FY 2023 – Progress Report Global Carbon Data Management and Synthesis Project

PMEL Cover Sheet

Period of Activity: 01 October 2022 - 30 September 2023

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FY 2023 – Progress Report Global Carbon Data Management and Synthesis Project AOML Cover Sheet

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FY2023 Annual Report [Global Data Management and Synthesis Project] Page 2 of 30

Global Data Management and Synthesis Project

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Table of Contents

Global Data Management and Synthesis Project		
1. Project Summary	4	
1.1. Project justification	4	
1.2. Project overview	4	
2. Scientific and Observing System Accomplishments	6	
2.1. Surface ocean pCO_2 measurements	7	
2.1.1. SOCAT	7	
2.1.2. Moored pCO_2 network	10	
2.1.3. SOCOM and RECCAP2	11	
2.1.4. Production of seasonal air-sea CO_2 flux maps	12	
2.1.5. Global Carbon Project (GCP) assessment	13	
2.2. Ocean interior synthesis	13	
2.2.1. Quality control of data from recent cruises	13	
2.2.2. Global Data Analysis Project v2 updates	14	
2.2.3. Anthropogenic carbon storage and concentration estimates	14	
2.2.4. Ocean carbonate system inter-comparison	19	
2.3. BAMS State of the Climate report	21	
2.4. Collaborations		
2.5. Performance measures	21	
3. Outreach and Education	22	
4. Publications and Reports		
4.1. Grant funded publications	23	
4.1.1. Publications by Principal Investigators	23	
4.1.2. Publications by Principal Investigators in preparation	24	
4.2. Related publications	24	
4.3. All Cited publications	24	
5. Data and Publication Sharing	28	
6. Project Highlight Slides		

1. Project Summary

1.1. Project justification

Over the past two and a half centuries, the surface oceans have absorbed approximately 30% of humankind's carbon dioxide (CO₂) emissions (Prentice et al. 2001; Canadell et al. 2007; Le Quéré et al. 2009). Ocean CO₂ uptake has reduced the accumulation of greenhouse gases in the atmosphere and slowed the rate of climate change (IPCC 2019; Sabine and Feely 2007; Feely et al. 2012; Gruber et al. 2019). The current consensus measurements-based estimate of ocean uptake for 2022 is 2.8 ± 0.4 Pg C (Friedlingstein et al. 2023).¹ This estimate gets updated annually, in part with data and synthesis products from this project. When anthropogenic CO_2 is absorbed by seawater chemical reactions occur that reduce both seawater pH and the concentration of carbonate ions in a process known as "ocean acidification." The pH of surface ocean waters has decreased by about 0.11 units since the beginning of the industrial revolution (Feely et al. 2009; Jiang et al. 2019), and it is continuing to decrease at a rate of 0.0021 ± 0.0007 year⁻¹ (Woosley et al. 2016). Questions remain regarding the details, mechanisms, feedbacks, and consequences of ocean carbon uptake and acidification. Continued monitoring and scientific analysis of the ocean carbon cycle is critical for understanding how this important sink for anthropogenic CO₂ is functioning; how ocean carbon storage might change in the future; and how we can best anticipate, mitigate, and adapt to potential future changes.

Carbon data synthesis is essential for monitoring ocean carbon uptake due to the global scale of uptake, the complexities of interpreting ocean carbon measurements, and the variety of ways carbon content is measured. Measurement programs from numerous participating nations contribute measurements of many different aspects of seawater chemistry made with a wide variety of sensors and analytical techniques. Data from these diverse measurements are ultimately used with Earth system model assessments, data-assimilating models, forecasts, property budgets, and measurement inversions designed to address scientific questions related to ocean carbon uptake. A common element of all of these analyses is that they benefit from consistently-formatted and quality-controlled ocean carbon measurements with well-constrained uncertainties. Data synthesis is therefore necessary to translate the wealth of information provided by the measurement community into the quality controlled and assessed data products needed for advancing and communicating global carbon cycle science.

1.2. Project overview

The global ocean carbon Data Management and Synthesis Project (DMSP) exists to provide resources and leadership to efficiently address the ocean carbon data needs of the global scientific community, decision makers, and the public. DMSP scientists are also charged with conducting original ocean carbon cycle research. DMSP investigator tasks include:

- 1. measuring ocean carbon;
- 2. quality controlling ocean carbon data;
- 3. providing ocean carbon data in common, convenient, and accessible formats;
- 4. assessing ocean carbon data uncertainty;
- 5. interpreting ocean carbon data;
- 6. and communicating relevant findings to decision makers and the broader public.

¹ Global Carbon Budget 2023 https://doi.org/10.5194/essd-15-5301-2023

FY2023 Annual Report [Global Data Management and Synthesis Project]

The DMSP brings together ocean carbon measurement and information technology experts from the Atlantic Oceanographic and Meteorological Laboratory (AOML) and the Pacific Marine Environmental Laboratory (PMEL). These scientists work closely with data managers at the National Center of Environmental Information (NCEI) and the CLIVAR and Carbon Hydrographic Data Office (CCHDO) to address the oceanographic community's carbon data access and synthesis needs. The DMSP prioritizes workup and analysis of data obtained through efforts funded by the Global Ocean Monitoring and Observation (GOMO) including the Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP), the partial pressure of CO₂ (pCO_2) on ships of opportunity effort (SOOP-CO₂), and the pCO_2 on moorings effort. Appreciable efforts are also made to incorporate data from other investigators worldwide. Investigators in the DMSP are leaders in design, automation, and quality control of the annual Surface Ocean Carbon Atlas release (SOCAT), and contributed to a surface water fCO₂ data collation that provide an updated monthly climatology centered on 2010 following the procedures of the Takahashi group at Lamont-Doherty Earth Observatory (Fay et al. 2023, submitted). Data synthesis efforts are aimed at addressing the core questions as described in the US Carbon Cycle Science Plan (Michalak et al. 2009):

1. Where has the anthropogenic carbon (i.e. carbon produced by human activities) entered the ocean?

2. ... and where is it stored?

3. How are these patterns of uptake and storage changing?

4. How is ocean carbon uptake impacting marine inorganic carbon chemistry?

The DMSP aims to quantify global anthropogenic CO_2 storage to within 2 Pg C decade⁻¹ and regional sea-air CO_2 fluxes to within 0.2 Pg C year⁻¹. The DMSP pursues this goal directly through original research, and indirectly by developing educational programs, methods, datasets, and data products to aid research efforts by the broader scientific community. DMSP scientists engage in additional outreach and educational programs tailored to the broader public with the goal of informing the public of significant advances in understanding the role of the ocean in climate.

Transparency and accessibility are critical for DMSP research, data, and data products. Data and data products are made available online at CCHDO², NCEI³, the AOML/PMEL⁴ institutional websites, and elsewhere⁵. Quality controlled data are not currently provided in real-time due to the need for post-measurement calibration and data quality control and synthesis, but an automated near-real-time data check, reduction and QC program for surface water CO₂ measurements is pursued in collaboration with investigators at the Ocean Thematic Center (OTC) of ICOS. Instead, preliminary data and finalized data are provided following timetables specified by guidelines of the measurement programs. Once submitted, data and data products are continually updated and archived, and efforts have been made to verify these websites are providing up-to-date versions. This has led to significant improvements in delivery time and quality control of the GOMO-sponsored underway and repeat hydrography data. Data use

² <u>http://cchdo.ucsd.edu/</u>

³ https://www.ncei.noaa.gov/products/ocean-carbon-acidification-data-system

⁴ <u>https://www.aoml.noaa.gov/ocd/ocdweb/occ.html</u> and <u>http://www.pmel.noaa.gov/</u> ⁵ <u>https://www.glodap.info/</u> and <u>https://www.socat.info/</u>

FY2023 Annual Report [Global Data Management and Synthesis Project]

statistics and bibliographies are kept by the US Repeat-Hydro and GO-SHIP.⁶ Acknowledgement of GOMO/NOAA and NSF funding is made on the front page of the CCHDO website. Publications, that include GOMO fund reference

http://data.crossref.org/fundingdata/funder/10.13039/100018302, can be found online for both AOML and PMEL⁷.

2. Scientific and Observing System Accomplishments

DMSP scientists contributed to several notable advances in carbon data synthesis in FY-23. These DMSP accomplishments directly enhance the COD deliverable of providing continuous instrumental records for global analyses of ocean carbon uptake and content. These major accomplishments include:

- an annual release of SOCAT, the Surface Ocean Carbon Atlas;
- improvements to the automation of the SOCAT data submission, quality control, and use-tracking;
- Sea-air CO₂ flux maps (including efforts in updating monthly climatologies and modeling) (Fay et al. 2023, submitted);
- contributions to the 2023 Global Carbon Budget⁸ (Friedlingstein et al. 2023);
- continued routine interior carbon measurement processing and synthesis (Müller et al. 2023);
- continued research into methods for filling in gaps in existing measurements;
- involvement in the Global Ocean Data Analysis Project version 2 (GLODAPv2.2023)⁹ semi-annual update process (Lauvset et al. *submitted*);
- contributions to the Bulletin of the American Meteorological Society annual State of the Climate report (SoC BAMS) (Wanninkhof et al. 2023).
- and participation in the second Regional Carbon Cycle Assessment and Processes (RECCAP2) carbon data synthesis effort¹⁰ (DeVries et al. 2023; Perez et al. 2023, submitted, Ishii et al., *in prep*).

Synthesis activities by the AOML¹¹ and PMEL¹² ocean carbon groups are discussed together due to the close working relationships maintained for and through this effort. Synthesis activities for surface ocean fCO_2 measurements (made from moorings, and underway measurements) and for ocean interior measurements (made on hydrographic cruises) are discussed separately from one another because these measurements are processed in different ways and typically used to answer different questions: Surface fCO_2 measurements are primarily used to determine where carbon enters the ocean through determination of the air-sea CO_2 fluxes (question 1 from section 1.2) and carbon measurements from repeat hydrography are primarily used to determine where in the ocean carbon resides and accumulates (question 2). The difference between ocean carbon uptake and storage results from the redistribution of carbon by interior ocean mixing and biogeochemical cycling. Reconciling these two approaches is a goal of the GOMO carbon

⁶ <u>oco.noaa.gov/resources/Progress_Reports/FY13/Swift_CCHDO_FY13_ProgressReport.pdf</u>

⁷ http://www.aoml.noaa.gov/publications/ and pmel.noaa.gov/public/pmel/publications-search/

⁸ http://www.globalcarbonproject.org/index.htm

⁹ https://www.glodap.info/

¹⁰ <u>https://www.globalcarbonproject.org/reccap/</u>

¹¹ http://www.aoml.noaa.gov/ocd/ocdweb/occ.html

¹² <u>http://www.pmel.noaa.gov/co2/</u>

FY2023 Annual Report [Global Data Management and Synthesis Project]

efforts. Doing so requires an up-scaling of the flux results over a decade and improving our understanding of interior ocean and lateral land-ocean carbon transports. Recent papers with DMSP scientist contributions (Gruber et al. 2019) assesses global changes in anthropogenic carbon inventory from 1994-2007, and 1994-2014, respectively, using data obtained on hydrographic cruises and methods introduced in DMSP-led research (Carter et al. 2017) and are the first major global updates on anthropogenic CO₂ changes in the ocean since the seminal paper of (Sabine et al. 2004). This is a good example of how this data synthesis effort has been able to use components of the GOMO-funded observing systems to address key issues. Continued collaborations aimed at refining and assessing the observational record produced by the Southern Ocean Carbon and Climate Observations and Modeling (SOCCOM) program and the growing Global Ocean Biogeochemical Argo (GO-BGC) program are providing insights into how to link the questions of air-sea flux and storage. The biogeochemical floats deployed by the SOCCOM and GO-BGC efforts provide both the interior measurements required to quantify storage changes and the frequent and broadly-distributed surface measurements required to assess air-sea fluxes. DMSP scientists are actively involved in assessing the capacity of this novel observing system for meeting DMSP objectives (Williams et al. 2017; Carter et al. 2018, 2021).

