# <sup>1</sup> Ocean Alkalinity Enhancement Data Management <sup>2</sup> Protocol

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## <sup>4</sup> Revision History

Date	Version	Revision Description	Notes
01/23/2025	0.1.0	Original draft document published for public review	

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- 6 The first open comment review period is January 23, 2025 March 07, 2025.
- 7 Notes for reviewers are highlighted in orange font.

## 8 Acronyms and Abbreviations

8a	mCDR	Marine carbon dioxide removal
8b	OAE	Ocean alkalinity enhancement
8c	DOI	Digital object identifier

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## 10 Definitions of Selected Terms

10a	Metadata	Metadata is structured information that describes and provides context for a data resource, helping to ensure that the dataset remains discoverable and usable in the future.
10b	Data standards	Data standards are a set of agreed-upon rules, formats, and conventions used to define and structure data, ensuring consistency, interoperability, and clarity across different systems, datasets, and organizations. They help maintain data quality, facilitate data sharing, and enable effective analysis by establishing uniformity in how data are collected, represented, and exchanged.

10c	Column header names	Standardized column header terms describing a parameter, these may be an abbreviation of the measured parameter.
10d	Controlled vocabulary	Controlled vocabularies are standardized lists of terms and definitions used to ensure consistency in the naming and classification of concepts within a specific domain. By limiting the use of predefined terms, controlled vocabularies help avoid ambiguity, enhance data interoperability, and improve the accuracy of data retrieval and analysis across different systems and datasets.
10e	Ocean alkalinity enhancement	Ocean alkalinity enhancement (OAE) is a climate change mitigation strategy that involves increasing the alkalinity of seawater to enhance its capacity to absorb and store atmospheric carbon dioxide.
10f	Platform	Any physical structure or system used to support and deploy instruments, sensors, or other equipment for collecting data in the ocean. Platforms can include research vessels, ships of opportunity (SOOP), profiling floats, buoys, underwater vehicles, and moorings.
10g	Sensor data	Sensors refer to instruments or devices used to measure and collect data on various physical, chemical, and biological parameters of the ocean environment and are typically deployed on ships from rosettes or underway systems, buoys, underwater vehicles, or autonomous platforms. Data collected from these systems are considered sensor data and do not refer to data from autosampling devices.
10h	Quality control	Methods or procedures involving validating and verifying collected data to identify and correct errors, inconsistencies, or outliers, ensuring that the measurements are accurate and suitable for analysis. This typically includes tasks such as instrument calibration, data validation checks, and cross-referencing with other datasets to

		maintain the integrity of scientific results.
10i	Model data	The model data referenced in this protocol refers to code, configuration and output from mathematical simulations that discretise the equations for fluid motion and energy transfer and integrate these over time on a realistic three-dimensional grid. This encompasses model output relevant to OAE projects on nearfield and regional scales, as well as global circulation models (GCMs) and Earth System Models (ESMs). This could include ocean circulation models with or without coupling to biogeochemical, sediment, sea ice, or atmospheric models. This does not currently cover data standards for conceptual, process models, 1D or 2D models, or simplified plume mixing zone models.
10j	Data file	Refers to a file containing values of some measurements. File format type may vary (e.g., NetCDF, xlsx, xml), however all data files will contain quantitative values with associated column header names.
10k	Baseline	Baseline refers to the initial set of data or conditions that are recorded before any interventions or modifications are made to the ocean environment. This baseline field data serve as a reference point for comparing future measurements, allowing for the assessment of the effectiveness and impacts of the OAE interventions over time, such as changes in ocean alkalinity, CO <sub>2</sub> absorption, or ecosystem health.
101	Intervention	An intervention refers to the intentional action or process applied to the ocean to alter its chemical or physical properties in order to enhance its capacity for carbon dioxide removal. This could include adding alkaline substances to the water or implementing other methods aimed at increasing ocean alkalinity and improving the ocean's ability to absorb and store atmospheric CO <sub>2</sub> .
10m	Control	A control site refers to a designated area in proximity to an intervention site, with shared

	characteristic waters, but that remains unaffected by the OAE intervention, serving as a baseline for comparison during intervention. The purpose of a control site is to isolate and account for natural variability in oceanographic conditions, biogeochemical processes, and carbon fluxes, enabling the evaluation of changes directly attributable to OAE activities.
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12 Additionally, observation types are provided in Jiang et al., 2023b and are archived by NOAA for 13 reference (<u>link</u>).

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## 15 Background and Introduction

16 This document outlines recommendations for producing consistent data and metadata for

17 Ocean Alkalinity Enhancement (OAE) field trial projects. Its first iteration was produced in

18 partnership with the ocean sciences community, with the intention to remain a living document

19 and continually improve to reflect best known scientific practice.

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## 21 Objectives & Guiding Principles

22 The objective of the OAE Data Management Guidelines and this OAE Data Protocols document

23 are to enable marine Carbon Dioxide Removal (mCDR)-OAE data collected from academia,

24 government, non-profit, and industry to be documented in a consistent way, and make them

25 findable and discoverable from shared data repositories to facilitate future data synthesis efforts.

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27 OAE introduces unique challenges and opportunities for data standardization. Traditional

28 oceanographic data standards, while robust, require updates to address the specific needs of 29 OAE projects.

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31 The main updates and recommendations are driven by these Guiding Principles:

- Project Comparability: Developing guidelines that ensure data from different OAE projects are intercomparable, enabling meta-analyses and large-scale assessments of OAE effectiveness and environmental impact.
- **Minimal Burden on Data Providers:** Establishing streamlined protocols and tools that simplify data submission while ensuring high-quality, standardized outputs.
- Flexibility for Innovation: Allowing for innovation in project designs by creating standards that accommodate diverse methodologies and intervention scales without imposing restrictive requirements.
- Transparency and Accessibility: Promoting open and transparent data sharing, with appropriate metadata, to facilitate peer review, collaboration, and public trust in OAE efforts.

43 By building on existing standards and addressing these updates, the goal is to create a system 44 that supports rigorous science while remaining practical and adaptable for data providers. This 45 ensures that OAE projects contribute meaningfully to the collective understanding of marine 46 carbon dioxide removal while fostering collaboration across the community.

## 47 Methodology

48 This protocol was developed by the OAE community in a multi-process method, starting with a 49 workshop during OCEANS 2024 with participants representing academia, government, 50 non-profit, and industry to gather initial feedback and input for sensor output, model output, and 51 discrete carbonate and nutrient data. This feedback was developed into a first outlined draft of 52 recommendations, which were reviewed by attendees and developed into the first draft OAE 53 Data Protocols 0.1.0.

55 Working Groups were formed to capture input from biological sciences, sediment processes, 56 and social science data, each hosting virtual meetings to gather community feedback, which 57 further informed the initial draft. The recommended variable column header names and 58 controlled vocabularies are made to mirror existing naming conventions, and long-standing 59 recommendations by the Ocean Acidification Community. The draft was then provided to the 60 Steering Team members for internal review. The resulting draft was presented at a second 61 workshop during AGU in December 2024 for additional mCDR-community feedback, followed 62 by additional internal revisions to create the draft that was presented during an open public 63 review period. This document represents the final conclusions developed by the OAE 64 community to ensure projects will be standardized, findable, openly accessible, and 65 intercomparable.

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67 We are grateful for the contributions of the workshop participants, working group members, the 68 Steering Committee and those who provided comments during the open review period. For a list 69 of contributors and contributing authors, please see the Acknowledgements section.

### 70 Intended users

71 This protocol is designed to assist data producers involved in OAE projects that include model 72 output, and/or field data from commercially available sensors, discrete observations, social 73 sciences, sediment processes, and/or biological processes, in consistently documenting their 74 datasets, while also providing guidance on selecting appropriate repositories, submission 75 timelines, controlled vocabularies, and best practices for ensuring data intercomparison. 76

77 Projects compliant with this protocol will at minimum meet the requirements below, however 78 additional recommendations provided are strongly encouraged. The guidelines and 79 recommendations outlined in this document may be applicable to a wider range of mCDR 80 methods outside of OAE. The protocols outlined are presented as best practice

81 recommendations, leaving the decision to adopt them at the discretion of individual mCDR 82 researchers.

85 The protocol is organized into five chapters:

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- 1. Metadata Building on existing metadata guidelines that accompany each repository, this protocol requires OAE Metadata to provide essential context unique to OAE field trials. It also includes a *Model Description Template* to introduce and define key fields for documenting model and model output data details.
- 2. Guidelines for Data Submission This chapter outlines how to set up, manage and submit data across a range of data types.
- 3. Column Header Names and Controlled Vocabularies Recommendations are provided for column header names as well as controlled vocabularies and definitions, including OAE-specific fields.
  - 4. Emerging Standards This section outlines future work of the Data Management Guidelines project.
  - 5. Deprecated Standards and Practices Versioning control for the Data Protocol is outlined here.

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#### 101 Metadata

102 Depending on your choice of repository, there may be a structured metadata interface required 103 with data submission. In cases where this is optional, it is recommended to refer to the 104 metadata contents provided by the NOAA OCADS (Jiang et al., 2023a) metadata form 105 (https://www.dropbox.com/scl/fi/8lrsyufqljs1qi7ut9fji/Metadata\_template\_4.1.xlsx?rlkey=nfusfv7cw 106 3khsrmrvaup7zf88&st=2v3c69sf&dl=0). This form includes both metadata that are general to any 107 oceanographic project (e.g., cruise id, experiment id, data submitter, investigators, etc.), 108 specific metadata for discrete, sensor, and model data, as well as OAE-specific fields that have 109 been recommended by the OAE community and are presented below (see OAE Metadata for 110 field data, and Model Description Template for model data). If provided as a separate file, this 111 information can be provided in xlsx, netCDF, json, or XML format and can be named 'metadata'. 112

#### 113OAE Metadata

114 mCDR research, particularly OAE, involves creating deliberate perturbations to study their 115 effects. Given the diversity of approaches to raising alkalinity or reducing acidity, along with the 116 site-specific nature of OAE field data, additional metadata fields are needed on top of existing 117 metadata templates that are designed for ocean carbon and acidification studies. OAE 118 Metadata provides the necessary context for the research community to effectively find, 119 interpret, compare, and use the data across different studies and methodologies.

121 For ease of use, the OAE-relevant fields are provided in the OAE Metadata table below. Note 122 that most of these OAE-relevant metadata fields are integral to the updated OCADS metadata 123 template except for modeling output studies. If you are submitting your data to a repository that 124 has required structured metadata fields, the information below can be provided in plain text, 125 netCDF, or XML format as a separate upload titled 'OAE\_metadata\_supplement'. If there is no 126 required metadata structure, please refer to the NOAA-OCADS full metadata table (see 127 Metadata).

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129 Note to reviewers: Our goal is to identify key fields and examples that make the metadata useful 130 and searchable, without overwhelming the data submitter. Please review for missing fields, 131 missing [inputs] that you'd like to be searchable, inconsistencies in vocabulary and areas that 132 are too detailed. We are also looking for feedback on which fields should be required vs 133 optional.

134a	OAE Metadata		
134b	Fields	Input descriptions for each metadata field are provided below, inputs shown in [brackets] should match the exact vocabulary given.	Illustrative example (not based on a real study).
134c	Project ID:	The project to which the submitted data belong. A unique project identifier that can be used to link project data across data submissions, and link baseline data to intervention data, for example.  If no Project ID has been assigned, one may be generated by combining the following fields, as described in Cross-linking Data Sets with Common Identifiers.  Any method that creates a unique ID that will link all project data (e.g., a project's baseline data to intervention data, and various data	<ul> <li>Project beginning August 05, 2025</li> <li>Hvalfjordur, Iceland Carbondive_20250805 _Hvalfjordur</li> </ul>

		submissions within an experiment type) is acceptable.	
134d	Experiment type:	[natural] [manipulated] [model output]	manipulated
		Note to reviewers: Other options for 'manipulated' might include 'adjusted', 'modified', 'engineered'. Please provide your feedback on these controlled vocabularies.	
		See <u>Controlled</u> <u>Vocabularies</u> section for definitions.	
		For model generated data, move to <u>Model</u> <u>Description Template</u> .	
134e	Experiment ID:	The experiment to which the data belong. The recommended naming convention is:  - Project ID - Project condition - Numerical indicator to differentiate between various experiments of the same type for a project. A two digit consecutive number beginning with 01	- First intervention (experiment type = manipulated) for this project  Carbondive_20250805_ Hvalfjordur_manipulate d01
134f	Observation type:	Please select any of the following that describe the submitted data: [profile] [surface	field experiments

		underway] [time series] [laboratory experiments] [pelagic mesocosms] [benthic mesocosms] [field experiments] [natural analogues]  See <u>Controlled</u> <u>Vocabularies</u> section for <u>Observation type</u> definitions. Model output metadata should use the <u>Model Description</u> <u>Template</u> .	
134g	mCDR Pathways:	[ocean alkalinity enhancement] [macroalgal cultivation for CDR] [direct ocean capture] [ocean fertilization] [artificial upwelling and downwelling] [coastal blue carbon] [marine ecosystem recovery]  See <u>Controlled</u> <u>Vocabularies</u> section for definitions.	ocean alkalinity enhancement
134h	Site description:	Provide information to help characterize the field site and provide context when interpreting the data. For example, descriptions of tidal patterns, climatological conditions, notable geological characteristics, the geographical and marine setting (coastal, intertidal, island region, sheltered environment),	Hvalfjordur, Iceland  The proposed field site is in Hvalfjordur, Iceland. The fjord is approximately 35 km long, 3.5 km wide and 15 - 50 m deep. The site has a sheltered physical environment with predictable circulation and water residence time. The flow in the fjord is

local sentiment surrounding coastal activities and climate change, notable events that may impact local sentiment to mCDR (for example: site had significant toxic spill in past decade, local positive support for offshore wind farming, frequent HAB site), ecologically protected species, economically significant operations in the marine environment. characteristic meteorological events. If possible based on the file type of this submission, please include useful maps or figures here.

Links to relevant social science surveys, cruise reports, or protected species observer notes may be provided here. characterized by inflow at depth and outflow at the surface, with primarily counterclockwise circulation. Water temp ranges from 0° C in winter and 10° C in summer. Hvalfjordur experiences a subpolar oceanic climate characterized by strong downslope winds, increased rainfall due to its fjord-mountain landscape, and maritime temperature moderation from the North Atlantic current. The local community is represented in project governance (board) and is engaged actively via town halls, information sessions, a website and newsletter. Cultural activities in the fjord include mussel harvesting, though the toxicity of the mussels is monitored by the food agency in Iceland and is not always permitted. Global Attitude Surveys were conducted in 2010 and 2020 and reported in the Bjarnadóttir et al report What do Icelanders think about the environment and climate change? Economic activity in the fjord includes several

			areas zoned for sediment mining, a port in Grundertangi and an aluminum smelting plant, among others. Usually no pelagic fish in fishable quantities with the exception of winter 1947 - 1948 where large schools of summer spawning herring led to high catches. Moderate harbour seal population has rebounded in recent years.
134i	Project description:	A narrative description of the project. For example, what were the goals of the project? What were the research questions? What were the processes to achieve these goals and answer these questions? Who were the key stakeholders, organizers, project leaders? Was this building off a previous or ongoing project, or is this a new region/experiment/mech anistic study?	A baseline study beginning in 2024 captured the physical, biogeochemical, atmospheric and biological data of the site over the course of a year. It included autonomous and vessel-based samples as well as public data sources. Building on this year-long baseline study, Dual Tracer study, and Dye Tracer Study, an interdisciplinary project team under the leadership of Dr. Jane Doe conducted research to establish and test a prototype MRV System Pilot. The

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			research questions were: 1) Can adding NaOH effectively increase seawater alkalinity, 2) Can increased alkalinity reduce surface ocean $pCO_2$ , 3) Does reducing surface ocean $pCO_2$ result in CDR, and 4) is there an impact on local species and natural communities as a result?
134j	Experiment description:	A narrative description of the experiment. For example, what part of the project do these data represent (e.g., baseline, intervention, control) and what do they contribute to the overall project? Are all project research questions listed in <i>Project description</i> relevant? What were the processes to achieve these goals and answer these questions?	On August 10, 2025 the project team released 23 tons of diluted NaOH solution over 96 hours and observed the results for 14 days. This experiment represented the first intervention conducted in the region and for this project. All project research questions above are relevant as the intervention will allow these questions to be answered. To effectively monitor these study regions in order to answer these questions, 10 repeat ship surveys were conducted to collect grab samples, underway sensor data, and profile data from rosettes. 12 buoys were deployed with sensor arrays including

			temperature, salinity, oxygen, chlorophyll, particulate information, pH, and pCO <sub>2</sub> . These data will be used to monitor the change in seawater pCO <sub>2</sub> and local species impact due to dissolved alkalinity addition.
134k	Other datasets collected from this project:	If multiple data sets were produced out of the same experiment, please list all related unique identifiers (e.g., DOI's) to these datasets. Also include links to additional experimental data produced from this Project ID.	All data for the current experiment (CarbonModel_202508 05_Hvalfjordur_manipul ated01) are provided in this submission, with the current draft doi: http://doi.org/xx.xxx  Additional experimental project data include: Baseline study: Carbondive_20250805_Hvalfjordur_natural01 http://doi.org/xx.xxx  Dye Tracer Study: CarbonModel_2025080 5_Hvalfjordur_manipula ted02 http://doi.org/xx.xxx  Counterfactual model run: CarbonModel_0101202 4_iceland_modeloutput 01 http://doi.org/xx.xxx  Earlier biological research relevant to mCDR operations can

			be found via the Marine and Freshwater Research Institute.
1341	Previous mCDR research in the area:	If previous or on-going mCDR field operations have occurred in the study domain by any project developer, they may be mentioned here either as a description, and/or if a reference to the study exists in the form of a data set, publication, etc, the DOI or other identifying information should be provided. Please provide direct links to data when available.	mCDR company Algae Lock was headquartered near the fjord and conducted some proprietary carbonate chemistry and algae farming research in the fjord.
134m	Co-located operations:	A description of any nearby operations that may influence the waters over the time period covered by this data. This might be a nearby mCDR project, a facility that discharges water with different characteristics than the inflow (e.g., a desalination plant), frequent boating operations, etc.	Aluminum smelting plant co-located in fjord, activities and plans unknown.
134n	Data conflicts and unreported data:	If data exist that are not provided by the project due to conflicts (e.g., geopolitical or other), data availability (e.g., a dataset is no longer available), it may be noted here.	Data from a citizen-based water quality effort were available between the years 2021 - 2023 and are informed by Carbon Dive project planning,

			but are no longer accessible.
1340	Meteorological and tidal conditions:	Include links to relevant datasets and/or a narrative description.	Wind data:  Vindatlas.vedur.is  Bathymetry data: Coast Guard Data from Atlas.lmi.is  Land and water usage map: Vefsja.is  Tide & weather data (sea level, wind, air pressure, temperature, salinity: Vedur.mogt.is
134p	Permit number:	Associated permit number(s).	permit #XYZ (permit pending, example is illustrative)
134q	Permit approval document:	Link to permit or document reference.	permit #XYZ (permit pending, example is illustrative)
134r	Permitting authority:	Name of organization or authority related to permitting, if applicable.	Ministry for Foreign Affairs (Utanríkisráðuneytið) Environmental Agency of Iceland (Umhverfisstofnun)
134s	Additional details:	Open text area to include additional information. These may include information for sediment processes data, biological data, or any other required information if not included in the main metadata or data files; see <i>Guidelines for Data Submission</i> for relevant sections of your data. Additional informational	See https://samplewebsite.is /data for a field blog and additional data from this site.

blogs, etc., may be linked here.
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134t	Intervention Only:		
134u	OAE treatment type:	[electrochemical alkalinity addition] [mineral alkalinity addition] [dissolved alkalinity addition] [river alkalinity addition] [coastal enhanced weathering]  See <u>Controlled Vocabularies</u> section for definitions.	dissolved alkalinity addition
134v	Alkalinity feedstock type:	[olivine] [potassium hydroxide] [lime] [portlandite] [calcium carbonate] [anorthite] [dolomite] [periclase] [brucite] [magnesite] [forsterite] [sodium hydroxide] [natrite] [nahcolite]  See <u>Controlled</u> <u>Vocabularies</u> section for definitions.	sodium hydroxide
134w	Alkalinity feedstock description:	Information such as feedstock source, characteristics, concentration, impurities, dilution prior to dosing, and for feedstock other than NaOH; trace metal	30% NaOH solution (commercially acquired) mixed with freshwater to achieve 1050 kg/m³ density. Tagged with 32g of inert gas SF <sub>6</sub> , dissolved in 1000 liters of freshwater

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		composition and particulate grain size.	
134x	Dosing location:	For point source location, provide latitude and longitude in decimal degrees. For coastal dispersal, provide the maximum and minimum latitude and longitude positions. If the location varies, such as a ship deployment, provide the location as a latitude and longitude vector with the dosing data and time stamps, with column headers named 'intervention_location_lo n' and 'intervention_location_lat' and state 'dosing location is provided as a variable' here. Latitude and longitude should be provided in decimal degrees (negative for southern and western hemispheres). In some cases, the dispersal may vary by only a few meters and a point location may be provided, however, in all cases, the decimal accuracy provided here should reflect the accuracy of known position.	64.394426, -21.465808
134y	Alkalinity dosing effluent density:	Fixed density or provide link/source to effluent density data if applicable. Please	1050 kg/m³ density, measured directly

		include whether density is directly measured or a derived value. If this is a variable included with your data, please note so here as 'alkalinity dosing effluent density is provided as a variable' and use 'dosing_effluent_density' for your column header name.	
134z	Dosing depth(s):	Depth(s) in meters. If this is variable, please include the schedule of depth changes and depths, or as a vector in meters with the data, named 'dosing_depth'. Please note here that 'dosing depth is provided as a variable'.	3 meters below surface
134aa	Dosing mechanism:	E.g., point source, outflow from pipe, coastal distribution, pier-based diffuser. Please be descriptive.	Pier-based diffuser
134ab	Dosing regimen:	At a minimum, please provide the schedule and timeline of dosing, including the time between doses, the duration of treatment and the amount used each time. More optimally, this information would be provided as a vector of binary data in the data file where 1 = dosing 'on' 0 = dosing 'off', using the	August 5, 2025: 3 IBC Test 09:00 - 12:00 August 6, 2025: 7 IBC dosing 09:00 - 16:00 August 7, 2025: 13 IBC dosing 09:00 - 22:00 August 8, 2025: 7 IBC dosing 09:00 - 16:00  Dosing regimen is also provided as a variable.

		column header name 'dosing_onoff'. If provided as a vector state here as 'dosing regimen is provided as a variable'.	
134ac	Dosing rate data:	To link dosing rate data that are provided a vector data (e.g., 'flow_rate', 'mineral_mass_addition 'mineral_mass_addition rate', or any of the fields above), provide the source or filename (if provided with the currendata submission) to access these variables. If these are included in the data file, that should be stated here with the associated column header names listed.	d01_dosingdata.csv Variables include: flow_rate (L/s)

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135a	Physiological Response Studies		
135b	Targeted acidity or alkalinity levels:	Description of the alkalinity range targeted.	NA
135c	Manipulation method:	A description of the manipulation method that was used. Associated DOIs can be noted here, but should be supplemental.	NA
135d	Location where the experiment was carried out:	City, state, and research facility name in which the experiment took place.	NA
135e	Treatment duration:	Start and end date and time (UTC)	NA

## 137 Model Description Template

138 The following template outlines key fields and examples for documenting model and model 139 output data details in OAE research. It provides a structured framework to ensure clarity, 140 consistency, and completeness in describing model components, grid details, boundary 141 conditions, and project-specific protocols. This standardized approach supports the required 142 model reproducibility goals of the Protocol.

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144 Note to reviewers: Our goal is to ensure model runs can be as reproducible as possible. Please 145 review for missing fields, conflicts with vocabulary or areas of unnecessary/overly granular 146 detail. We are also looking for feedback on which fields should be required vs optional.

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147a	Model Description Template		
147b	Fields	Input descriptions for each metadata field, inputs shown in [brackets] should match the exact vocabulary given.	Illustrative example (not a real project).
147c	Project ID:	The project to which the submitted data belong. A unique project identifier that can be used to link project data across data submissions and link baseline data to intervention data, for example.  If no Project ID has been assigned, one may be generated by combining the following fields, as described in <i>Cross-linking Data Sets with Common Identifiers</i> .  Any method that creates a unique ID that will link all project data (e.g., a project's baseline data to intervention data, and various data submissions within an experiment type) is acceptable.	- Lead organizer:     CarbonModel - Project beginning January     01, 2024 - Iceland  CarbonModel_01012024_iceland d
147d	Experiment type:	[natural] [manipulated] [model output]	Model output

		See <u>Controlled Vocabularies</u> section for definitions.	
147e	Model run experiment type:	[counterfactual] [perturbation] [counterfactual and perturbation] [other]  See <u>Controlled Vocabularies</u> section for definitions.	perturbation
147f	Experiment ID:	The experiment to which the data belong. The recommended naming convention is:  - Project ID - Experiment type - Numerical indicator to differentiate between various experiments of the same type for a project. A two digit consecutive number beginning with 01.	First model alkalinity run for this project  CarbonModel_01012024_icela nd_modeloutput01
147g	Experiment description:	A narrative description of the experiment. For example, what were the research questions and goals? What were the processes to achieve these goals and answer these questions?	The goals of this model run are to support an OAE field trial in Iceland by Carbon Dive in order to model the spread of alkalinity released and air-sea CO <sub>2</sub> exchange over time in the region.
147h	Other datasets collected from this project:	Include links or DOI's to associated field data and model runs for this Project ID.	Counterfactual model run: CarbonModel_01012024_icela nd_modeloutput01 http://doi.org/xx.xxx  Baseline field study: Carbondive_20250805_Hvalfjo rdur_natural01 http://doi.org/xx.xxx  Dye Tracer Study: CarbonModel_20250805_Hvalf jordur_manipulated02 http://doi.org/xx.xxx

147i	Model configuration:	Links to model configuration files (e.g. roms_application.h, roms.in, and build_roms.sh files for a ROMS simulation)	https://github.com/parkermac/ LO_roms_user/tree/main/upw elling
47j	Model Physics Component		
147k	Name:	Name of model (e.g. ROMS, Oceananigans)	ucla-roms
1471	Version:	Model release version	tag-1
147m	Codebase:	Link to model code repository	https://github.com/CESR-lab/ucl a-roms
147n	Description:	A description of the physical model characteristics, including version of equations being solved (hydrostatic vs non-hydrostatic), tracer advection scheme, how bottom drag is represented, mixed layer parameterizations, sub-grid mixing parameterizations if applicable, etc. Associated links to data, DOIs, or publications can be noted here, but should be supplemental.	The circulation model is a regional implementation of the Regional Ocean Modelling System (ucla-roms) Configured for the North Atlantic, centered on Iceland. The outer grid has a 3.3 km horizontal resolution and 100 vertical layers, while an inner nested grid has 40 m resolution and 100 vertical layers. ROMS is a free-surface, terrain-following, primitive equations ocean model, the hydrostatic primitive equations for momentum are solved using a split-explicit time-stepping scheme. All 2D and 3D equations are time-discretized using a third-order accurate predictor (Leap-Frog) and corrector (Adams-Molton) time-stepping algorithm. The primitive equations are discretized over variable topography using stretched terrain-following coordinates. The circulation model uses the 3rd-order upstream-biased (horizontal) and 4th-order centered differences (vertical) advection schemes for temperature and

			salinity. The model includes 12 freshwater inputs and is forced by the ERA5 atmospheric product (https://doi.org/10.1002/qj.3803) at the surface and by GLORYS at the boundaries. Vertical mixing is parameterized using the K-profile parameterization (KPP) from Large et al. 1994, and the air-sea interaction boundary layer in ROMS is based on the bulk parameterization of Fairall et al. (1996). Bathymetry is from GLORYS, the model T and S are initialized from GLORYS, and the model includes tides from the TPXO atlas.
1470	References:	Reference for model physics description	https://doi.org/10.1016/j.ocemod .2004.08.002
147p	Model BGC/Ecosystem Compone	ent	
147q	Name:	Name of BGC/Ecosystem component	MARBL
147r	Version:	Version of BGC/Ecosystem component used	Cesm2.2-n00 (imbedded in C-Star)
147s	Codebase:	Url link to where code can be found, the link to the specific commit (GitHub) or version should be provided.	https://github.com/marbl-ecosys /MARBL.git
147t	Description:	A description of the biogeochemical/biological model characteristics, including which parameters are modeled explicitly, derived carbonate system parameters, advection scheme for biological tracers, CO <sub>2</sub> solver protocol (e.g., CO2SYS), links to data/code with biological model parameters (e.g., growth and mortality rates), etc. Include details on whether	The Marine Biogeochemistry Library (MARBL) is a prognostic ocean biogeochemistry model that simulates marine ecosystem dynamics and the coupled cycles of carbon, nitrogen, phosphorus, iron, silicon, and oxygen and is a component of the Community System Earth Model 2 (CESM2). The ecosystem includes multiple phytoplankton

dissolution and precipitation of calcium carbonate are considered, how exchanges between sediment and overlying water are represented (if applicable), and whether active feedbacks between biological processes and the carbonate system are represented.

Associated links to data, DOIs, or publications can be noted here, but should be supplemental.

functional groups (diatoms, diazotrophs, small phytoplankton, and coccolithophores) and multiple potentially growth limiting nutrients (nitrate, ammonium, phosphate, silicate, and iron. There is one zooplankton group, dissolved organic material (semi-labile), sinking particulate pools and explicit simulation of the biogeochemical cycling of key elements (C, N, P, Fe, Si, O, plus alkalinity) (Moore et al. 2004). The ecosystem component is coupled with a carbonate chemistry module based on the Ocean Carbon Model Intercomparison Project (OCMIP) (Doney et al. 2009) allowing dynamic computation of surface ocean pCO2 and air-sea CO<sub>2</sub> flux. Photoadaptation is calculated as a variable phytoplankton ratio of chlorophyll to nitrogen based on Geider et al. 1998. Phytoplankton N/P ratios are fixed at the Redfield value of 16. but the diazotroph group has a higher N/P atomic ratio of 50. The model parameterizes a prognostic phytoplankton calcifier in MARBL that is modeled on coccolithophore physiology (Krumhardt et al., 2019). The ratio of calcification to photosynthesis by the coccolithophore functional type is responsive to environmental conditions, where the calcification to photosynthesis ratio is a function of

temperature, nutrients, and

CO<sub>2</sub>. Carbonate chemistry is explicit and there are two parallel carbonate systems including DIC and alkalinity tracers; applying fixed-preindustrial and time-evolving atmospheric CO<sub>2</sub> to these parallel systems enables cleanly computing anthropogenic CO<sub>2</sub> concentrations. MARBL computes burial and denitrification losses of material at the seafloor according to empirical relationships. Particulate organic carbon burial is computed using a relationship between burial efficiency and POC flux from Dunne et al. (2007), with an imposed maximum burial efficiency of 80%. Burial of SiO<sub>2</sub> at the seafloor is based on observations in Ragueneau et al. (2000). In MARBL, 4% of Si incidents on the seafloor are buried, except where the incident flux of Si to the seafloor exceeds 2 mmol m-2 d-1; then, 20% of Si is buried. As described above, sedimentary denitrification depends on the incident POC flux and is computed based on an empirical relationship from Bohlen et al. (2012). Burial of CaCO<sub>3</sub> on the ocean floor occurs where  $\Omega > \Omega crit$  in the model's bottom layer; where  $\Omega$  < Ωcrit, all CaCO<sub>3</sub> reaching the model's bottom layer is dissolved. All CaCO3 is assumed to be calcite, thus ignoring the distinction between

147u	Air-sea CO2 flux parameterization:	Description and/or references of air-sea CO <sub>2</sub> flux parameterization used, gas transfer velocity formulation and atmospheric CO <sub>2</sub> details (e.g., fixed or time varying, and if time varying which data were used).	the mineral forms calcite and aragonite, which may be important in modulating dissolution depths (Gangstø et al., 2008).  Air-sea CO2 gas exchange is parameterised as a function of temperature (T) and wind speed (u10), and the concentration of the gas in the air (Ca) and in the surface water (Cw) in the form:  F = k(u10 T)(Cw-Ca), where k is the gas transfer velocity. Gas transfer velocity is parameterized using the 4th order polynomial formulation of Wanninkhof (2014). Quadratic k <sub>660</sub> parameterisation is calibrated to give 16.5 cm/hr global average (recommended Naegler, 2009) for the ERA5 wind product by SeaFlux/Luke Gregor et al. (2023).  Atmospheric CO <sub>2</sub> is assumed fixed and spatially uniform at 428 ppm.
147v	References:	Links or DOIs to any reference(s) relevant to the model components/development, specific model configuration, model validation etc.	https://doi.org/10.1029/2021MS00 2647
147w	Other model components:	Additional components such as sea ice, sediment, atmosphere, etc., following the structure above if applicable (e.g., Name, Version, Codebase, Description, References).	Not applicable
147x	Grid Details:		

147y	Grid type:	Descriptive structure of grid (e.g., latitude-longitude grid, unstructured triangular, tripolar)	Rectangular x-y grid with rotation:  Central longitude: -19 Central latitude: 65 Grid Rotation: 20
147z	Region:	A description of the region modeled, include the latitude and longitude boundaries if they are not provided in another field. Latitude and longitude should be provided in decimal degrees (negative for southern and western hemispheres).	North Atlantic centered on Iceland Longitude range = -17° to -20° Latitude range = 60° to 70°
147aa	Arrangement:	The grid arrangement of orthogonal physical quantities (e.g. Arakawa A, Arakawa B, Arakawa C)	Arakawa C-grid
147ab	Nx:	Number of x grid points	800
147ac	Ny:	Number of y grid points	800
147ad	Nz:	Number of vertical coordinate levels	100
147ae	N nodes:	Number of grid nodes (if using an unstructured grid)	5285
147af	Horizontal resolution range:	Range of horizontal resolution (m or km)	3.3 km (for the outer nest)
147ag	Vertical resolution range:	Range of vertical resolution (m)	Max. 4 m (topography following vertical grid)
147ah	Input Details:		
147ai	Bathymetry:	Data source for bathymetry used (including links to data if available)	GLORYS bathymetry data- https://doi.org/10.48670/moi-00 021
147aj	Initial conditions	Data sources for initial conditions of all model state variables (including links to data if available)	Initial conditions from GLORYS (mercatorglorys12v1_gl12_mea n)
147ak	Boundary conditions:	Data source for boundary conditions for all model state	GLORYS (mercatorglorys12v1_gl12_mea

		variables (including links to data if available)	n)
147am	Atmospheric forcing data used:	Data source for atmospheric forcing if applicable (including links to data if available). Examples include, wind fields, shortwave and longwave radiation, air temperature, humidity, etc.	ERA5 hourly (https://doi.org/10.24381/cds.14 3582cf)
147an	Tidal forcing:	Data source for tidal forcing (including links to data if available)	TPXO atlas (https://www.tpxo.net/global/tpxo 10-atlas)
147ao	River & sediment flux details:	Description of river and sediment flux data used to force the model (including links to data if available)	River fluxes for the inner nest sourced from the Icelandic Met Office (https://en.vedur.is/) for 12 rivers, no river fluxes used for the outer nest. No sediment fluxes applied.
147ap	Experiment Details:		
147aq	Spin-up protocol:	A description of the spin up process chosen for the model initiation, including an explanation for how appropriate spin up was defined to be achieved.	2 weeks per nest
147ar	Start date and time:	Start date and time of model experiment in UTC	01-Jan-2024 01:20:30
147as	End date and time:	End date and time of model experiment in UTC	01-Jan-2034 01:20:30
147at	Output frequency:	Time frequency at which model fields are saved (e.g. hourly mean, daily mean)	Monthly means
147au	Time stepping scheme:	Method used to discretize time domain (e.g., Euler, Runge-Kutta, leapfrog)	10 second for spin-up - up to 3 minutes per timestep for outer nest
147av	Description of alkalinity addition:	A description of how alkalinity perturbation was applied in the model	Applied over multiple grid cells in initial conditions to ALK_ALT_CO2 variable in MARBL (only in inner nest, no Alk experiment in outer nest)

147aw	Hardware Configuration:		
147ax	Machine:	Machine name of hardware used to run model	Perlmutter
147ay	Operating system:	Operating system of hardware used to run model	Linux
147az	CPU/GPU details:	Details on CPU or GPU hardware	Details here: https://docs.nersc.gov/systems/ perlmutter/architecture/#cpu-no des
147ba	Memory:	Memory capacity of machine	512 GB of DDR4 memory total
147bb	Storage:	Storage capacity of operating system	44 PB
147bc	Parallelization:	Description of processors used in parallel, including number or processors and MPI version if used.	3 nodes and 108 ntasks per node

#### 149 Guidelines for Data Submission

150 This section outlines the specific requirements and recommendations for submitting data 151 associated with OAE research. It covers general guidelines for adjusted and raw data, in situ 152 sensor data, sediment processes, and biological/physiological data. Additionally, it provides 153 instructions for creating unique Project IDs to facilitate cross-linking of datasets, particularly for 154 research cruises and other projects, and timelines for archiving data. These standards ensure 155 data consistency, reproducibility, and compatibility across studies while allowing for flexibility to 156 include supplementary details in the OAE Metadata when repository fields are insufficient.

158 In this section, a indicates requirements in order to be considered compliant with this 159 protocol. "Recommendations" are strongly suggested best practices to support quality data 160 sharing, but may not always be possible.

## 161 General Guidelines for your Data

162 The following recommendations and requirements are general for both discrete and sensor 163 data.

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165 Requirements:

When preparing your data, refer to the data file templates provided in <u>Column Header</u>

Names that include recommended column header names and units for various data types.

169

When filling out your metadata, refer to the <u>Controlled Vocabularies</u> for inputs.

171 Field data representing baseline conditions, control conditions, or intervention conditions 172 will be uploaded separately. 173 174 The unique project ID must be included in any data upload's metadata in order to link 175 e.g., the model output to other affiliated project data, baseline data to intervention data, 176 etc. 177 178 A unique sample identification number should be assigned to vector data (use column 179 header name = 'sample ID'). These can simply be consecutive numbers. 180 181 If not included in the metadata (e.g., see fields under Observed Properties in NOAA's 182 OCADS metadata file), a ReadMe file should be provided in plain text format. Contents 183 may include the following as text, figures, charts, etc. (as applicable): 184 Description of calibrations or adjustments performed to data. 185 Any information needed to reproduce adjusted data or derived variables. This may 186 include, but is not limited to, equations, coefficients (e.g., if using CO2SYS for carbonate 187 parameter calculations; see *Derived Variables*). 188 References on data QA/QC processing steps (e.g., DOI, software and software settings 189 190 used, etc). For sensor data, include the sensor ID and/or serial number, certification number, as 191 available. 192 Analysis protocols should be described, or a DOI provided. 193 194 195 Missing values should be reported as '-999'. 196 Associated quality flags for measured variables should be indicated as 197 <parameter name> flag and follow the following flagging definitions (Jiang et al., 2022; 198 Table 2). 199 0 = interpolated or calculated data 200 1 = not evaluated/quality unknown 201 2 = acceptable 202 3 = questionable 203 4 = known bad 204

#### 208 Recommendations:

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6 = median of replicates

9 = missing value

- + If processing software were used, include firmware version in *ReadMe*.
- + Sampling protocols should be listed in the *ReadMe* file.
- + Providing meteorological data that provides context to the results of the project and interpretation of data is strongly encouraged. For example, rain accumulation (as it impacts salinity).

+ Point by point uncertainty/precision values should be included with data (indicated as <parameter\_name>\_uncertainty or <parameter\_name>\_precision). For sensor data, if no uncertainty or precision analyses were performed during the project, these may be estimated using the manufacturers calibration sheets, for example, a factory calibrated sensor may have an accuracy specification of "+/-2 uM or 1.5% of measurement, whichever is greater." This information can be converted into a point-by-point uncertainty value.

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#### 222 Guidelines for In Situ Sensor Data

#### 223 Requirements:

If adjusted data are provided, raw data must be provided for sensor and discrete data (indicated as <parameter\_name>\_raw and <parameter\_name>\_adjusted).

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224

Manufacturer calibration files are required with submission, if the sensor ID is not included, it should be included in the metadata or *ReadMe* file.

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#### 230 Recommendations:

+ It is strongly recommended that sensor data are provided in netCDF, especially when reporting data from a multi-sensor platform.

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+ Profile data may have associated standard deviation profile or median profile values (indicated as <parameter\_name>\_std and <parameter\_name>\_med).

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## 237 Guidelines for Model Output

238 Model output data plays a crucial role in interpreting and predicting the outcomes of OAE 239 interventions. Adhering to established data standards ensures that model configurations and 240 outputs are consistent, interoperable, and easily integrated with observational data. This section 241 outlines the requirements to maximize the usability and reproducibility of model output, as well 242 as to facilitate meaningful comparisons across studies and datasets.

243

#### 244 Requirements:

245 All model code, including software versions (e.g., compiler information), model configuration, experiment codes and input/forcing data wherever possible must be 246 shared publicly. Given data storage costs and limitations, it is not expected that large 247 input datasets (e.g. atmospheric forcing data or boundary conditions) that are publicly 248 available elsewhere be archived along with model code, but model code should link to 249 public data repositories containing forcing. If model forcing datasets are not already 250 stored publicly, it is recommended that they be publicly archived and linked to the model 251 code wherever possible. 252

- Documentation outlining the model components, code versions, configuration, forcing, and parameterizations named 'model\_description' if uploaded separately and provided in, xlsx, netCDF, or plain text format. An example template for this information is provided in the *Model Description Template*.
- Parameter names may refer to <u>Column Header Names and Controlled Vocabularies</u> for common naming conventions.
- The parameters modeled, spatial, and temporal frequency of model output data will vary substantially for specific model projects, and archiving large quantities of model output is impractical due to data storage limitations and costs. However, in cases where a biogeochemical model is used to quantify net CDR (using a baseline and intervention experiment), we recommend publicly archiving the following parameters from models from both baseline and intervention model experiments at minimum:
- 2D Air-sea CO<sub>2</sub> flux (mol/m<sup>2</sup>/s or mmol/m<sup>2</sup>/day) time series
- 3D Dissolved Inorganic Carbon (μmol/kg) time series
- 3D Total Alkalinity (μmol/kg) time series
- 3D Temperature (°C) time series
- 3D Salinity time series

To save space, derived variables do not need to be included, however the inputs needed to derive those variables (e.g. for CO2SYS) should be included. It is recommended that model output is archived on the original model grid, but the temporal frequency of the

provided data is project dependent and left to the data provider to decide what to supply.

280 Recommendations:

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- + The data from a counterfactual run and the intervention run may each be provided separately, as this can decrease the data storage needed.
- + It is recommended that model outputs are provided in netCDF format, following recommended naming conventions (see <u>Column Header Names and Controlled Vocabularies</u> for parameter naming conventions).
- + Additional recommended parameters to archive include:

289 Physical transport vectors (u, v, w)

Biological tracers (chlorophyll, phytoplankton, zooplankton, dissolved oxygen,

NO<sub>3</sub>- and NH<sub>4</sub>+, as available)

#### 293 Guidelines for Intervention Data

294 An intervention refers to the deliberate action taken to alter ocean chemistry, such as adding 295 alkalinity or reducing acidity, as part of an Ocean Alkalinity Enhancement (OAE) study. This

296 section builds on the metadata requirements by detailing the additional intervention-specific 297 data needed to fully document and contextualize the action, ensuring consistency and utility 298 across studies. The following Requirements and Recommendations are given for intervention 299 data, in addition to those listed under *General Guidelines for your Data*.

300 301 Requirements:

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307 308

Data related to dosing must be included\*, for example:

Flow rate

304 Mineral mass addition

Mineral mass addition rate

\*These can be detailed in a separate file, with associated links provided in the <u>OAE</u>

*Metadata*, or as data vectors (see Recommendations below).

309 Recommendations:

- + Providing the dosing information above as a vector, interpolated to the intervention data is suggested, using variable names: 'flow\_rate', 'mineral\_mass\_addition', and 'mineral\_mass\_addition\_rate'.
- + For usability, a binary vector describing whether the dosing is on/off is recommended with the data submission, e.g.,

  'dosing\_onoff': 0 = no dosing is occurring, 1 = dosing is active.

317

313

#### 318 Guidelines for Sediment Processes Data

#### 319 Requirements:

A description and/or reference to methods used for total carbon values must be included in the metadata. If there is no appropriate field to include this information in the data submitter's repository, it can be included in the OAE Supplemental Metadata file under the field 'Additional information'.

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Sediment sampling method should also be included. If there is no appropriate field to include this information in the data submitter's repository, it can be included in the OAE Metadata under the field 'Additional details'.

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#### 329 Recommendations:

+ Local sediment type should be included in the OAE Supplemental Metadata under 'Site description'.

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+ Information on water depth at the sediment collection site and core length should be provided in the data file.

#### 336 Guidelines for Biological/Physiological Data

#### 337 Recommendations:

Information on time scales and species level should be provided. If there is no appropriate field to include this information in the data submitter's repository, it can be included in the OAE Metadata under the field 'Additional details'.

338

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340 341

#### 342 Derived Variables

343 Derived variables refer to those that are estimated from measured variables. These may be 344 estimated utilizing software or additional calculations.

#### 345 Carbonate Parameters

346 When using CO2Sys to derive carbonate parameters, the user has a choice of equilibrium 347 constants. Please refer to the documentation in <a href="PyCO2Sys">PyCO2Sys</a> for recommended constants 348 appropriate to your oceanographic conditions. A general recommendation for seawater with 349 temperature between 2° and 35°, and salinity between 19 to 43, is to use the carbonic acid 350 dissociation constants of Leuker et al. (2000) and Waters et al. (2014) for brackish water (with 351 the salinity range 1 to 50 and temperature range 0 - 50). The boron-salinity ratio from Lee et al 352 (2010) is recommended, and for the dissociation constants of bisulfate (HSO<sub>4</sub><sup>-</sup>), Dickson (1990) 353 is recommended. For the dissociation constants of hydrofluoric acid (HF), Perez and Fraga 354(1987) is recommended. See Jiang et al. (2022) for further discussion of these 355 recommendations and associated uncertainties.

357 See fields under xCO<sub>2</sub>/pCO<sub>2</sub>/fCO<sub>2</sub> in NOAA's OCADS metadata file for additional required 358 metadata fields for continuous data of calculated pCO<sub>2</sub>/fCO<sub>2</sub>.

#### 359

#### 360 TEOS-10 Calculations

361 Software to calculate common ocean properties (e.g., density, absolute salinity, potential 362 temperature) based on thermodynamic equations can be downloaded for use with most coding 363 languages here: https://www.teos-10.org/software.htm and for use with excel here: 364 https://github.com/dpierrot/GSW Sys.

365

## 366 Cross-linking Data Sets with Common Identifiers

#### 367 Project ID

368 An ID that is unique based on the project's key attributes may be created using the following 369 fields, separated by an underscore character, however any method that creates a unique ID that 370 will link all project data (e.g., a project's baseline data to intervention data, and various data 371 submissions within an experiment type) is acceptable.

- Lead organizer surname and first initial, or company 372
- A unique date with the primary purpose to ensure a unique Project ID, as such the 373 guidelines here are not strict. Please choose a date most reasonable to the data, for 374 example, this may be the date that data were first collected for this project (likely the 375

```
beginning of baseline sampling). Provide the date in Coordinated Universal Time (or
376
          UTC) using ISO-8601 format (YYYYMMDD)
377
          Location (descriptive)
378
379
380 Example 1: Carbon Dive is submitting project data beginning January 20, 2023 for their study
381 site in San Francisco Bay where they collected baseline and intervention data, their resulting
382 Project ID is carbondive 20230120 sanfranciscobay.
383
384 Experiment ID
385 An experiment ID is provided for each unique Experiment type as well as unique experiments
386 within a single Experiment type. Options include using EXPOCODE (for research cruise
387 projects), or generating one by combining the following:
          Project ID (see above for how to generate)
388
          Experiment type (see Controlled Vocabularies)
389
          A numerical indicator starting at 01 to differentiate between experiments of the same
390
          type for a project.
391
392
393 In the example for Carbon Dive above, their Project ID is
394 carbondive 20240120 sanfranciscobay.
396 Carbon Dive collected baseline and intervention data during this project.
397 For the baseline experiment, the Experiment ID is
398 carbondive 20240120 sanfranciscobay natural01, and the Experiment ID for their intervention
399 is carbondive 20240120 sanfransiscobay manipulated01.
400
401 They also conducted an intervention experiment that was deemed reasonably distinct from the
402 first (e.g., the details under OAE Metadata Supplement for
403 carbondive sanfransiscobay manipulated01 were not representative of this intervention
404 experiment, however it was still considered to be under the same project), and used Experiment
405 ID carbondive_20240120_sanfransiscobay_manipulated02.
406
407 Example 2: Dr. Jane Smith is providing model output from two global studies, one from a
408 counterfactual model run and one from a baseline model run, their resulting Project ID is
409 smith 20241004 global, and Experiment IDs are smith 20241004 global modeloutput01 and
410 smith 20241004 global modeloutput02
411
412 Guidelines for Archiving
```

#### 413 Naming convention of data files:

414 It is recommended that individual data files are named by combining the Experiment ID with the 415 data type. For example, a file containing data from discrete carbonate bottle samples during the 416 first OAE intervention of project carbondive\_20250805\_Hvalfjordur will be titled 417 carbondive\_20250805\_Hvalfjordur\_manipulated01\_discrete. If multiple discrete bottle files will

- 418 be uploaded, appending a numerical value to the end starting with 01 can differentiate these.
- 419 However, it is recommended that data of a single type are uploaded together.
- 420 Other examples of data types include: profile (e.g., data files containing discrete and sensor
- 421 data from a CTD cast), field (for field data files containing a mix of data types), autonomous,
- 422 underway, discrete, physiological, and model output.

#### 424 Timeline for data submission:

425 Deadlines for submitting data depend on the intended use of the data. For example, data 426 submitted for regulatory purposes often required a faster turnaround to meet the demands of 427 project development, while data for academic investigations may not face the same external 428 pressures. However, the results of academic projects are fundamental to advancing mCDR 429 safely and responsibly and have therefore been allocated appropriate timelines to reflect this 430 importance.

431

- 432 Reporting and sharing model output may largely be dictated by project and registry timelines,
- 433 and verifiers will need to verify model results prior to credit delivery, requiring models to be
- 434 rigorously tested and validated before the intervention project begins to ensure that accurate
- 435 model-based quantification of CDR can be executed and shared on a scale of weeks,
- 436 depending on planned reporting periods.

437

438 Data for all purposes should be submitted by the earlier of the deadlines set by the project 439 funders, regulators, registry, and other stakeholders, or the following:

440

441 Sensor data: Delayed-mode (e.g., quality controlled and adjusted) data should be made 442 available within 3 months from collection (when the sensor is placed in-situ). It is recommended 443 that real time sensor data be archived within 1 month.

444

445 Model output: Within 3 months of completion of model experiments.

446

447 Discrete data: Discrete data from samples including carbonates, sediment processes, nutrients, 448 biological data etc. should be made available within 3 months from collection.

449

#### 450 Where to store data:

451 Data can be stored in any scientific data repository that provides long-term preservation of data 452 (ideally with version control capabilities), rich metadata management supporting the mCDR 453 metadata template as outlined previously, and that provides data citations with a unique DOI. 454 The choice of data repository may often be dictated by funder requirements. However, we make 455 the following suggested recommendations for data repositories.

456 457

458

- Discrete and sensor data are recommended to be stored at <u>NOAA's Ocean Carbon and</u> Acidification Data System (OCADS).
- Raw eDNA data are suggested to be archived at the <u>National Center for Biotechnology</u> Information (NCBI).

