RECCAP2-ocean: Protocol for observation-based products

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Overview

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The majority of this protocol is based on the <u>RECCAP2 model protocol</u> to ensure congruence between data sets. Thus, if in doubt, consult the modelling protocol for naming conventions, file formatting, etc. Many of the data and data products that will be used in RECCAP2 already exist. These products should be formatted to match the RECCCAP2 protocal by the relevant author/data provider if required. In addition, the data provider should add documentation as specified later in this section.

RECCAP2 ocean data will include the product categories as listed below (see the RECCAP2 ocean scoping document for details).

- Surface ocean pCO₂ products e.g., CMEMS-FFNN by Denvil-Sommer et al. (2019)
- Ocean interior products e.g., MOBO-DIC_MPIM by Keppler et al. (2020)

Product specific protocols

Below we detail the protocols for each of the categories. For protocols common to all products, see the <u>File specifications</u> section. Note that each product should also include a product description (a.k.a. README) file - requirements for this description is also listed under each product.

Surface ocean pCO₂ products

The pCO₂ product must meet the following requirements to be included in the RECCAP-2 study:

- be available from 1985 to 2018 (exceptions can be made)
- 90% of the ice free ocean must be available for all time steps of the product (OISST sea-ice fraction will be used to determine the ice free region)
- Contain all variables that are listed as Priority 1 in the table below

We strongly encourage data submitters to also include variables that are listed as Priority 2. *Note that fluxes should be positive for uptake and negative for outgassing. Also note that the dimensions are [lon, lat, time] which may differ from the usual [time, lat, lon].*

Variable Name	Units	Output frequenc y	Shape	Priority	Long name
fgco2_glob	Pg C yr ⁻¹	monthly	Т	1	Globally integrated air-sea CO ₂ flux (positive downward)
fgco2_reg	Pg C yr ⁻¹	monthly	iT	1	Regionally integrated air-sea CO ₂ flux (positive downard) (using regional bounds), i: number of regions. (<u>Regional mask available on the website</u>)
fgco2	mol m ⁻² s ⁻¹	monthly	XYT	1	Flux density of the total air-sea CO2 exchange (positive downward)
spco2	μatm	monthly	XYT	1	Surface ocean pCO2
fice	-	monthly	XYT	1	fractional ice-cover (=sea-ice concentration) used for the computation of the air-sea exchange flux [0-1]
area	m ²		XY	1	Total surface area of each grid cell
Kw	m s ⁻¹	monthly	XYT	2	Air-sea piston velocity
pco2atm	μatm	monthly	XYT	2	Atmospheric pCO2 ('pco2atm' [uatm] will vary spatially, as opposed to the spatially uniform 'xco2atm' [ppm] atm CO2 forcing due to corrections for atm pressure and vapor pressure)
alpha	mol m ⁻³ µatm ⁻¹	monthly	XYT	2	CO2 solubility
tos	degC	monthly	XYT	3	sea-surface temp
sos	-	monthly	XYT	3	sea-surface salinity

Requirements for **README**:

- Original study citation and dataset citation if applicable
- Gas transfer velocity (*Kw*) formulation used (e.g. Nightingale et al. 2000). What wind product was used. What was the scaling factor for *Kw*
- The temperature, salinity, and wind products used to calculate *Kw* and *alpha* should be listed.
- Handling of sea-ice with respect to air-sea CO2 fluxes (product and application).

- The procedure used to calculate *pco2atm* with details of the following: xCO₂ product, interpolation, pH₂O correction used and pressure product.
- Other comments or idiosyncrasies in the dataset that will affect global or regional comparison

Watson et al. (2020) approach

Watson et al. (2020) present an approach to adjust $p\mathrm{CO}_2$ to the vertical gradients of temperature in the water column between the ship intake depth and the skin temperature measured by satellites. $F\mathrm{CO}_2$ is calculated from the adjusted atmospheric and seawater $p\mathrm{CO}_2$. We do not require that $p\mathrm{CO}_2$ data product providers submit a second version calculated with this approach, but we would welcome these results. Below is a brief summary of how to calculate $F\mathrm{CO}_2$ as done in Watson et al. (2020):

- 1. correct SOCAT intake pCO_2^{sea} to the subskin temperature using for example the takahashi rule of thumb as in the Holding et al product. Interpolations of pCO_2^{atm} are performed on these corrected data.
- 2. calculate $C_{sea} = S_{subskin} \cdot pCO_2^{sea}$ at subskin T, where $S_{subskin}$ (alpha in table above) is calculated at the subskin temperature and salinity.
- 3. Calculate $C_{atm} = S_{skin} \cdot pCO_2^{atm}$ where S_{skin} is calculated at the skin temperature and salinity.
- 4. calculate flux $FCO_2 = K_w \cdot (C_{sea} C_{atm})$ where Kw is the gas exchange coefficient.

For an in depth description please see the <u>linked pdf document</u> as described by Andrew Watson.

Ocean interior products

The ocean interior products are diverse and thus the minimum requirements are not stringent.

At least one of the following variables is required in addition to the volume per grid cell:

- Dissolved inorganic carbon (dissic)
- Total alkalinity (talk)
- Anthropogenic carbon (cant)

The file formatting and naming conventions have to adhere to the table below and the <u>File/Grid specifications and naming</u> specifications. *Please note that the dimensions should be in the order [lon, lat, depth, time].*

Variable Name	Units	Output frequency	Shape	Priority	Long name
dissic	mol m ⁻³	monthly	XYZT	(1)	Dissolved inorganic carbon
cant	mol m ⁻³	periodic	XYZT	(1)	Anthropogenic CO2
talk	mol m ⁻³	monthly	XYZT	(1)	Total Alkalinity
volume	m^3		XYZ	1	Total volume of each grid cell
thetao	degC	monthly	XYZT	3	seawater potential temperature
so	-	monthly	XYZT	3	Salinity (PSS-78)
no3	mol m ⁻³	monthly	XYZT	3	Dissolved Nitrate Concentration
po4	mol m ