The Ocean Carbon and Acidification Data System

- Li-Qing Jiang^{1,2}, Alex Kozyr^{1,2}, John Relph², Errol Ronje³, Linus Kamb⁴, Eugene Burger⁴,
- Jonathan Myer⁵, Liem Nguyen⁶, Krisa M. Arzayus⁷, Tim Boyer², Scott Cross⁸, Hernan
 Garcia², Patrick Hogan³, Kirsten Larsen³, and A. Rost Parsons³
- ⁶ ¹Cooperative Institute for Satellite Earth System Studies, Earth System Science
- 7 Interdisciplinary Center, University of Maryland, College Park, Maryland 20740,8 United States.
- 9 ²NOAA/NESDIS National Centers for Environmental Information, Silver Spring,
- 10 Maryland 20910, United States.

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- ³NOAA/NESDIS National Centers for Environmental Information, Stennis Space
- 12 Center, Mississippi 39529, United States.
- ⁴NOAA/OAR Pacific Marine Environmental Laboratory, Seattle, Washington 98115,
 United States.
- ⁵NOAA/NESDIS National Centers for Environmental Information, Asheville, North
- 16 Carolina 28801, United States.
- ⁶Department of Computer Science, University of Maryland, College Park, Maryland
 20740, United States.
- ⁷NOAA/NOS Integrated Ocean Observing System, Silver Spring, Maryland 20910,
 United States.
- ⁸NOAA/NESDIS National Centers for Environmental Information, Charleston, South
- 22 Carolina 29412, United States
- 23 Corresponding author: Li-Qing Jiang (Liqing.Jiang@noaa.gov).

24 Abstract

- 25 The Ocean Carbon and Acidification Data System (OCADS) is a data management
- 26 system at the National Oceanic and Atmospheric Administration (NOAA) National
- 27 Centers for Environmental Information (NCEI). It manages a wide range of ocean
- 28 carbon and acidification data, including chemical, physical, and biological
- 29 observations collected from research vessels, ships of opportunity, and uncrewed
- 30 platforms, along with laboratory experiment results, and model outputs.
- 31 Additionally, OCADS serves as a repository for related Global Ocean Observing
- 32 System (GOOS) biogeochemistry Essential Ocean Variables (EOVs), e.g., oxygen,
- 33 nutrients, transient tracers, and stable isotopes. OCADS endeavors to be one of the
- 34 world's leading providers of ocean carbon and acidification data, information,
- 35 products, and services. To provide the best data management services to the ocean
- 36 carbon and acidification research community, OCADS prioritizes adopting a
- 37 customer-centric approach and gathering knowledge and expertise from the
- 38 research community to improve its data management practices. OCADS aims to
- 39 make all ocean carbon and acidification data accessible via a single portal, and
- 40 welcomes submissions from around the world:
- 41 https://www.ncei.noaa.gov/products/ocean-carbon-acidification-data-system/.

42 Introduction

43 With \sim 71% of its surface area covered by the ocean, the Earth is sometimes called a "Blue Planet" or "Water Planet". The ocean plays a critical role in climate 44 45 regulation by sequestering and storing approximately 25% of anthropogenic carbon dioxide (CO₂), one of the primary greenhouse gases emitted by human activities ¹⁻⁶. 46 47 Furthermore, the ocean absorbs about 90% of the excess heat trapped in the Earth 48 system and transports heat from the equator to the poles^{7,8}. Additionally, the ocean 49 provides various ecosystem goods and services that are essential to our society. 50 Billions of people, especially those living in the coastal communities, depend on the 51 ocean for their food security^{9,10}, recreation¹¹, livelihood^{12,13}, and natural and cultural 52 heritage¹⁴.

Since the beginning of the Industrial Revolution around 1750, human activities have released ~2.5 trillion metric tons of carbon dioxide¹⁻⁶, resulting in an atmospheric CO₂ increase of ~50% (~419 parts per million, or ppm, 2022 annual average)¹⁵ compared to the 1750 level of ~277 ppm¹⁶, causing our climate to change^{17,18}. Without the carbon capture and sequestration services provided by the ocean, the atmospheric CO₂ today would have been ~80 ppm higher than the current level³.

60 This large influx of carbon dioxide is altering the ocean's chemistry. After CO₂ is 61 absorbed by seawater, a portion of it will react with water to form carbonic acid, 62 which will then dissociate and release hydrogen ions (H⁺). The extra H⁺ will associate 63 with carbonate ions (CO_3^{2-}) to increase the concentration of bicarbonate ions 64 (HCO₃[−]). The net result is that the mildly alkaline ocean is becoming more acidic (and 65 less alkaline), and its carbonate ion (CO_3^{2-}) , a building block for many marine organisms, has been decreasing. This process is commonly referred to as "ocean 66 acidification (OA)"¹⁹⁻²⁶. Ocean acidification is making it harder for marine calcifiers 67 68 (e.g., mollusks, crustaceans, coral) to build and maintain their shells and skeletal 69 structures, endangering coral reefs and marine ecosystems more broadly²⁷⁻³⁰. It can 70 also negatively affect non-calcifying organisms, e.g., disrupting the use of chemical 71 sensations to find food or avoid predators for certain species, thus potentially 72 shifting the food web, and changing the community composition and structure^{31,32}. 73 Even apex predators (e.g., large whales) may experience the effects of ocean 74 acidification in the future as decreasing pH levels could change the acoustic 75 characteristics of the ocean, thus alter or disrupt their communication and foraging 76 behaviors as the ocean becomes noisier³³⁻³⁵.

77 On timescales of decades to millennia, the ocean imposes a dominant control 78 over atmospheric CO₂ levels, due to its vast size and efficient exchange of CO₂ with the atmosphere^{5,36,37}. It contains the majority (~95%) of the total active pool of 79 80 inorganic carbon in the Earth's surface, at \sim 38,000 billion tons of carbon, which is 81 \sim 45 times that of the atmosphere³⁸⁻⁴⁰. Geoengineering efforts, such as marine 82 carbon dioxide removal (mCDR), could potentially change the ocean's chemistry and impact the marine ecosystems⁴¹. Therefore, understanding carbon cycling in the 83 84 ocean is critical for the research of global climate change, ocean acidification, marine 85 CDR, and their downstream effects on the marine ecosystems, and the final impact on the human socio-economic structure^{28,42}. 86

87 Effective data management is a crucial aspect of the research efforts mentioned 88 above^{43, 44}(Figure 1). After all, the ocean is a global system, and data collected from 89 individual research cruises often need to be compiled into regional and global data products, before they can be used to support further oceanographic research, enable 90 91 the Measurement, Reporting, and Verification (MRV) of mCDR for carbon credit 92 accounting, and produce reports that can guide society's strategies for mitigating and 93 adapting to environmental changes⁴⁵. Data management provides an avenue where 94 all data are (a) safeguarded for long-term access; (b) documented with common 95 metadata and data standards and controlled vocabularies; and (c) findable and 96 accessible. It plays a very important role in data reuse and valorization, model 97 verification, and most importantly, quality control (QC), synthesis, and data product 98 developments.

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101 **Figure 1.** A schematic diagram showing the importance of ocean data management 102 in promoting oceanographic research and product developments. (Credit: This figure

103 is adapted from a diagram generated by Guidi et al.⁴⁶).

104 The Ocean component of the Carbon Dioxide Information Analysis Center (CDIAC-Oceans, Oak Ridge National Laboratory, Tennessee, USA) played a very important 105 106 role in the management of ocean carbon data from 1993 to 2016. Two factors 107 contributed to the success of CDIAC-Oceans: its customer-centric approach, and the 108 accessibility of all ocean carbon data collected by the global research community 109 through a single data portal. However, CDIAC-Oceans' data holdings were not backed 110 with a long-term archive. Its portfolio was focused on ocean carbon data and related 111 hydrographic variables only. Its infrastructure was not designed to manage other 112 types of OA data, such as physiological response biological studies. Worst of all, 113 CDIAC-Oceans lost its funding from the Department of Energy (DOE) in 2016. 114 NCEI's OA data management efforts started with an OAP funded project called

115 Ocean Acidification Data Stewardship (OADS) in 2012. By leveraging a modern 116 community-driven rich metadata template⁴⁷ and NCEI's enterprise long-term archive

- 117 management system with version control and controlled vocabulary management
- 118 capabilities, OADS built state-of-the-art technical infrastructure that helped

transform NCEI's OA data management efforts from a top-down government task toa bottom-up community-driven service.

121 In November 2015, NCEI was notified that CDIAC-Oceans would lose its funding 122 by the end of September 2016. To continue the service that was provided by CDIAC-123 Oceans, a new project called Ocean Carbon Data System (OCADS) was established at 124 NCEI in January 2017, using the same technical infrastructure that was built by OADS. 125 All CDIAC's data holdings and webpages were transferred to NCEI, and the CDIAC-126 Oceans staff member was hired by NCEI as a cooperative institute employee to 127 continue his work on the management of international ocean carbon data. The 128 Ocean Carbon Data System could be considered as CDIAC-Oceans 2.0. All data 129 holdings were upgraded with a much-improved modern metadata template⁴⁷. 130 Controlled vocabularies were applied to all aspects of the metadata to ensure 131 accurate data findability. All data files were published into NCEI's long-term archive 132 with version control capabilities.

133 In September 2022, a new integrated system called the Ocean Carbon and 134 Acidification Data System (OCADS) was formed at NCEI out of a merger of the former 135 Ocean Acidification Data Stewardship Project (OADS) and Ocean Carbon Data System 136 (OCADS). This merger was a response to feedback from the research community, 137 who had encountered difficulties in choosing between the two systems for 138 submitting and accessing data purposes. With the merger, the entire suite of ocean 139 carbon and acidification data services offered by NCEI became available to the global 140 research community, ushering in a new era of collaborative research possibilities. It's 141 worth noting that the acronym OCADS remains the same, even though the new 142 OCADS is a consolidation of the two previous systems.

143 Besides NCEI, current data management systems that have ocean carbon or 144 acidification data in their portfolios include the CLIVAR and Carbon Hydrographic 145 Data Office (CCHDO, U.S.A.), Biological and Chemical Oceanography Data 146 Management Office (BCO-DMO, U.S.A.), the Ocean acidification International 147 Coordination Center (OA-ICC, Monaco), PANGAEA (Germany), European Marine 148 Observation and Data Network (EMODnet, Belgium), British Oceanographic Data 149 Center (BODC, U.K.), Bjerknes Climate Data Centre (Norway), International 150 Oceanographic Data and Information Exchange (IODE) Sustainable Development 151 Goals (SDG) Portal (France), OceanOPS (France), and Joint European Research 152 Infrastructure for Coastal Observatories (JERICO).

The Ocean Carbon and Acidification Data System has been the choice of data management services for most of the recent ocean carbon and acidification data product developments, e.g., the Surface Ocean CO₂ Atlas Version 2022 (SOCATv2022)⁴⁸, Global Ocean Data Analysis Product Version 2 (GLODAPv2.2022)⁴⁹, the Coastal Ocean Data Analysis Product in North America (CODAP-NA)⁵⁰, and the CARbon, tracer and ancillary data In the MEDiterranean sea (CARIMED).

- 159 OCADS excels in this arena because:
- 160
 1. It is backed with a state-of-the-art long-term archive. All data are guaranteed
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 to be available for at least 75 years, thanks to the NOAA records management
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 requirements.
- 163 2. It has a stringent version control mechanism that ensures permanent

1	64		preservation of all historical versions.
1	65	3.	OCADS provides a community-driven metadata display interface that is
1	66		tailored to the needs and preferences of the oceanographic research
1	67		community.
1	68	4.	Controlled vocabularies are applied to all aspects of its data management to
1	.69		ensure accurate data findability.
1	70	5.	OCADS manages a wide range of ocean carbon and acidification data,
1	71		including chemical, physical, and biological observations, along with
1	72		laboratory experiment results, and model outputs.
1	.73	6.	OCADS hosts one of the largest ocean carbon and acidification data
1	74		repositories in the world, thanks to the data holdings transferred from CDIAC-
1	75		Oceans.
1	76	7.	OCADS has established mechanisms to support existing ocean carbon and
1	77		acidification data product developments, e.g., SOCAT, and GLODAP.

178 Results

179 Mission

180 At its core, the mission of OCADS is to provide data management services that 181 facilitate and support research on ocean carbon cycling and ocean acidification. This 182 is accomplished through:

- Safeguarding their data in a well-supported federal archive to ensure long term (≥75 years) access and version control,
- Serving as one of the world's leading providers of ocean carbon and acidification data, information, and products, and
- Providing data management support for quality control, synthesis, and data
 product development activities.

The OCADS data management services include dedicated support for acquiring data, publishing data into the archive, managing rich metadata with controlled vocabularies, and enabling online data retrieval and access. Another aspect of the OCADS portfolio is QCing data and developing coastal and open ocean data products^{23,50,51}. In addition, OCADS has been playing a leading role in establishing numerous international standards for both metadata and data^{47,52}.

195 Data scope

196 OCADS manages a wide range of ocean carbon and acidification data (Table 1). 197 Here, ocean carbon and acidification data are defined as data that contain at least 198 one of these variables: carbon dioxide molecular ratio (xCO_2), pressure (pCO_2) or 199 fugacity (fCO₂), total dissolved inorganic carbon content (DIC), total alkalinity content 200 (TA), pH, hydrogen ion content ($[H^+]$), carbonate ion content ($[CO_3^{2-}]$), and calcium 201 carbonate mineral saturation states for aragonite (Ω_{arag}) and calcite (Ω_{cal}). Besides 202 these variables, OCADS also serves as a repository for other Global Ocean Observing 203 System (GOOS) biogeochemistry Essential Ocean Variables (EOVs), i.e., oxygen, 204 nutrients (e.g., Silicate, Phosphate, Nitrate), Transient Tracers (e.g., 205 chlorofluorocarbons, or CFCs), nitrous oxide, particulate matter, stable carbon

- 206 isotopes, and dissolved organic carbon⁵³.
- 207 **Table 1**. An inventory of the OCADS data holding by observation type as of January
- 208 15, 2023.

Observation type	Number of datasets
Profile/CTD	1173
Surface underway	822
Time-series	101
Laboratory experiment	29
Total	2230

209 Common types of data OCADS manages include:

- In situ observational ocean carbon and acidification data, including chemical,
 physical, and biological observations collected from research vessels, ships of
 opportunity, moorings, and other uncrewed platforms.
- Results from physiological response studies, including laboratory experiments,
 mesocosm studies, field experiments, and natural analogues.
- Model outputs.
- Data products (See Table 2 for examples)

217 Product development support

OCADS provides data management support for numerous ongoing projects focused on developing ocean carbon and acidification data products (Table 2). This service comprises archiving individual datasets from various cruises, producing tables with comprehensive lists of these datasets, and providing access to the developed data products. At present, OCADS can only provide support for data product development activities related to ocean carbon and acidification research due to limited resources.

Table 2. Major regional and global ocean carbon and acidification data product development efforts, with OCADS providing data management support.

Data product	Abbreviation	Area	Citation
The Surface Ocean CO₂ Atlas	SOCAT	Global	Bakker et al.48
The Global Ocean Data Analysis Project Version 2	GLODAPv2	Global	Lauvset et al.49
Coastal Ocean Data Analysis Product in North America	CODAP-NA	Coastal	Jiang et al. ⁵⁰
CARbon, tracer and ancillary data In the MEDiterranean sea	CARIMED	Regional	Álvarez et al.

227 SOCAT is a global data product that provides surface ocean *f*CO₂ measurements,

228 primarily obtained from ships of opportunity (SOOP)⁴⁸. It represents one of the most

229 extensive collections of observational ocean carbon data. The latest release

230 (SOCATv2022) contains 33.7 million fCO_2 values with an accuracy of better than 5

231 μ atm. A further 6.4 million *f*CO₂ sensor data with an estimated accuracy of 5-10 μ atm

are available separately. GLODAP is a full water column open ocean data product,

- 233 containing high-quality data from discrete bottle based measurements⁴⁹. GLODAP
- 234 covers 14 oceanographic variables, i.e., temperature, salinity, oxygen, nitrate,
- silicate, phosphate, DIC, TA, pH, chlorofluorocarbon (CFC-11), CFC-12, CFC-113,
- carbon tetrachloride (CCl₄), and Sulfur hexafluoride (SF₆). The most recent release,
- GLODAPv2.2022, includes measurements from close to 1.4 million water samples
- collected on 1085 cruises. CODAP-NA is an internally consistent data product for
 discrete inorganic carbon, oxygen, and nutrients on the North American ocean
- discrete inorganic carbon, oxygen, and nutrients on the North American ocean
 margins⁵⁰. CODAP-NA's initial release (v2021) contains 3391 oceanographic profiles
- from 61 research cruises covering all continental shelves of North America, from
- Alaska to Mexico in the west and from Canada to the Caribbean in the east from 6
- 243 December 2003 to 22 November 2018.

244 Best practice data standards

245 Common data standards are crucial in facilitating future data utilization, 246 particularly for quality control and synthesis efforts. Adhering to such standards can 247 minimize uncertainties and errors that may result from ambiguous variable 248 abbreviations, inconsistent quality control flags, and non-standardized calculations. A 249 recently released best practice data standard for discrete chemical oceanographic 250 observations⁵² provides guidelines on various topics such as column header 251 abbreviations, quality control flags, missing value indicators, standardized calculation 252 methods for carbon system parameters, new tools for calculating thermodynamic 253 variables using the International Thermodynamic Equations of Seawater 2010 (TEOS-254 10) equations⁵⁴, and new tools for calculating fCO_2 from dry-air mixing ratios.

255 Components

OCADS comprises three primary user interfaces that have been tailored to
provide optimal data management support for research related to ocean carbon and
acidification (Figure 2):

- The Scientific Data Information System (SDIS), a digital data submission
 interface,
- The Rich Metadata Management System (RMMS), a user-friendly metadata
 management and display interface, and
- The Ocean Carbon and Acidification Data System Portal (OCADS_portal), a data
 search and access interface.

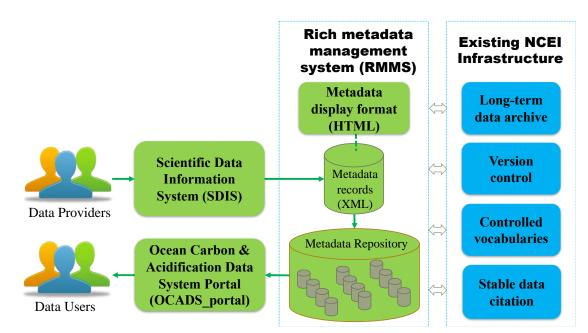




Figure 2. A schematic diagram showing the major components of the Ocean Carbon and Acidification Data System (OCADS).

268 The Scientific Data Information System (SDIS) is a digital data submission interface 269 developed by NOAA's Pacific Marine Environmental Laboratory (PMEL) to streamline 270 the process of submitting ocean carbon and acidification data to NCEI. (Figure 3). It 271 enables a user to input metadata, upload data files, and submit the resultant data 272 package to NCEI for review and eventual archival. The SDIS integrates rich metadata 273 management capabilities that are designed to satisfy the research needs and 274 requirements of the global ocean carbon and acidification research community⁴⁷. 275 The SDIS incorporates a user profile management system that permits data 276 submitters to (a) maintain a record of all their prior submissions, (b) start a new 277 submission by duplicating an existing record, and (c) save their work midway through 278 a submission and resume later. In addition to new submissions, the SDIS also 279 supports revision requests.

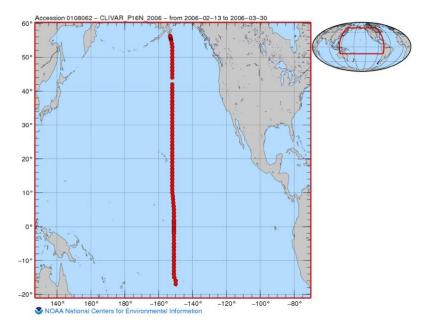
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	Metadata Preview Download Save Upload OADS Metadata File (XML,	123-456-7890	Extension Extension	ion	First.L	idress * ast@noaa.g	jav		0
	Excel, or CSV)		Resear						

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- 281 **Figure 3.** A screenshot showing the metadata interface of the Scientific Data
- 282 Information System (SDIS, https://data.pmel.noaa.gov/sdig/oap/Dashboard/).

283 The Rich Metadata Management System (RMMS) is a metadata management 284 and display interface that has been created to present the collected rich metadata 285 information in a user-friendly format. At present, the RMMS is comprised of these 286 sections: title, investigators, package description, data citation, identification 287 information, types of study, a browse graphic, temporal coverage, spatial coverage, 288 platforms, research projects, variable metadata sections, datasets related to this 289 current dataset, and funding information⁴⁷. The RMMS plays a crucial role in 290 providing data management experiences that meet the needs and preferences of the

291 global oceanographic research community.



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Figure 4. An example of a browse graphic from a dataset collected in the Pacific
 Ocean from 2006-02-13 to 2006-03-30 (Cruise_ID: CLIVAR_P16N_2006) (Credit:
 https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0108062.html).

296 To ensure uniformity and ease of understanding, all OCADS dataset titles adhere 297 to the template of "[observed properties] collected from [observation categories] 298 using [instruments] from [research vessels or other platforms] in [sea names] during 299 [research projects] from [start date] to [end date]. An example of an OCADS data title is: "Dissolved inorganic carbon, total alkalinity, pH, temperature, salinity and other 300 301 variables collected from profile and discrete sample observations using CTD, Niskin 302 bottle, and other instruments from R/V Wecoma in the U.S. West Coast California 303 *Current System during the 2011 West Coast Ocean Acidification Cruise (WCOA2011)* 304 from 2011-08-12 to 2011-08-30". Each OCADS dataset is accompanied by a browse 305 graphic, providing users with a visual representation of the sampling locations or 306 experiment setup, facilitating a quick understanding of the data. (Figure 4).

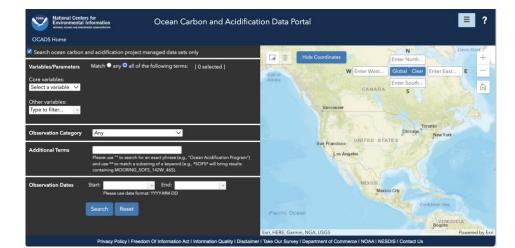
The "variable metadata section" is a one of the most important components of the RMMS, as it allows for the detailed documentation of all ancillary information related to a particular observed property, e.g., dissolved oxygen. This section can be repeated as many times as needed to document rich metadata information for all observed properties in the dataset. Information contained in this section will assist data users in comprehending the measurement details, such as the instruments

313 used, methods applied, calibration procedures, and the associated data quality and 314 uncertainty (accuracy/precision). Accuracy refers to how close the measurements are 315 to the true or known values. Precision, on the other hand, refers to how close the 316 measurements are to each other. Future improvements include the inclusion of a 317 new metadata field that specifies whether a measurement is of weather or climate 318 quality⁵⁵, as well as additional elements aimed at supporting marine carbon dioxide 319 removal (CDR) research, e.g., types of alkalinization. An illustration of a variable 320 metadata section is presented in Figure 5. Note that only the metadata elements 321 that have been filled out by the data provider are shown, although the RMMS has

322 the capacity to display all metadata elements as described in Table 2 of Jiang et al⁴⁷.

	bottle dissolved oxygen
Abbreviation:	OXYGEN_UMOL_KG
Unit:	micromol/kg
Observation type:	Discrete measurements from samples collected on CTD casts
In-situ / Manipulation / Response variable:	In-situ observation
Measured or calculated:	Measured
Sampling instrument:	Niskin bottle
Analyzing instrument:	Brinkman Dosimat automated titrator
	The analysis method is based upon the Carpenter (1965) whole flask titration of iodine, which is produced by ar equivalent amount of dissolved oxygen. An automated titrator (Brinkman Dosimat) uses an amperometric end point detection as described by Culberson and Huang (1987) and modified for IBM-PC computers by Knapp et a (1990). The nominal 125-ml iodine flasks are used for sampling are pre-calibrated so their volumes are precisely known. Samples were titrated within a few hours of being collected. 685 discrete oxygen samples were run to validate sensor O2 observations on the CTD package.
Quality flag convention:	OXYGEN_FLAG, WOCE quality control flags are used: 2 = good value, 3 = questionable value, 4 = bad value, 5 = value not reported, 6 = mean of replicate measurements, 9 = sample not drawn.
Researcher name:	Ann Swanson
Researcher institution:	Oregon State University, College of Earth, Ocean, and Atmospheric Sciences; PI: Burke Hales

- 323
- 324 **Figure 5.** An example of a "variable metadata section" from a dataset during the
- 325 2011 West Coast Ocean Acidification Cruise
- 326 (https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/0123467.html).



327

- **Figure 6.** A screenshot showing the Ocean Carbon and Acidification Data System
- 329 Portal (or OCADS_portal, https://www.ncei.noaa.gov/access/ocean-carbon-
- acidification-data-system-portal/).

331 The Ocean Carbon and Acidification Data System Portal (OCADS_portal)

provides an interface for users to search and access all data holdings within OCADS

(Figure 6). It uses user-friendly technologies, such as auto-complete, dropdown
menus, and OpenLayers maps, to enhance the user experience of searching for data.
Currently, the Portal enables users to search for datasets based on five criteria:

- Variables/Parameters: The observed properties, e.g., water temperature, total alkalinity content, etc. A user can select one or multiple observed properties.
- Observation Category: How the observed properties are measured, e.g.,
 surface underway, time-series, CTD profile, laboratory experiment, etc.
- Additional Terms: A powerful free-text search box allowing users to use any other elements of the metadata record to assist with the search, e.g., a
 research vessel name, the last name of an investigator, an expedition code (EXPOCODE), a cruise identifier (Cruise ID), etc.⁵²
- Observation Dates: The start and end dates of the observation. Only cruises
 with at least one data point collected during the period will show up in the
 search results.
- Spatial Coverage: A user can either input the bounding box information
 (longitudes and latitudes) or draw a rectangle on the map to define a
 geographic area that will constrain the spatial parameters of the query.
 Similarly, only cruises with at least one sampling station within the bounding
 box will show up in the search results.

352 Customers

OCADS recognizes the significance of (a) documenting all ocean carbon and acidification data with common metadata and data standards and controlled vocabularies, and (b) making them available through a single data portal. The program encourages the submission of data from across the globe and provides this service at no cost to all data producers, regardless of their location. In addition to data producers, OCADS also serves data users and consumers, including researchers, educators, decision-makers, private industry, and the general public from all nations.

- 360 Helpful tips
- 361 Here are some additional tips that will help users access data at NCEI:
- An "accession" refers to a dataset published at NCEI's archives. The accession
 number is a 7-digit numerical number used to uniquely identify a dataset
 archived at NCEI.
- A "landing page" refers to NCEI's generic metadata page, in contrast to the
 RMMS page that is served through OCADS. The former covers bare minimum
 elements such as title, abstract, citation, and keywords. The latter is much
 richer and is focused on providing the best metadata to meet the data needs of
 ocean carbon and acidification research.
- If only an accession number is available, below is how to access its metadata:
 Link to the RMMS (available only if the dataset is published through OCADS,
 NNNNNN is the accession number):
- 373 https://www.ncei.noaa.gov/data/oceans/ncei/ocads/metadata/NNNNNNN.
 374 html

375 376	 Link to NCEI's landing page will be: https://accession.nodc.noaa.gov/NNNN NNN. This link works for all datasets within NCEI's archives.
377 378 379 380 381	 If a user is taken to the landing page first by the search engine, here is how to access the rich metadata page: first click the "Documentation" tab, then click "Project metadata". To see the version history of an Accession: first go to the landing page, then click the "Lineage" tab.
382	Links & Email
383 384	 Ocean Carbon and Acidification Data System (OCADS): https://www.ncei.noaa.gov/products/ocean-carbon-acidification-data-system/.
385 386 387	 Scientific Data Information System (SDIS): Link: https://data.pmel.noaa.gov/sdig/oap/Dashboard/. Video tutorial: https://www.youtube.com/watch?v=ZZL_wQWr38A.
388 389 390	 Rich Metadata Management System (RMMS): An example:
391 392 393	 Ocean Carbon and Acidification Data System Portal (OCADS_portal): Link: https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system-portal/.
394	\circ Video tutorial: https://www.youtube.com/watch?v=DYFI0aH00FU.
395 396	 OCADS contact: Email: noaa.ocads@noaa.gov.