### 462 Column Header Names and Controlled Vocabularies

463 A fundamental principle of data standardization is ensuring consistent naming across data
464 submissions, projects, and repositories. If your chosen repository does not enforce a
465 vocabulary, please refer to the references below for recommended naming conventions.
466 Recommended units are also frequently provided for each variable, which significantly eases
467 the process of synthesizing data across projects when standardization is maintained.
468

#### 469 Column Header Names

470 Column header names are the labels given to specific data types, variables, or measurements 471 in a data set, commonly presented as abbreviated names in column headers. Standardizing 472 column header names significantly eases syntheses projects and ensures that a user can find 473 data of interest. Data file templates are provided below that include recommended column 474 header names. It is recommended to use the following data submission templates for the 475 following data types (provided in .xlsx files), this will ensure column header names and units are 476 standardized across projects.

477

478 Note to reviewers: Please select any of the following data types that you are most familiar with 479 to provide feedback on the column header names for these data.

480

#### 481 Discrete data:

- 482 Column Header Names Description
- Data File (.XLSX) Example

#### 484 Autonomous data:

- Column Header Names Description
- Data File (.XLSX) Example
- Further naming conventions of less-common and diagnostic variables are <u>provided by</u>
- 488 Argo

#### 489 Underway data:

- 490 Column Header Names Description
- Data File (.XLSX) Example
- 492 Physiological response data:
- Column Header Names Description
- Data File (.XLSX) Example

#### 495 Controlled Vocabularies

496 Controlled vocabularies are separate from column header names. These are controlled 497 definitions of whole descriptive words that may be used for metadata input, for example. 498

499 Note to reviewers: the motivation of the controlled vocabularies for experiment type is to be able 500 to pull out un-perturbed data from a large database (or in this example 'natural' data), for 501 example. This may relate to mCDR experiments, but there are many experiments that would be 502 considered 'manipulated' data. As such, this needs to be broad and not only mCDR-applicable 503 (as is the case with many of the controlled lists that follow).

504			
504a	Controlled Vocabularies for Experiment Type		
504b	Experiment type	Definition	
504c	Natural	Refers to measurements representing its natural environment or context. This includes gridded or calculated values. For example, the gridded SOCAT data product is considered an in-situ data product.	
504d	Manipulated	This refers to data or measurements representing conditions that have been adjusted, or transformed from their original state. For example, observations from mCDR field trial, mesocosm, laboratory experiment, are all considered manipulated values.	
504e	Model output	Model output refers to the results or data generated by numerical or computational models.	

505a	Controlled Vocabularies for mCDR Pathways		
505b	mCDR Pathway	Definition	
505c	Ocean alkalinity enhancement	Ocean Alkalinity Enhancement (OAE) is a method to help mitigate climate change by increasing the alkalinity of seawater to enhance its capacity to absorb and store atmospheric carbon dioxide (CO <sub>2</sub> ).	
505d	Macroalgal cultivation for CDR	Macroalgal Cultivation refers to the process of farming large seaweeds (macroalgae) such as kelp, sargassum, or other marine plants to absorb atmospheric carbon dioxide (CO <sub>2</sub> ) and potentially sequester it over the long term.	
505e	Direct ocean capture	Direct Ocean Capture (DOC) is a technology-driven approach to extract carbon dioxide (CO <sub>2</sub> ) directly from seawater.	
505f	Ocean fertilization	Ocean Fertilization is a mCDR strategy that involves adding nutrients, such as iron, nitrogen, or phosphorus, to the ocean to stimulate the growth of phytoplankton or other microscopic plants that absorb carbon dioxide (CO <sub>2</sub> ) through photosynthesis.	

505g	Artificial upwelling and downwelling	Artificial Upwelling and Downwelling are mCDR strategies that involve manipulating ocean water movement to enhance natural carbon sequestration processes.
505h	Coastal blue carbon	Coastal Blue Carbon refers to the carbon captured and stored by coastal ecosystems, such as mangroves, salt marshes, and seagrasses. These ecosystems absorb carbon dioxide (CO <sub>2</sub> ) from the atmosphere and store it in their biomass (leaves, roots, stems) and sediments, making them natural and effective solutions for mCDR.
505i	Marine ecosystem recovery	Marine Ecosystem Recovery refers to the restoration and protection of marine ecosystems to enhance their natural ability to capture and store carbon dioxide (CO <sub>2</sub> ). This approach leverages the natural carbon-sequestering processes of marine habitats like coral reefs, kelp forests, seagrass meadows, oyster beds, and deep-sea ecosystems, aiming to rebuild biodiversity, ecosystem functions, and carbon storage capacity.

506
507 Note to reviewers: please review the suggested vocabulary list and definitions below. We aim to 508 create easily recognizable categories of OAE treatment types while grouping activities that may 509 be relevant for field data synthesis.

510a	Controlled Vocabularies for OAE Treatment Types		
510b	Treatment type	Definition	
510c	Electrochemical alkalinity addition	Uses electrochemistry to increase seawater alkalinity. This process typically involves separating seawater into acidic and alkaline streams, with the alkaline stream being released into the ocean to enhance carbon sequestration, with the acidic stream neutralized on land or used as a byproduct.	
510d	Mineral alkalinity addition	Involves adding alkaline minerals or particulate slurry (such as MgOH <sub>2</sub> , MgO, or CaO) to seawater either directly or through coastal outfalls (such as wastewater) to increase its alkalinity.	
510e	Dissolved alkalinity addition	Involves the addition of dissolved or aqueous alkaline feedstocks (e.g. NaOH solution) into seawater either	

		directly in coastal waters, through coastal outfalls or in the open ocean.
510f	River alkalinity enhancement	Involves adding alkaline substances (such as limestone) in rivers before they flow into the ocean for the purposes of carbon removal or emission reduction.
510g	Coastal enhanced weathering	Introduces alkaline mineral sand (e.g. olivine), boulders or berms in coastal areas to promote the absorption of CO <sub>2</sub> from the atmosphere into carbonate minerals (e.g., calcium carbonate, CaCO <sub>3</sub> ).
510h	Pre-equilibrated alkalinity addition	Involves pre-treating seawater with alkalinity in a controlled setting, allowing equilibration with the atmosphere before returning into the marine system.

5	1	1
J	+	+

511a	Controlled Vocabularies for Model Experiment Types		
511b	Model Experiment Types	Definition	
511c	Counterfactual	A counterfactual model experiment describes a simulation created to mimic current oceanic conditions without interventions, such as mCDR treatment.	
511d	Perturbation	A perturbed model experiment describes a simulation created to mimic an intervention or change from the natural ocean conditions.	

513 <u>Mineral feedstock source materials for OAE</u> (based on Renforth and Henderson, 2017; Caserini 514 et al., 2022). This list includes input options to the 'Alkalinity feedstock type' field of the <u>OAE</u> 515 <u>Metadata</u>.

516

517 Note to reviewers: The controlled vocabularies below are previously vetted and provided for 518 reference only. (No additional review is needed)

- 520 Additional relevant vocabularies may include the following categories:
- 521 Observation types (Jiang et al., 2023b)
- 522 Instrument type (Jiang et al., 2023b)
- 523 Platform type (Jiang et al., 2023b)
- 524 Country: provided by the NERC vocabulary server
- 525 Sea names: provided by SeaDataNet C16 (sea areas)
- 526 <u>Institutions</u>: provided by the Research Organization Registry (ROR)

527 Research Vessel Platform Codes: provided by the International Council for the Exploration of 528 the Sea (ICES) 529 530 Emerging Standards 531 This section describes in-work standards, file structures, etc., that are supplementary or 532 complimentary to the OAE Data Management Protocol. 533 534 There are multiple areas that are currently under development or have not been covered within 535 the current version of the protocol. However, work is ongoing to broaden the current protocol to 536 be a more robust resource for the OAE community. 537 538 If you are interested in providing input or leadership on the development of data management 539 guidelines for these emerging areas, please reach out to Irene Polnyi, Director of Strategy and 540 Partnerships at Carbon to Sea Initiative (irene@carbontosea.org). 541 542 Content expanded in updated protocol versions may include: 543 Sensor quality control recommendations: Consensus on the best practices for sensor quality 544 control and calibration will be documented, with the goal to provide a list of useful resources 545 (guides, publications, tools, software, etc.), starting with the common biogeochemical sensors 546 (nitrate, pH, pCO<sub>2</sub>, dissolved oxygen, particle backscatter, chlorophyll fluorescence, and 547 irradiance). 548 549 Biological experimental best practices: During the drafting of the current protocol, the OAE 550 Data Standards Biological Working Group highlighted the need for standardized best practices 551 in methods, calibrations, and sampling specific to OAE projects. Insights and outcomes from 552 focused efforts in this area will be integrated into future iterations of the protocol. 553 554 Sediment processes data best practices: Work is in progress by the sediment processes 555 community to standardize methodological approaches. Guidelines will be added to this protocol 556 as their work develops. 557 558 Social sciences data best practices: Work is in progress by the social science community to 559 develop further recommendations. Guidelines will be added to this protocol as these 560 recommendations develop. 562 Laboratory and mesocosm studies: Although the current protocol focuses on field data, 563 laboratory and mesocosm experiments play a crucial role in advancing OAE research. These 564 data come with unique standardization challenges that need to be addressed. As 565 recommendations become available, future iterations of this protocol will incorporate tailored 566 guidelines for laboratory and mesocosm data, informed by input from experts in these areas. 567

```
568 Version control: A section on "recommendations for version control" that includes
569 recommendations for updating data due to errors found in previous versions, updated methods,
570 and/or bad data found will be discussed in future versions of the protocol.
571
572 Deprecated Standards and Practices
573 Previous versions of this protocol can be found on the host site.
574 The versioning format is defined as follows.
575 Update definitions:
           MAJOR: Significant changes, such as new sections, substantial revisions, or breaking
576
           changes to existing recommendations.
577
           MINOR: Additions or refinements to existing recommendations that are
578
           backward-compatible.
579
           REVISION: Small edits like fixing typos, formatting, or minor clarifications without
580
581
           changing the meaning or scope.
582
583 Triggers for updates:
584 1. MAJOR Version (e.g., `2.0.0`):
585 - Introduced a new framework or restructured the document.
586 - Added entirely new priority levels or sections.
587 - Removed or deprecated previous recommendations in a way that could affect adoption.
588 - Example: Moving from draft to the first official release ((0.1) \rightarrow (1.0)).
589
590 2. MINOR Version (e.g., `1.2.0`):
591 - Added new recommendations that complement existing ones.
592 - Updated examples, case studies, or appendices without altering the core content.
593 - Clarified ambiguities in key recommendations while maintaining backward compatibility.
594
595 3. REVISION (e.g., `1.1.3`):
596 - Corrected grammar, typos, or formatting.
597 - Reworded text for readability without changing intent.
598 - Fixed links or citations.
599 Acknowledgements
600 Coordination Team
601 The coordination team was responsible for the conceptualization and delivery of the protocol.
602
603 Leads: Jacki Long, LiQing Jiang, Veronica Tamsitt
604 With funding and steering support from: Irene Polnyi, Anna Madlener, David P. Keller
606 Data Initiative Steering Committee
```

- 607 The steering committee comprises members who are active in OAE field work to provide
- 608 strategic guidance to the Data Management initiative coordination team as they assess the
- 609 landscape of field data, surface areas of existing alignment and identify areas of opportunity.