2.1. Surface ocean pCO₂ measurements

The ocean absorbs carbon from the atmosphere where the atmospheric fCO_2 exceeds ocean fCO_2 , and releases carbon to the atmosphere where the reverse is true. Sea surface fCO_2 measurements are therefore critical for determining the spatial and temporal patterns of ocean CO_2 uptake. Ocean fCO_2 measurements are made on buoys and other sensor platforms such as wind-propelled autonomous surface vehicles (ASVs) (e.g., Saildrones), Ships of Opportunity (SOOP-CO₂), including research ships. DMSP scientists work to gather fCO_2 observations into global datasets, quality control and assess fCO_2 measurements, improve the routines used to estimate air-sea CO_2 flux from air-sea fCO_2 differences, improve the relationships used to estimate fCO_2 from satellite measurements, and use the combined quality-controlled products for original science. Data are posted on publicly-accessible websites^{13,14}. Data and metadata are also sent to the NCEI¹⁵ and SOCAT databases (Bakker et al. 2016; Pfeil et al. 2013).

2.1.1. SOCAT

The Surface Ocean CO_2 Atlas (SOCAT)¹⁶ is a quality controlled, global surface ocean carbon dioxide (CO₂) data set compiled from data gathered on research vessels, SOOP, buoys, and now Saildrones. SOCAT is comprehensive; it draws together and applies uniform QC procedures to all such observations made across the international community. It is extensively used as input for machine learning approaches to create air-sea CO_2 flux maps and in model comparisons. Previous releases occurred in 2011, 2013, and annually in June since 2015 (Bakker et al., 2014, 2016a, 2016b, 2017, 2018, 2019, 2020, 2021, 2022, 2023¹⁷).

¹³ <u>http://www.aoml.noaa.gov/ocd/ocdweb/occ.html</u>

¹⁴ pmel.noaa.gov/co2/story/Volunteer+Observing+Ships+%28VOS%29

¹⁵ https://www.ncei.noaa.gov/access/ocean-carbon-data-system/oceans/

¹⁶ <u>https://www.socat.info/</u>

¹⁷ https://socat.info/wp-content/uploads/2023/06/2023_Poster_SOCATv2023_release.pdf

With over 35.6 million surface CO₂ observations and 7449 datasets (e.g., cruise tracks, Saildrone tracks, and mooring deployments), including 333 new or updated submissions, SOCATv2023¹⁸ spans from 1957 to 2023. Figure 2.1a shows a global snapshot of the newly-added data and the full version 2023 collection. In addition to the 2nd-level quality controlled, global surface ocean fCO₂ (fugacity of CO₂) cruise data collection, SOCAT also produces gridded summary fields on 1° x 1° (open ocean) and ¹/₄° x ¹/₄° (coastal) resolutions. The SOCAT data products are archived with data citations (DOIs) provided at both Pangaea and NCEI. For the v2023 release, it was ensured that NOAA data received NOAA DOIs through NCEI OCADS, and not additional DOIs from Pangaea.



Figure 2.1. SOCAT v2023 data collection accessed through the SOCAT Live Access Server. (left) Newly added since V2023 and (right) all quality-controlled surface water *f*CO₂ observations (µatm) in v2023. Squares indicate mooring locations.

SOCAT continues to leverage the efficiencies of the data ingestion automation system developed through DMSP funded efforts. The submission system has again proven its worth as the SOCAT data team was able to accomplish the annual release with no delays - even though the Bjerknes

¹⁸ DOI:10.25921/1h9f-nb73

FY2023 Annual Report [Global Data Management and Synthesis Project]

Climate Data Centre (BCDC) no longer supported the SOCAT data submission in any capacity. Due to the efficiency of the submission system, SOCAT was able to meet the annual release requirement of the Global Carbon Project's Annual Carbon Budget.¹

DMSP scientists Kevin O'Brien and Linus Kamb, from PMEL, and Denis Pierrot of AOML continue to lead the development and enhancement of the SOCAT automated data ingestion and QC software, with partners from NOAA's National Center for Environmental Information (NCEI). All development is done with the oversight of the SOCAT global group to ensure SOCAT needs are fully met. During FY23, the SOCAT automation team was busy supporting the community as they engaged in submission and quality control of data to support SOCATv2023 and v2024. As noted above, SOCAT v2023 has been released officially, while data submission for v2024 is ongoing and ends in January 2024. Data QC for v2024 is occurring in parallel with data submission and final data QC must be performed by March 31, 2024. We anticipate the release of v2024 in June 2024, timed to continue supporting the creation of the Global Carbon Project's Annual Global Carbon Budget.

The AOML and PMEL groups are the largest contributors to SOCAT and lead several of the regional quality control groups.¹⁹ All members of the group are involved in quality control, providing corrections, and commenting on the quality of data following SOCAT protocols with particular emphasis on metadata and dataset quality control.

During FY23, DMSP scientist Kamb was busy finalizing the SOCAT metadata submission tool. This metadata entry tool, which has been leveraged from work done for the NOAA Ocean Acidification Program (OAP), will, for the first time, provide a uniform way for SOCAT submitters to include required metadata when submitting datasets. Work was completed to integrate SOCAT specific fields into the metadata editor, identified through previous OADS XML work. In addition to supporting manual creation of metadata through the on-line editor, the tool supports uploading of existing excel spreadsheets in the OADS/OCADS/SDG14.3 formats, as well as continuing to support OME-style metadata which is used by a handful of important SOCAT partners. This metadata editor was presented and its use demonstrated to the surface carbon community at the November 2023 meeting in Oostende and it was well received. The tool is now available on-line for SOCAT submitters in time for the v2024 submissions.²⁰

Also in FY23, DMSP scientist O'Brien was heavily involved in the organization of the "Surface Carbon Summit" in Oostende, Nov, 2023. During the submission period for the previous version, there were several submission issues that were directly related to the inexperience of new data submitters. This meeting offered a wonderful opportunity to reintroduce the SOCAT data submission system and demonstrate the new metadata editor tool, as previously mentioned. The additional burden to DMSP scientists for SOCATv2023 submission issues also emphasized the loss of support from the Bjerknes Climate Data Center group, which no longer supports SOCAT. However, thanks to the robust submission system that has underpinned the SOCAT data product for the last several years, DMSP scientists were able to manage well enough and ensure that there was no delay of the SOCAT annual release. The loss of BCDC support meant that O'Brien

¹⁹ https://socat.info/index.php/groups-for-socat-version-2023/

²⁰https://data.pmel.noaa.gov/sdig/socat/MetadataEditor.html

FY2023 Annual Report [Global Data Management and Synthesis Project]

and Dr. Bakker were also required to pick up extra tasks having to do with reporting submissions statistics, etc. to the Global Carbon Project.