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398 Discussions

399 OCADS and international OA data management

400 OCADS operates within the Oceanographic Science and Development Branch 401 (OSDB) of NCEI. As a component of the federal government, OCADS enjoys stable 402 funding, which sustains its data management system. However, this does not imply 403 that OCADS is biased towards NOAA or the United States. NCEI, the parent 404 organization of OCADS, is a World Data Center for Oceanography designated by the 405 International Council for Science (ICSU) through a resolution of the 29th United Nations General Assembly in 2008⁵⁶. Like all other data that NCEI handles, 100% of 406 407 the data that OCADS obtains will be made available to all users worldwide.

408 OCADS recognizes the importance of collaborating with other Data Analysis 409 Centers (DACs) to achieve the common goal of offering top-notch data management 410 services to the global oceanographic research community. Such partnerships not only 411 help distribute the burden of international ocean carbon and acidification data 412 management efforts, but also help overcome any regional or geopolitical barriers 413 that could potentially prevent direct interaction between OCADS and local data 414 producers. For DACs that need the support of a long-term archive, OCADS is eager to 415 cooperate with them to transfer a copy of their data to NCEI's archive. This process is 416 generally automated.

417 Ideally, all DACs, including OCADS, should function as regional nodes, aiding in the 418 availability of all ocean carbon and acidification data via a centralized one-stop data 419 portal. This can be accomplished by providing standardized metadata to the search 420 engine of the agreed-upon one-stop portal. The most recent U.N. Ocean Acidification 421 Research for Sustainability (OARS) data management initiative suggests designating 422 the GOA-ON Portal as the envisioned one-stop OA data portal. Once this is 423 implemented, users can employ the GOA-ON Portal to search for and retrieve all 424 ocean carbon and acidification data of a specific type. After finding a dataset via the 425 Portal, a user can then return to the respective regional DAC to access the data files 426 and locate any pertinent metadata information. 427 For such a federated system to work properly, the participating DACs must fulfill 428 the following minimum requirements: 429 1. Maintain a long-term archive to ensure uninterrupted data access into the 430 future. 431 2. Provide strict version control capabilities, preserving all historical versions of 432 a dataset on a permanent basis. 433 3. Utilize a community-driven common metadata template, e.g., the one used 434 by OCADS, to collect comprehensive metadata information needed for ocean 435 carbon and acidification research. 436 4. Present the collected metadata in: 437 a. A user-friendly interface for metadata readability (e.g., HTML). 438 b. A technical format to facilitate machine-to-machine interoperability (e.g., 439 XML, SQL). 440 5. Employ common controlled vocabularies for successful data findability and 441 easy machine-to-machine metadata exchange. 442 6. Support data citation with DOIs. 443 7. Establish a mechanism for sharing metadata with the agreed-upon one-stop 444 portal, making the data searchable and accessible through the portal.

Before such a federated system is implemented, it is recommended that data
producers share a copy of their data with OCADS to ensure timely inclusion in data
products like SOCAT and GLODAP.

448 Data management vs. data product development

449 The concepts of "data management" and "data product development" are often 450 conflated, but they are fundamentally different. It is true that they both involve 451 working with data, but their similarities end there. Data management refers to the 452 process of ingesting, storing, and disseminating data⁴³. It includes tasks such as establishing long-term archives, maintaining version control, using metadata 453 454 templates, adhering to data standards, and implementing controlled vocabularies. 455 Data management is frequently mandated by government regulations and carried 456 out by specialized national data centers.

Data product development, on the other hand, refers to the process of
developing products and services (e.g., synthesis products, gridded climatologies,
models, or predictions) out of data for the purpose of providing value to users.
Unlike data management, data product development is rarely mandated by federal
or local regulations. It can be carried out by anyone, including academic institutions.

- 462 Like other research activities, data product development also needs data
- 463 management support.