611 Steering Committee: Gabby Kitch, David "Roo" Nicholson, Ruth Musgrave

612

### 613 Advisory and Consultation

- 614 Strategic guidance and consultation was provided from a range of experts via interview,
- 615 document feedback and thought partnership.

616

- 617 Advisory and consultation: Jing He and Sophie Gill, Isometric; Tannis Thorlakson and Vilas Rao,
- 618 Cascade Climate; Aaron Olson, Planetary Technologies; Jonathan Sharp, UW/PMEL.

619

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- 621 Participants of the OAE Data Dive Workshop (Halifax, September 2024) provided valuable input
- 622 into the first draft of the protocol, including thoughtful discussion around important trade-offs,
- 623 surfacing key areas of alignment and driving towards internal consensus.

624

Grace Andrews, Hourglass Dariia Atamanchuk, Dalhousie Alice Benoit-Cattin, HAFRO

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### 654 Contributing Authors during the Open Comment Review Period

655

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## 695 Appendix

### 696 Appendix A: Column header names for discrete data:

697 OCADS Column Header standards for Profile Data. Recommended column header

698 abbreviations, recommended units, and brief descriptions, for discrete chemical oceanographic

699 observations. In this table, CTD refers to the group of instruments for measuring conductivity

700 (salinity), temperature, and depth, and CTD-rosette to the complete system of Niskin bottles

701 (used for seawater sampling) on a frame together with the CTD. "N/A" means not applicable.

702 "DP" is short for decimal places, or the number of digits after the decimal point. For more

703 information, please check out Jiang et al., 2022.

Column Header standards for Profile Data				
Abbreviation [unit]	Full unit	DP	Description	
EXPOCODE	N/A	N/A	Expedition code consists of the four-digit International Council for the Exploration of the Sea (ICES) platform code and the date of departure from port (UTC) in ISO8601 format (YYYYMMDD). For example, a research expedition onboard NOAA Ship Ronald H. Brown (ICES code: 33RO) leaving the port on August 27, 2015 (Coordinated Universal Time, or UTC) would have an EXPOCODE of 33RO20150827.	
Cruise_ID	N/A	N/A	Cruise identification is the particular ship cruise number or other alias for the cruise. A Cruise_ID (e.g., A16N2013) could consist of a Section_ID (A16N) and the sampling year (e.g., 2013), if only one section is covered during the cruise.	
Section_ID	N/A	N/A	Identification for a cruise section/leg (e.g., A16N, or P02).	
Station_ID	N/A	N/A	Station identification. Numerical Station_IDs without letters are recommended to facilitate future QC efforts.	

Cast_number	N/A	N/A	Cast number, where a cast is the lowering of equipment over the side at one station, e.g., CTD, net tow, etc. Cast_number should be sequential and restart with 1 for each station.
Rosette_position	N/A	N/A	Rosette position refers to the position number around the CTD-rosette (e.g., 1 of a 1-12, or 1-24, or 1-36 number).
Niskin_ID	N/A	N/A	Niskin_ID is a unique alphanumeric identifier assigned to only that Niskin bottle over the duration of the expedition.
Niskin_flag	N/A	N/A	Quality control flag for tracking problems with Niskin closure and integrity.
Sample_ID	N/A	N/A	A sample identifier (Sample_ID), which uniquely identifies a row of data during the subsequent QC and interpretation process, is often generated by concatenating the Station_ID, Cast_number, and Rosette_position, according to: Sample_ID = Station_ID × 10000 + Cast_number × 100 + Rosette_position. For example, at station 15, the 2nd cast, a Rosette_position of 3 will have a Sample_ID of 150203.
Year_UTC	N/A	0	Calendar year in UTC when Niskin bottles at a specific depth are triggered
Month_UTC	N/A	0	Calendar month in UTC when Niskin bottles at a specific depth are triggered
Day_UTC	N/A	0	Calendar day in UTC when Niskin bottles at a specific depth are triggered
Time_UTC	[hh:mm:ss]	N/A	Time in UTC (hh:mm:ss) when Niskin bottles at a specific depth are triggered
Yearday_UTC	N/A	2	Yearday refers to the day number in an annual cycle. (e.g., 06:00 on Jan 1 means yearday = 1.25, 18:00 on Dec 31 means yearday = 366.75 in a leap year). Note, Yearday_UTC starts with 1, instead of 0. It can be calculated according to this equation: Yearday_UTC = datefunction(Year_UTC, Month_UTC, Day_UTC)

			- datefunction(Year_UTC, 1, 1) + Time_UTC + 1, where, "datefunction" is the date function of a program (e.g., in Excel, the data function would be "DATE").
Latitude	decimal degrees	4	Latitude in decimal degrees North (negative for southern hemisphere) when Niskin bottles at a specific depth are triggered
Longitude	decimal degrees	4	Longitude in decimal degrees East (negative for western hemisphere) when Niskin bottles at a specific depth are triggered
Depth_bottom	m	0	Bottom water depth of the sampling station
CTDPRES	dbar	1	Hydrostatic pressure recorded from CTD at the depth where the sample is taken
Depth	m	1	Depth at which a sample is taken. It can be approximated from CTDPRES and Latitude using the TEOS-10 equation.
CTDTEMP_ITS90	deg_C	3	In situ temperature recorded from CTD on the ITS-90 scale. If the temperature scale is IPTS-68, this term should be replaced with "CTDTEMP_IPTS68".
CTDTEMP_flag	N/A	N/A	Quality control flag for CTDTEMP
CTDSAL_PSS78	N/A	3	Salinity calculated from conductivity recorded with CTD using the equation of the Practical Salinity Scale of 1978. CTDSAL_PSS78 is unitless.
CTDSAL_flag	N/A	N/A	Quality control flag for CTDSAL
Salinity_PSS78	N/A	3	Salinity calculated from conductivity measured from discrete bottles using the equation of the Practical Salinity Scale of 1978. Salinity_PSS78 is unitless.
Salinity_flag	N/A	N/A	Quality control flag for Salinity_PSS78
CTDOXY	umol/kg	1	Dissolved oxygen (O <sub>2</sub> ) content from oxygen sensors mounted on the CTD
CTDOXY_flag	N/A	N/A	Quality control flag for CTDOXY

Oxygen	umol/kg	1	Dissolved oxygen (O <sub>2</sub> ) content measured from discrete-bottle-based Winkler titration
Oxygen_flag	N/A	N/A	Quality control flag for Oxygen
DIC	umol/kg	1	Total dissolved inorganic carbon content
DIC_flag	N/A	N/A	Quality control flag for DIC
TA	umol/kg	1	Total alkalinity content
TA_flag	N/A	N/A	Quality control flag for TA
pH_T_measured	N/A	4	pH measured on Total Scale (T) at measurement temperature and 1 atmosphere pressure (0 dbar applied pressure) using spectrophotometric methods. If the pH is measured on the seawater, free, or NBS scale, replace "T" with SWS, F, or NBS, respectively. For pH measurements made using electrodes, "pH_T_measured (electrode)" should be used instead.
TEMP_pH	deg_C	2	Temperature at which the pH_TS_measured value is measured
pH_flag	N/A	N/A	Quality control flag for pH_TS_measured
Carbonated_measured	umol/kg	1	Dissolved carbonate ion content ([CO <sub>3</sub> <sup>2-</sup> ]) at measurement temperature and 1 atmosphere pressure (0 dbar applied pressure).
TEMP_Carbonate	deg_C	2	Temperature at which the Carbonate_measured value is measured
Carbonate_flag	N/A	N/A	Quality control flag for Carbonate_measured
fCO2_measured	uatm	1	Fugacity of carbon dioxide ( $fCO_2$ ) in air that is in equilibrium with seawater measured from discrete bottles at measurement temperature and 1 atmosphere pressure (0 dbar applied pressure).
TEMP_fCO2	deg_C	2	Temperature at which the fCO2_measured value is measured
fCO2_flag	N/A	N/A	Quality control flag for fCO2_measured

Silicate	umol/kg	2	Silicate (total dissolved inorganic silicate: Si(OH) <sub>4</sub> , H <sub>4</sub> SiO <sub>4</sub> , SiO2, Sil) content
Silicate_flag	N/A	N/A	Quality control flag for Silicate
Phosphate	umol/kg	2	Phosphate (total dissolved inorganic phosphate: H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> , HPO <sub>4</sub> <sup>2-</sup> , PO <sub>4</sub> <sup>3-</sup> ) content
Phosphate_flag	N/A	N/A	Quality control flag for Phosphate
Nitrate	umol/kg	2	Nitrate (NO <sub>3</sub> -1) content. This term should not be used to indicate nitrate plus nitrite content, although the distinction is generally small because nitrate >> nitrite.
Nitrate_flag	N/A	N/A	Quality control flag for Nitrate
Nitrite	umol/kg	2	Nitrite (NO <sub>2</sub> -1) content
Nitrite_flag	N/A	N/A	Quality control flag for Nitrite
Nitrate_and_Nitrite	umol/kg	2	Nitrate plus nitrite content
Nitrate_and_Nitrite_flag	N/A	N/A	Quality control flag for Nitrate_and_Nitrite
Ammonium	umol/kg	2	Ammonium (NH <sub>4</sub> <sup>+</sup> and NH <sub>3</sub> ) content
Ammonium_flag	N/A	N/A	Quality control flag for Ammonium

## 706 Appendix B: Column header names for autonomous data:

- 707 OCADS Column Header standards for autonomous sensor data. Column header abbreviations,
- 708 their preferred units and brief descriptions for continuous measurements of oceanographic
- 709 variables using autonomous or remotely operated platforms, e.g., time-series mooring,
- 710 Saildrones, gliders, and Argo floats, instead of traditional manned research vessels. "N/A" is
- 711 short for "not applicable". Users can go to the "Resources" tab and click the "Quality Control
- 712 Flags" collapsible to access the definitions of the quality control flags.