In addition to the above enhancements and submission efforts, DMSP scientists continued to support SOCAT users through account management, submission questions, resolution of any submission difficulties and updates. This support is often challenged by the enhanced IT security requirements for NOAA IT infrastructure.

The SOCAT automation team continues to provide SOCAT releases through interoperable web services²¹ and archive the data with NCEI using the structures put in place in FY-19. DMSP scientists continue working with NCEI to ensure that there is no lapse in archival, and that Digital Object Identifiers (DOIs) are properly attached to the individual synthesis files. Including DOIs improves cite-ability and reusability for SOCAT data.

On the data visualization side of SOCAT, DMSP researchers continue to enhance the Live Access Server software to provide effective visualizations of the SOCAT data, both for the SOCAT community and the larger public.

2.1.2. Moored pCO₂ network

Measurements of fCO_2 from moorings are an important component of global carbon cycle monitoring. These platforms provide the long-term temporally-resolved datasets needed to study processes responsible for sub-seasonal to decadal fCO_2 variability. The platforms also provide cost-effective data from remote data-limited regions. Data from these systems were shared and led to scientific advances in FY23 as discussed in the *High-Resolution Ocean and Atmosphere* pCO_2 *Time-Series Measurements* progress report (PI: Sutton) (e.g., Knor et al. 2023; Sutton et al. 2022; Wynn-Edwards et al. 2023). Mooring data synthesis activities in FY23 included data ingestion into the SOCATv2023 release, and data from the CO₂ mooring network are included in the most recent release of SOCAT and the annual release of the Global Carbon Budget. As a result of the recent mooring additions to these data synthesis products and assessments and the cumulative 132 years of NOAA CO₂ mooring data now available at OCADS, we expect the CO₂ mooring project to continue to make a large impact on our efforts to model and understand the global carbon cycle in the coming years. Autonomous Surface Vehicle CO₂ data²² were submitted to SOCAT for the first time in FY2019 and now appear in versions 2020 through 2023. The ASVCO2 system and data sets are described in detail in (Sabine et al. 2020).

²¹ <u>http://ferret.pmel.noaa.gov/socat/erddap/</u>

²² https://www.ncei.noaa.gov/access/ocean-carbon-data-system/oceans/ASV/index.html

FY2023 Annual Report [Global Data Management and Synthesis Project]

2.1.3. SOCOM and RECCAP2



Figure 2.2 Global climatological maps of (top) net air–sea CO_2 fluxes centered on 2010 using the approach of Takahashi, using the SOCAT dataset with ocean CO_2 uptake regions shown in the blue colors and outgassing regions in red, for December, January and February (top); and June, July, August (*from:* Fay et al. 2023, submitted).

DMSP scientists at AOML and PMEL are actively engaged in the Surface Ocean pCO_2 Mapping intercomparison (SOCOM) group and related efforts on a comparison of the global sea-air fluxes based on new methodologies to extrapolate the observations in time and space (Rödenbeck et al. 2015). For this effort J. Triñanes and R. Wanninkhof have analyzed and synthesized optimal remotely sensed (winds, SST, Chl-a, and salinity) and model output (MLD) products to be used in these efforts. These data are used in an artificial intelligence (AI) construct to create global flux maps. We have processed the updated and extended CCMP wind product through 2022²³ (Atlas et al. 2011) and determined monthly average wind velocities and their 2nd and 3rd moments at 0.25° resolution for the 6-hourly product. The resulting monthly timeseries from 1997-2020

²³ <u>http://www.remss.com/measurements/ccmp/</u>

FY2023 Annual Report [Global Data Management and Synthesis Project]

has been submitted for analysis in the RECCAP2 effort. A summary of net air-sea CO₂ fluxes for the different products, including the AOML-ET method developed with DMSP support, is shown in Figure 2.3. The AOML-ET product along with a monthly time series of pCO_2 produced by P. Landschützer from the SOCAT data are used to provide the monthly to decadal changes in CO₂ uptake for the annual State of the Climate Report of BAMS²⁴.

2.1.4. Production of seasonal air-sea CO_2 flux maps

Improved methods are being developed using AI approaches while we maintain the monthly flux product as it faithfully reproduces the general patterns of anomalies. For quantitative analyses we are using the neural network-based approach of (Landschützer et al. 2013) as default, but are investigating different AI methods to create improved flux maps. In particular, Dr. Triñanes has led an effort to apply a novel neural network approach, and Extra Trees to create monthly global CO₂ flux maps from 1997 onward. Results suggest that the overall patterns with our approach compare more favorably with observations, particularly at high latitudes, than patterns estimated with other approaches, but the overall long-term trend is greater (Figure 2.3).

²⁴ <u>https://journals.ametsoc.org/view/journals/bams/104/9/BAMS-D-23-0076.2.xml</u> FY2023 Annual Report [Global Data Management and Synthesis Project]



Figure 2.3. Comparison of different AI approaches to estimate net annual CO_2 uptake by the ocean. The method developed as part of the DMSP effort (AOML-ET) is shown by a black line. The annual average update for the Takahashi 2010 climatology scaled by area is shown as a black circle. The results from other AI approaches as obtained from the Global Carbon Project

(https://www.globalcarbonproject.org/carbonbudget/22/data.htm) are listed in the legend (Wanninkhof et al. 2023, submitted).

An updated monthly air-sea CO₂ flux climatology centered on 2010 following the methods of the late T. Takahashi was created in collaboration with D. Munro (U. Colorado), S. Sutherland (LDEO-Columbia (ret)) and A. Fay (LDEO-Columbia). Climatologies were created with both the dataset compiled by T. Takahashi and colleagues, and the larger SOCAT V2020 dataset. *FY2023 Annual Report [Global Data Management and Synthesis Project]* Page 13 of 30

While overall fluxes were similar, the comparison showed improved regional depictions with the SOCAT data. Summer and wintertime depictions of the air-sea CO_2 fluxes are shown in Figure 2.2 with as notable feature the regions of outgassing in Southern Ocean in Austral wintertime.