464 Methods

- 465 OCADS was designed and built with the following rationales in mind:
- 466 (a) A customer-driven service: OCADS was designed to meet the data 467 management needs and requirements of the global ocean carbon and 468 acidification research community. We believe data management is a scientific 469 effort that requires close collaboration with the research community. To 470 ensure that our service is customer-driven, we rely on researchers to help us 471 define many aspects of the OCADS data management, including metadata 472 templates, controlled vocabularies, data standards, website design, and data 473 submission and access interfaces.
- 474 (b) Rich metadata management: OCADS utilizes a community-driven rich
 475 metadata template⁴⁷ to collect detailed metadata information to enable data
 476 users, especially the synthesis community, to comprehend the measurement
 477 uncertainty and other sampling and calibration details, e.g., instrumentation,
 478 calibration, scales, units, biological subject, life stage, etc. of each variable.
 479 Rich metadata management is applied to the submission interface, metadata
 480 display interface, and the data search and access interface.
- 481 (c) Controlled vocabularies: Controlled vocabularies are lists of standardized 482 terms. For example, some scientists could report their dissolved inorganic 483 carbon measurements as "total dissolved inorganic carbon content", while others may call it "dissolved inorganic carbon", or "total carbon dioxide". 484 485 Multiple variations of terms for the same variable may cause confusion or 486 decreased discoverability. Therefore, controlled vocabularies play a very 487 important role to ensure successful data search. At OCADS, controlled 488 vocabularies are applied to many groups of metadata elements, including 489 observed properties (e.g., dissolved oxygen), observation types (e.g., surface 490 underway, time-series), platforms (e.g., research vessels), sea names, 491 instruments, institutions, people, countries, etc.
- 492 (d) Stable data citation: Each dataset archived at NCEI has an associated data 493 citation. The citation contains information such as author list, title of the data, 494 data repository, publication year, and an optional persistent identifier (e.g., 495 DOI). DOI is strongly recommended for all OCADS datasets, although OCADS 496 gives data providers the discretion of whether a DOI should be assigned or not. 497 According to the NOAA Plan for increasing Public Access to Research Results 498 (PARR)⁵⁷, "NOAA National Data Centers are the only entities authorized to issue 499 NOAA dataset identifiers.". This important guideline ensures that the same 500 dataset will not be assigned multiple DOIs, potentially causing unnecessary 501 confusions.
- (e) Long-term archive: All OCADS datasets are archived using the NCEI enterprise
 archival infrastructure, ensuring the data will be available into the future (≥75
 years). Besides a digital copy at NCEI's server, all published datasets in NCEI's
 archives are backed up to a staging disk on a backup server, as well as two

- 506offline tape-based repositories. Any data that are either new or changed are507first backed up to the staging disk at a frequency of once per day, 7 days per508week. Data on the staging disk is then migrated to tape copy #1 (on-509premises). The same data are later copied to tape copy #2 (off-site).
- 510 (f) Version control: Unlike journal publications, datasets are often updated after 511 they are published. This can happen after further QC is conducted or after 512 additional data or metadata are gathered. While it is critical to provide future 513 users with the latest version of the data, it is equally important to preserve all 514 historical versions. Otherwise, research based on historical versions of the 515 data can no longer be verified. In rare cases, the data may need to be 516 reverted to a historical version. NCEI's enterprise archival infrastructure 517 provides strict version control. After a dataset is published, no further 518 changes can be made to the published version. Any changes to the data will 519 trigger a new version of the dataset.
- 520 (g) Preserving the original data: In an era when the Findable, Accessible, 521 Interoperable, and Reusable (FAIR) Data Principles⁵⁸ are often emphasized 522 over traditional data formats like Microsoft Excel, OCADS recognizes the 523 importance of preserving the original data. They often contain embedded QC 524 comments, equations between different columns, color-coding, etc., which 525 are critical to the future data use. Such information can often get lost during 526 the conversion to FAIR-compatible data formats, e.g., NetCDF. Therefore, 527 OCADS always ensures the preservation of the original data.

528 Data availability

- 529 All data presented in this article are available at
- 530 https://www.ncei.noaa.gov/products/ocean-carbon-acidification-data-system/.

531 Code availability

532 Not applicable.

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754 Author contributions

755 L-QJ created the first draft of the paper, and all authors contributed to the writing 756 of the manuscript. L-QJ designed and coordinated the development of many OCADS 757 components, including the metadata template, the Rich Metadata Management 758 System, its underlying XML, XSL, and HTML formats, the OCADS portal, the SDIS, 759 main pages of the OCADS website, and the international data standard for discrete 760 bottle-based data. L-QJ also designed and led the efforts to transfer a total of 2,296 761 data sets serving from 1,193 FTP directories at cdiac.ornl.gov (corresponding to 1,190 762 NCEI accessions) from the Carbon Dioxide Information Analysis Center (CDIAC-763 Oceans) to NCEI. OCADS was built on the success of the CDIAC-Oceans, which was 764 first launched in 1993 by AK. AK processed the majority of the OCADS accessions, 765 including all CDIAC-Oceans datasets that were later transferred to OCADS. AK helped 766 review the design of the new OCADS website and created the many data access 767 pages including the clickable maps and numerical data packages brought to NCEI 768 from the former CDIAC-Oceans. AK also contributed tremendously to the transfer of 769 data and webpages to NCEI. JR helped build the RMMS, the backend automation 770 program for the SDIS, the automation programs to transfer data from CDIAC-Oceans 771 to NCEI, along with many other IT aspects of OCADS. ER tested SDIS after its initial 772 deployment and provided comments that improved the SDIS archive appraisal and 773 ingest process and other aspects of OCADS. ER has been the subject matter expert 774 working on the flow of biological OA data. LK and EB developed the Scientific Data 775 Information System. JM created the Drupal portion of the OCADS website. LN wrote 776 the code for the html pages of the new OCADS website, and the new OAP research 777 project management system. KMA, TB, SC, HG, PH, KL and ARP (ranked alphabetically

- based on their last names) provided resources and guidance for many aspects of
- 779 OCADS.

780 **Competing interests**

781 The authors declare no conflict of interest.