or the Joint IMBeR/Future Earth Coasts Continental Margins Working Group (CMWG), in particular within the Chinese marginal seas.

On the side of “end users” of modern ocean $\delta^{18}\text{O}$ and $\delta^{13}\text{C}$ -DIC data in the paleoclimate and modelling communities, strong links exist with the CLIVAR water isotopes WG and the PAGES 2k Phase 4 program, in particular the CoralHydro2k WG, which is currently producing the CoralHydro2k $\delta^{18}\text{O}$ ($\delta^2\text{H}$) database, and its sister WG Iso2k. Potential links, especially if involving modelling of the hydrological cycle and isotopic changes in moisture source regions, could also exist with PAGES WG SISAL (Speleothem Isotopes Synthesis and Analysis) and the ice core research community. Seawater isotope data are used to provide model boundary conditions and assess model performance and skill in isotope-enabled Earth system models (e.g., Schmidt et al., 2007; Brady et al., 2019; Cauquoin et al., 2019), thereby improving climate model projections of the future. On national levels, there exist (paleo)climate modelling efforts that use modern ocean water isotope or $\delta^{13}\text{C}$ -DIC data for model validation (e.g., Roche and Caley, 2013; Cauquoin et al., 2019; Kwon et al., 2021; Liu et al., 2021) and will profit from a quality assessment of the existing data.

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