2.1.5. Global Carbon Project (GCP) assessment

The global carbon project²⁵ provides annual "state of the carbon cycle" reports. This report includes active participation and recent data contributions from ocean carbon scientists (Le Quéré et al. 2013, 2015b,a, 2016, 2018a,b; Friedlingstein et al. 2019, 2020, 2022a,b). The pCO_2 from ships data that are quality controlled through the DMSP effort and provided to the SOCAT and Takahashi databases are key contributions to this effort. Co-authors on the 2023 assessments include DMSP scientists R. Wanninkhof and D. Pierrot of AOML, L. Barbero of CIMAS, and R.A. Feely, S. Alin and A. J. Sutton of PMEL.

2.2. Ocean interior synthesis

Dissolved inorganic carbon (DIC) is a direct measure of the carbon content of seawater and is therefore an ideal measurement for exploring changes in ocean carbon storage. At least two properties must be measured to determine the effect of changes in carbon storage on ocean chemistry, so total alkalinity (TAlk) is also routinely measured. Seawater pH, and on NOAA GO-SHIP cruises fCO_2 as well, are also often determined as very precise constraints and as an independent check on other measurements. DMSP scientists are working to gather interior ocean carbon observations into global datasets, quality control and assess these measurements, improve the routines used to estimate carbon storage from DIC changes, improve the relationships used to estimate TAlk and similar quantities from other measured properties, and use the combined quality-controlled products for assessments of ocean carbon uptake. This effort is performed in part under the aegis of GLODAP⁸.

2.2.1. Quality control of data from recent cruises

The CLIVAR/CO₂ Repeat Hydrographic cruise lines A16N_leg 1, A16N_leg 2, and I05 were conducted aboard the *NOAA ship Ronald H Brown and* RV *Roger Revelle, respectively* in FY23 as part of the Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP). The For I05, the DIC, and underway *f*CO₂ data were reduced and submitted to NCEI and CCHDO at the end of the cruise as stipulated in the GO-SHIP repeat hydrography data submission protocol, and final QC is ongoing. For A16N DIC, discrete *f*CO₂ and underway *f*CO₂ data were successfully obtained but final submission has been delayed because the final CTD/O₂ data has not been processed due to a family situation of the person responsible. During FY23 the DIC measurements from P02_W and P02_E were finalized. These efforts and reduction of the underway data are being undertaken by D. Greeley, J. Herndon, and A. Collins of PMEL and C. Featherstone, P. Mears, and K. Schockman at AOML.

2.2.2. Global Data Analysis Project v2 updates

Since the 2016 release of the GLODAPv2 global hydrographic cruise data product (Olsen et al. 2016), the GLODAPv2 team has been aiming for for a semi-annual release of an updated data product. The first updated the data product (extending through \sim 2012) to approximately 2016, and included >200 additional international cruise data sets. This effort was renewed in FY18 with a GLODAPv2.2018 reference group with data product update released in calendar year

²⁵ <u>http://www.globalcarbonproject.org/</u>

FY2023 Annual Report [Global Data Management and Synthesis Project]

2019 (Olsen et al. 2019). The updates have been annual since this release: GLODAPv2.2020, .2021, and .2022 were released with accompanying manuscripts (Olsen et al. 2020; Lauvset et al. 2021, 2022) with DMSP scientists B. Carter, R. A. Feely, and R. Wanninkhof as co-authors. As summarized in the abstract: "GLODAPv2.2022 is an update of the previous version, GLODAPv2.2021 (Lauvset et al., 2021). The major changes are as follows: data from 96 new cruises were added, data coverage was extended until 2021, and for the first time we performed secondary quality control on all sulfur hexafluoride (SF₆) data. In addition, a number of changes were made to data included in GLODAPv2.2021. These changes affect specifically the SF₆ data, which are now subjected to secondary quality control, and carbon data measured onboard the RV Knorr in the Indian Ocean in 1994–1995 which are now adjusted using CRM measurements made at the time. GLODAPv2.2022 includes measurements from almost 1.4 million water samples from the global oceans collected on 1085 cruises." The reference group meetings were conducted remotely in FY-21 and FY-22. The manuscript detailing the GLODAPv2.2023 product is now in peer review and the data product is available online⁵.

The GLODAPv2 effort is scheduled to conclude with .v2023. There is a planned one-year hiatus from annual releases while preparing for a major overhaul with the GLODAPv3 release, which is tentatively scheduled for FY25. Currently, the annual updates to GLODAPv2 adjust newer cruises to the body of cruise measurements that were available with the original release in 2016. GLODAPv3 will offer an opportunity to adjust the older cruises to be more in line with recent measurements (since ~2012) which are, in many cases, made using analytical approaches that are known to have reduced uncertainties. It will also afford an opportunity to resolve several outstanding questions that have been noted with the adjustment procedures used in the GLODAPv2 data release. Finally, it will offer an opportunity to formalize the relationship between GLODAP and its coastal partner project (CODAP). In anticipation of these major efforts, DMSP-PI Carter has agreed to take over the GLODAP co-Chair role from Toste Tanhua.

2.2.3. Anthropogenic carbon storage and concentration estimates

Two major new sets of products were released in FY-23, and progress was made on several additional products related to interior ocean anthropogenic carbon (C_{anth}) accumulation.

The first set of products is the global (DeVries et al. 2023), Atlantic (Perez et al. 2023, submitted), and the forthcoming Pacific (Ishii et al. in prep) chapters of the second REgional Carbon Cycle And Processes (RECCAP2) synthesis of model and observation based carbon cycle information. RECCAP2 provides a comprehensive overview of the state of the knowledge of air-sea C_{anth} and natural CO₂ fluxes and interior changes based on models and observations (Figure 2.4). These papers have/will have DMSP coauthorship. Two sets of analyses from the RECCAP2 synthesis found that there is a climate-forced acceleration of the ocean carbon sink of 0.34 ± 0.06 (global ocean biogeochemical model simulations, GOBMs) and 0.41 ± 0.03 PgC yr⁻¹ decade⁻¹ (inverse model assessments). The synthesis also shows that the carbon sink is dominated by anthropogenic carbon, but the variability in the carbon sink is driven by variations in natural carbon inventories.