Column Header Standards for Autonomous Sensor Data			
Abbreviation Unit Description			
EXPOCODE	N/A	Expedition code (EXPOCODE) consists of the four-digit International Council for the Exploration of the Sea (ICES) platform code	

		and the date of departure from port (UTC) in YYYYMMDD.
Platform_type	N/A	Controlled vocabularies for the types of the platform, e.g., research vessel, Saildrone, glider, argo, fish vessel, oil tanker, mooring, etc.
Platform_name	N/A	The name of the platform, e.g., Ronald H. Brown.
Year_UTC	N/A	Calendar year in Coordinated Universal Time (UTC)
Month_UTC	N/A	Calendar month in Coordinated Universal Time (UTC)
Day_UTC	N/A	Calendar day in Coordinated Universal Time (UTC)
Time_UTC	[hh::mm::ss]	Time in the format of hh:mm:ss
Yearday_UTC	N/A	Yearday refers to the day number in an annual cycle. (e.g., 12 pm on Jan 1 means Yearday = 1.50, 6 am on Dec 31 means Yearday = 366.25 in a leap year). Two digits after the decimal point are recommended.
Latitude	decimal degree	Latitude in decimal degrees North (negative for Southern Hemisphere)
Longitude	decimal degree	Longitude in decimal degrees East (negative for Western Hemisphere)
Depth	meter	Depth (in meters) at which the sensor is located
SST_ITS90	degrees Celsius	Sea surface temperature
SSS_PSS78	N/A	Sea surface salinity
Pressure_ATM_LICOR	hPa	Atmospheric pressure as recorded by LICOR
Temperature_LICOR_ITS90	degrees Celsius	Temperature as recorded by LICOR
xCO2_SW_wet	µmol/mol	Mole fraction of carbon dioxide in seawater in wet gas
xCO2_SW_flag	N/A	Quality control flags for mole fraction of carbon dioxide in seawater in wet gas
xCO2_ATM_wet	µmol/mol	Mole fraction of carbon dioxide in air in wet gas
xCO2_ATM_flag	N/A	Quality control flags for mole fraction of carbon dioxide in air in wet gas

xH2O_SW	µmol/mol	Mole fraction of H <sub>2</sub> O in the headspace of the equilibrator
xH2O_ATM	μmol/mol	Mole fraction of H <sub>2</sub> O in air
xCO2_SW_dry	µmol/mol	Mole fraction of CO <sub>2</sub> in seawater in dry gas
xCO2_ATM_dry	µmol/mol	Mole fraction of CO <sub>2</sub> in air in dry gas
fCO2_SW_sat	µatm	Fugacity of CO <sub>2</sub> in seawater at saturated water vapor pressure
fCO2_ATM_sat	µatm	Fugacity of CO <sub>2</sub> in air at saturated water vapor pressure
dfCO2	µatm	Difference of fCO <sub>2</sub> in water and air (fCO2_SW - fCO2_Air)
pH_T_insitu	N/A	pH on total scale at in situ temperature
pH_flag	N/A	Quality control flag for pH_T_insitu
Oxygen	μmol/kg	Dissolved oxygen measured from sensor
Oxygen_flag	N/A	Quality control flag for dissolved oxygen
Percent_O2	N/A	Percent O <sub>2</sub> measurement made in equilibrated air
Percent_O2_flag	N/A	Quality control flag for Percent_O2
Chl_a	μg/L	Chlorophyll a concentration
Chl_a_flag	N/A	Quality control flag for Chlorophyll a concentration

## 715 Appendix C: Column header names for underway data:

- 716 OCADS Column Header standards for underway data. Column header abbreviations, their
- 717 preferred units, and brief descriptions for surface underway based chemical oceanographic
- 718 data. "N/A" is short for "not applicable". Users can go to the "Resources" tab and click the
- 719 "Quality Control Flags" collapsible to access the definitions of the quality control flags.

Column Header Standards for Underway Data		
Abbreviation Unit Description		
EXPOCODE	N/A	Expedition code (EXPOCODE) consists of the four-digit International Council for the Exploration of

		the Sea (ICES) platform code and the date of departure from port (UTC) in YYYYMMDD.
Cruise_ID	N/A	Cruise identification
Year_UTC	N/A	Calendar year in Coordinated Universal Time (UTC)
Month_UTC	N/A	Calendar month in Coordinated Universal Time (UTC)
Day_UTC	N/A	Calendar day in Coordinated Universal Time (UTC)
Time_UTC	[hh:mm:ss]	Time in the format of hh:mm:ss
Yearday_UTC	N/A	Yearday refers to the day number in an annual cycle. (e.g., 12 pm on Jan 1 means Yearday = 1.50, 6 am on Dec 31 means Yearday = 366.25 in a leap year). Two digits after the decimal point are recommended.
Latitude	decimal degree	Latitude in decimal degrees North (negative for Southern Hemisphere)
Longitude	decimal degree	Longitude in decimal degrees East (negative for Western Hemisphere)
Depth	m	Depth in meters
SST_ITS90	degree Celsius	Sea surface temperature (usually intake temperature)
SSS_PSS78	N/A	Sea surface salinity
Pressure_ATM	hPa	Sea level atmospheric Pressure
Temperature_EQU_ITS90	degree Celsius	Water temperature recorded in the equilibrator
Pressure_EQU	hPa	Pressure inside the headspace of the equilibrator. 1 hPa = 1 mbar.
xCO2_EQU	µmol/mol	Mole fraction of carbon dioxide (dry) inside the headspace of the equilibrator
xCO2_ATM	µmol/mol	Mole fraction of carbon dioxide (dry) in the atmosphere
xCO2_ATM_interpolated	µmol/mol	Interpolated atmospheric $xCO_2$ to match with water analyses time
fCO2_SW_SST	µatm	Fugacity of seawater carbon dioxide at SST
fCO2_SW_flag	N/A	Quality control flag for fugacity of seawater carbon dioxide
fCO2_ATM_interpolated	µatm	Interpolated atmospheric fCO <sub>2</sub>
dfCO2	µatm	Delta fCO <sub>2</sub> between seawater and atmosphere (fCO2_SW - fCO2_ATM)

pH_T_insitu	N/A	pH on total scale at in situ temperature
pH_flag	N/A	Quality control flag for pH_T_insitu
Oxygen	µmol/kg	Dissolved oxygen measured from sensor
Oxygen_flag	N/A	Quality control flag for dissolved oxygen
Percent_O2	N/A	Percent O <sub>2</sub> measurement made in equilibrated air
Percent_O2_flag	N/A	Quality control flag for Percent_O2
Chl_a	μg/L	Chlorophyll a concentration
Chl_a_flag	N/A	Quality control flag Chlorophyll a concentration

# 722 Appendix D: Physiological response data:

- 723 OCADS Column Header standards for physiological data. Column header abbreviations, their
- 724 preferred units, and brief descriptions for physiological response studies (e.g., laboratory
- 725 experiment, mesocosm, field experiments, and natural analogues). "N/A" is short for "not
- 726 applicable".

Physiological Header Descriptions				
Abbreviation	Unit	Description		
Measurement_ID	N/A	A unique identification number of the measurement		
Type_of_study	N/A	The specific type of physiological response study. It can be laboratory experiment, mesocosm, field experiment, natural analogues, etc. Please be as specific as possible.		
Treatment_type	N/A	Whether this is an ocean acidification study or an ocean alkalinity enhancement study. The input can be a choice of "Acidification", or "Alkalinization".		
Treatment_method	N/A	How specifically the seawater acidity or alkalinity was manipulated. The input can be any of "Bubbling CO <sub>2</sub> ", "Adding hydrochloric acid", "Adding calcite", "adding magnesite", or "Electrochemical", etc.		
Treatment_details	N/A	The type, characteristics, and amount of alkaline or acid materials, e.g., addition of 100g of		

	hydrated lime (Ca(OH)₂) with a grain size <63μm in diameter to a tank with a capacity of 100L
N/A	Species of the marine organisms studied
N/A	It is recommended to use the species reference databases from the Integrated Taxonomic Information System (ITIS, <a href="http://www.itis.gov/">http://www.itis.gov/</a> ), World Register of Marine Species (WoRMS, <a href="http://marinespecies.org/">http://marinespecies.org/</a> ), Catalogue of Life (COL, <a href="https://www.catalogueoflife.org/">https://www.catalogueoflife.org/</a> ), or Paleobiology Database (PBDB, <a href="https://paleobiodb.org/classic/classificationForm">https://paleobiodb.org/classic/classificationForm</a> ).
N/A	This can be egg, embryo, larva, juvenile, or adult, etc.
N/A	Location where the organisms were collected. Please be as specific as possible
decimal degrees	Bounding box for the location of the organism collection
decimal degrees	Bounding box for the location of the organism collection
decimal degree	Bounding box for the location of the organism collection
decimal degree	Bounding box for the location of the organism collection
YYYY-MM- DD	Local date when the organisms were collected
hh:mm	Local time when the organisms were collected
N/A	Location where the experiment was carried out
N/A	Identification of the tank (if applicable)
N/A	The type of the tank.
L	The volume of the tank
N/A	Whether natural seawater or artificial seawater was used
N/A	If natural seawater was used, please specify the location where seawater was collected
N/A	Whether a flow-through system or a static system was used
	N/A  N/A  N/A  decimal degrees  decimal degrees  decimal degree  YYYY-MM-DD  hh:mm  N/A  N/A  N/A  N/A  N/A  N/A  N/A

Flow_rate	L/min	If a flow-through system was used, please specify the flow rate here
Target_treatment_level_fCO2	µatm	Target treatment level in terms of fugacity of carbon dioxide. If pCO <sub>2</sub> is used, please change the header name to reflect that.
Target_treatment_level_pHT	N/A	Target treatment level in terms of pH on total scale.
Target_treatment_level_TA	µmol/kg	Target treatment level in terms of total alkalinity content.
Exposure_type	N/A	Type of exposure
Date_experiment_start	YYYY-MM- DD	Local date when the experiment was started
Time_experiment_start	hh:mm	Local time when the experiment was started
Date_sampling	YYYY-MM- DD	Local date when the sample was collected
Time_sampling	hh:mm	Local time when the sample was collected
Exposure_duration	days	Duration of the exposure
Temperature_ITS90	degrees Celsius	Water temperature at ITS90 scale
Salinity_PSS78	N/A	Water salinity at the Practical Salinity Scale 1978
DIC	µmol/kg	Total dissolved inorganic carbon content
TA	µmol/kg	Total alkalinity content
рНТ	N/A	pH on total scale
fCO2	µatm	Fugacity of carbon dioxide. If partial pressure of carbon dioxide is reported instead, please change the header name to reflect that.
Omega_aragonite	none	Aragonite saturation state
Omega_calcite	none	Calcite saturation state
Oxygen	µmol/kg	Dissolved oxygen content
Silicate	µmol/kg	Silicate content
Phosphate	µmol/kg	Phosphate content
Nitrate	µmol/kg	Nitrate content

(F	Response variables)	variable dependent	