Figure 2.4. A comparison of the column inventory anthropogenic carbon accumulation rate as quantified from global ocean biogeochemical models (GOBMs, a), from data based approaches (b), and from ocean circulation inverse models (OCIM, d), as well as their differences (f) and the climate forced signals on natural (g) and anthropogenic (e) carbon.

A second major product from FY23 is the update of the eMLR(C*) estimates used by Gruber et al. (2019) for another decade by Müller et al. (2023). The update and the original both have DMSP coauthors. The recent update argues there is evidence that the global ocean C_{anth} accumulation rate slowed down from the 1994 to 2004 period to the 2004 to 2014 period (Fig. 2.5). Interestingly, the authors find a (statistically insignificant) slowdown in the South Pacific where, by contrast, earlier DMSP-led findings by Carter et al. (2019) showed a (statistically significant) increase in storage in the South Pacific in a regional analysis using different methods. Preliminary findings based on GOBM simulations from the RECCAP2 analysis show a modest increase in the anthropogenic carbon storage rate in the South Pacific during this period (Ishiii et al. *in prep*). These comparisons highlight the importance of quantifying the sources of uncertainties in these analyses and how they vary with different approaches. All three of these studies were assessed using observing system simulation experiments, wherein the technique uncertainty is inferred from reconstruction errors of exactly known modeled anthropogenic carbon accumulations. The uncertainty analysis by Müller et al. (2023) reveals unusually large Pacific Ocean uncertainties from the eMLR(C*) technique in the 1994-2004 period due to the unavailability of certain data types. The eMLR(C*) analysis also found moderate decreases in Indian Ocean anthropogenic carbon accumulation with a >0.5 PgC decade⁻¹ where there is added uncertainty due to adjustments made to alkalinity measurements.

Collectively, these comparisons show that it is beneficial to use a variety of data analysis approaches to resolve variations in anthropogenic carbon accumulation, and that it is desirable to apply the analysis of Carter et al. (2019) to the Indian and Atlantic Basins and test whether the "slowing global ocean C_{anth} accumulation" hypothesis is robust to methodological uncertainties. The Indian Ocean basin is doubly important to revisit because one of the central repeated sections of the Indian Ocean basin had not been reoccupied since 2009 at the completion of the analysis of Müller et al. (2023). At the end of FY23, PI Carter served as Chief Scientist aboard the I05 cruise, which successfully reoccupied the line. Thus, an updated set of estimates should be possible as soon as the data are finalized (see section 2.2.1). Early estimates reveal a modest decrease in the accumulation rate (Fig. 2.6), though a full analysis of uncertainty and final data are needed to make a more confident statement.



Figure 2.5. Global anthropogenic carbon inventory and its changes since 1994 from Müller et al. (2023).



Figure 2.6. Preliminary anthropogenic carbon accumulation rates R_{Canth} across the I05 section of the Indian Ocean from two ~14 year periods. Generally, accumulation was greater in the earlier period than in the more recent period. The middle section is missing from the top panel because the section was not fully occupied for carbonate chemistry variables during the 1990s.

With the comparison between methods being a central theme of upcoming research, it is urgent that we better understand the uncertainties in the methods and directly assess their strengths and weaknesses. To address this, at the end of FY-23, PI Carter started using DMSP funding to mentor a postdoctoral scholar (Dr. Xinyu Li). Dr. Li is externally funded but will contribute to DMSP research related to C_{anth} . Dr. Li aims to use the model simulations made publicly available as part of the RECCAP2 analysis (Müller 2023) to comprehensively compare both approaches, alongside several alternatives, across a large number of disparate model environments.

FY2023 Annual Report [Global Data Management and Synthesis Project] Page 19 of 30

2.2.4. Ocean carbonate system inter-comparison

FY-23 saw continued progress and new products and papers related to carbonate system inter-consistency, or the practice of using 3 or more measurements of the carbonate system in seawater (i.e., an over-constrained system) as the basis for assessing uncertainties in seawater carbonate system measurements. Previous DMSP-led research (Carter et al. 2018) noted a persistent pH-dependent discrepancy between measured and calculated pH that spans measurements and calculations from all laboratories that are making the highest quality open-ocean pH measurements across the United States and internationally. This discrepancy is particularly problematic for applications that require carbonate system intercomparability. Given this, the DMSP-led Ocean Carbonate System Intercomparison Forum (OCSIF) was formed as a working group through the Ocean Carbon and Biogeochemistry (OCB) program to coordinate and recommend research to quantify and/or reduce uncertainties and disagreements in measurable seawater carbonate system measurements and calculations, identify unknown or overlooked sources of these uncertainties, and provide recommendations for making progress on community efforts despite these uncertainties²⁶. FY-23 saw the preparation of two papers related to the findings of this working group (Carter et al. in press; in internal review at PMEL in anticipation of submission).

The first of these two papers (Carter et al., *in press*) aims to (1) summarize recent progress toward quantifying and reducing carbonate system uncertainties; (2) advocate for research to further reduce and better quantify carbonate system measurement uncertainties; (3) present new data, metadata, and analysis related to uncertainties in carbonate system measurements; and (4) restate and explain the rationales behind several OCSIF recommendations, and has been accepted for publication at *Limnology and Oceanography*.

The second paper (Carter et al., *in internal review at PMEL*) takes a more quantitative focus, and in it DMSP researchers review recent literature estimates of measurement and calculation uncertainties focusing on discrete open-ocean carbonate chemistry measurements in the Global Ocean Data Analysis Project 2022 update (GLODAPv2.2022). They also quantify random (R) and systematic (S) uncertainties using both an uncertainty propagation (UP) approach and a carbonate chemistry measurement "inter-consistency" (IC) approach that quantifies the disagreement between direct measurements of carbonate chemistry variables and calculations of the same variables from other carbonate chemistry measurements. The analysis reveals that the seawater carbonate chemistry measurement community has collected and released data with a random uncertainty that falls between the thresholds defined for "climate" and "weather" quality goals by the Global Ocean Acidification Observing Network (GOA-ON) (Newton et al. 2015). However, subsets of the available data show varied random uncertainty, and some subsets, including the subset of DIC measurements that have been QC'd by DMSP efforts (see: 2.2.1) show random variations consistent with the (most stringent) climate quality criteria. The paper includes a review of how uncertainty propagation results compare to our inter-consistency results and how the average inter-consistency varies across common carbonate chemistry thermodynamic constant options (Fig. 2.7). The paper concludes by providing general guidance for quantifying the effective uncertainty that matters for any given analysis.

²⁶ <u>https://www.us-ocb.org/ocean-carbonate-system-intercomparison-forum/</u>

FY2023 Annual Report [Global Data Management and Synthesis Project]



Figure 2.7. Distributions of ratios between the observed (in GLODAPv2.2022) and expected (from uncertainty propagation) random (top, $U_{R,\Delta,IC}/U_{R,\Delta,UP}$, where smaller values imply smaller uncertainties) and systematic (bottom, $U_{S,\Delta,IC}/U_{S,\Delta,UP}$, where values closer to 0 imply smaller uncertainties) disagreements between measured and calculated values of carbonate chemistry variables for each of the12 possible comparisons (distributions) and each of the 16 commonly-used sets of carbonate chemistry constants for seawater (x-axis). This analysis finds that the GLODAPv2.2022 data product as a whole is most consistent with the carbonate

chemistry constants from Lueker et al. (2000) and Uppström (1974). However, this finding varies between subsets of the data and comparisons.

2.3. BAMS State of the Climate report

The submission of an ocean carbon section to the BAMS SoC report, resumed after a 1-year hiatus, included comparison of approaches to determine air-sea CO_2 fluxes (see figure 2.3) (Wanninkhof et al. 2023). Furthermore, the section shows that ocean carbon uptake anomalies in 2022 relative to the 1990–2020 average are negative (i.e., more CO_2 going into the ocean) relative to expectations from atmospheric CO_2 increases, yielding a 0.6 Pg C greater annual uptake than the 30-year average. However, there are significant areas where there are positive anomalies, notably the equatorial Pacific, and section of the subtropical gyres caused by decadal changes in the ENSO pattern and sea surface warming, respectively.

The interior ocean section highlights the new approaches and methodologies to determine ocean interior carbon. These include algorithms that enable predictions of total dissolved inorganic carbon (DIC) and other carbonate chemistry parameters in the interior ocean from a variety of predictors, and BGC Argo. This points to a new frontier for interior ocean carbon cycle science that will likely see significant advances in the coming years with the advent of new data streams and continued iteration on machine learning mapping strategies.

2.4. Collaborations

DMSP scientists continued collaborations with researchers throughout the field. Of note for 2023 were the interactions in two OCB working groups. The "filling the gaps in observation-based estimates of air–sea carbon fluxes" working group led by G. McKinley of LDEO-Columbia U. and includes A. Sutton and R. Wanninkhof as members; and the Ocean Carbonate System Intercomparison Forum (OCSIF) led by B. Carter which includes L. Barbero as member. The "Gaps" working group focuses on knowledge gaps and uncertainties in the global inventory and flux products. The findings are contributing directly to the IPCC and RECCAP2 assessments. The OCSIF working group is discussed in section 2.2.4. There is a continued focus on the development of a Bio-GO-SHIP program, and DMSP scientists devoted some time to planning exercises for Bio-GO-SHIP in FY23.

Also in FY-23, Carter relied on DMSP funding to make contributions to several publications that were led by other institutions or by individuals funded on separate grants. In each instance, Carter's role centered around carbon data management and/or synthesis. Examples include the continued development of a new fCO_2 mapping methodology intended for coastal environments (Sharp et al. 2022) and its deployment to create an online indicators data product²⁷ (Sharp et al. *in prep*), the development of a global surface ocean acidification indicators data product (Jiang et al. 2023), and an analysis of the subsurface C_{anth} accumulation impacts (Fassbender et al. 2023). Each of these analyses relied upon previously developed DMSP data products.

2.5. Performance measures

Performance measures from the FY-23 work plan are summarized in Table 2.3. These performance measures have been accomplished in full and the rate of data return for viable

²⁷ <u>https://ecowatch.noaa.gov</u>

FY2023 Annual Report [Global Data Management and Synthesis Project]Page 22 of 30

measurements is effectively 100%. Products resulting from these efforts are provided in the last column.

Measure of	2023	Relevant website/papers
Performance		
CO ₂ flux maps	CO ₂ flux	See: Fig. 2.3. (Wanninkhof et al. 2023), also related:
	maps	(Sharp et al. 2022; <i>in prep</i>)
Ocean interior	No PM	(Carter et al. in press; DeVries et al. 2023; Müller et
synthesis		al. 2023; Perez et al. 2023)
Data	Processing	https://www.nodc.noaa.gov/oceanacidification/steward
processing of	surface data	ship/data_portal.html, socat.info
surface data		
Data	Preliminary	P02_W https://cchdo.ucsd.edu/cruise/33RR20220430
processing	and finalized	P02_E https://cchdo.ucsd.edu/cruise/33RR20220613
interior data	data from	A16N_1 https://cchdo.ucsd.edu/cruise/33RO20230306
	recent cruises	A16N_2 https://cchdo.ucsd.edu/cruise/33RO20230413
		I05 https://cchdo.ucsd.edu/cruise/33RR20230722

Table 2.3. A summary of performance measures as listed in the FY-23 work plan.

3. Outreach and Education

Synthesis Project investigators have been active in educating the public about ocean carbon changes. Several of the PIs are routinely asked to give invited seminars of their results at national and international meetings and symposia. Several of the PIs regularly teach graduate and undergraduate classes in ocean carbon chemistry. These classes incorporate the scientific results coming from this work. Several of the PIs have graduate students or post-docs that are exposed to the work accomplished through this project. Several of the Synthesis Project PIs also serve on national and international science committees that help guide and coordinate ocean carbon research. Interactions with the general public include presentations to local schools, open public lectures (both in the US and abroad), public "webinars" (seminars broadcast as streaming video onto the web e.g. for World Oceans Day), laboratory tours for groups ranging from school kids to Congressional Representatives, official congressional testimonies, and outreach blogs. DMSP PIs have also given numerous press interviews and have been quoted in printed and online media, radio, and television.

Dr. Wanninkhof has provided presentations to international scientific audiences on the science efforts and is advocating for a collaborative international surface CO_2 observing network, SOCONET. He works closely with GO-SHIP steering committee members, IOOCP and JCOMMOPS to provide community outreach in bulletins and presentations on the importance of the decadal global ocean surveys and the major accomplishments of this program. He is actively involved in developing SOCONET, the WMO Global Greenhouse Gas Watch (G³W), and the US Global Greenhouse Gas Monitoring Program. He is post-doc adviser of Katelyn Schockman who obtained her degree at USF in 2022.

FY2023 Annual Report [Global Data Management and Synthesis Project] Page 23 of 30

Dr. Feely is an Affiliate Professor at the UW School of Oceanography. In FY23, Dr. Feely gave 3 presentations of his carbon research at local, national, and international meetings, including the ECCWO-5 Symposium in Bergen, Norway.

In FY-23 Carter gave 4 scientific talks that featured DMSP research to various external audiences. He also served on the GO-SHIP executive committee, the GLODAP reference team, and the Biogeochemical Argo Steering committee, began as US GO-SHIP Co-Chair starting in FY23, and was nominated as the GLODAP co-chair starting in FY24. He peer-reviewed 12 research papers and proposals during the last 12 months. In FY-22 Carter became an affiliate faculty member of the University of Washington. He is now the primary advisor for two postdocs and two graduate students. He serves on the committee for a third graduate student. PI Carter also mentored numerous scientists at sea as part of the I05 research cruise, and co-hosted Hollings Scholar Jonathan Tran at PMEL in summer of 2023.

4. Publications and Reports

DMSP scientists comply with federal Public Access to Research Results requirements and list GOMO as a funding source in paper acknowledgements. The FundRef number 100007298 has been included in recent publications and will be included as well going forward.

4.1. Grant funded publications

4.1.1. Publications by Principal Investigators

- **Carter, B. R.**, and **Coauthors** (*in press*) Uncertainty sources for measurable ocean carbonate chemistry variables, *Limnol. Oceanography*
- DeVries, T., and **Coauthors**, 2023: Magnitude, Trends, and Variability of the Global Ocean Carbon Sink From 1985 to 2018. *Glob. Biogeochem. Cycles*, **37**, e2023GB007780, https://doi.org/10.1029/2023GB007780.
- Fassbender, A. J., B. R. Carter, J. D. Sharp, Y. Huang, M. C. Arroyo, and H. Frenzel, 2023: Amplified Subsurface Signals of Ocean Acidification. *Glob. Biogeochem. Cycles*, 37, e2023GB007843, <u>https://doi.org/10.1029/2023GB007843</u>.
- Fay, A. R., D. R. Munro, G. A. McKinley, **D. Pierrot**, S. C. Sutherland, C. Sweeney, and **R.** Wanninkhof, 2023: Updated climatological mean delta fCO₂ and net sea–air CO₂ flux over the global open ocean regions. *Earth Syst. Sci. Data Discuss.*, 1–35, https://doi.org/10.5194/essd-2023-429.
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- Wynn-Edwards, C. A., E. H. Shadwick, P. Jansen, C. Schallenberg, T. L. Maurer, and A. J. Sutton, 2023: Subantarctic pCO2 estimated from a biogeochemical float: comparison with moored observations reinforces the importance of spatial and temporal variability. Front. *Mar. Sci.*, **10**.
- 4.1.2. Publications by Principal Investigators in preparation
- Carter, B. R., and Coauthors, Random and systematic uncertainty in ship-based seawater carbonate chemistry observations, internal review at PMEL
- Carter, B. R., and Coauthors, (in prep) Tracer-based Rapid Anthropogenic Carbon Estimation (TRACE)
- Ishii, M, B. R. Carter and Coauthors, The Pacific Regional Carbon Cycle Assessment and Processes (RECCAP2) carbon data synthesis report, internal review at PMEL.
- Lauvset, S. K., and Coauthors, GLODAPv2.2023: the latest version of the global interior ocean biogeochemical data product, submitted for publication at Earth Syst. Sci. Data.
- Perez, F. F., and Coauthors, 2023: An assessment of CO2 storage and sea-air fluxes for the Atlantic Ocean and Mediterranean Sea between 1985 and 2018. Global Biogeochem Cycles, submitted.
- Schockman, K. M., R. H. Byrne, B. R. Carter, and R. A. Feely, (submitted 2023) Spectrophotometric Determination of the Bicarbonate Dissociation Constant in Seawater for $20 \le S_P \le 40$ and $3 \le t \le 35$ °C and CO₂ System Internal Consistency at Low Temperatures, Limnology and Oceanography
- Sharp, J. D., T. Boyer, B. R. Carter, S. Cross, L. Jiang, P. Lavin, and Hyelim Yoo (in prep), Ocean Acidification Indicators in Coastal US Ecosystems Over the Early 21st Century, Sci. Dat.
- Wanninkhof, R., J. Triñanes, D. Pierrot, D. R. Munro, C. Sweeney, and A. R. Fay, submitted 2023: Impact of Predictor Variables on Estimates of Global Sea-Air CO₂ Fluxes Using an Extra Trees Machine Learning Approach. Global Biogeochem Cycles.

4.2. **Related publications**

Numerous publications use DMSP-related data products. These are tracked by the data product distribution teams. A periodically-updated list can be obtained for SOCAT²⁸ and GLODAP²⁹ online. Empirical algorithm use-cases are tracked through citations of the associated validation

²⁸ https://www.socat.info/index.php/publications/

²⁹ https://www.glodap.info/index.php/glodap-impact/

FY2023 Annual Report [Global Data Management and Synthesis Project] Page 25 of 30

documents^{30,31}. The DOI-minting activities described above for SOCAT datasets will allow this tracking to become more automated for related datasets going forward.

4.3. All Cited publications

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³⁰ <u>https://scholar.google.com/scholar?cites=14510365232221234357&as_sdt=5,48&sciodt=0,48&hl=en</u> ³¹ <u>https://scholar.google.com/scholar?cites=17172330226054160354&as_sdt=5,48&sciodt=0,48&hl=en</u>

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FY2023 Annual Report [Global Data Management and Synthesis Project] Page 28 of 30

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FY2023 Annual Report [Global Data Management and Synthesis Project] Page 29 of 30

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5. Data and Publication Sharing

Data management, archival, and sharing are core priorities for DMSP activities, as described in the FY18 work plan. No updates have been made to this data management plan during FY21.

6. Project Highlight Slides

This has been provided as a .pptx file.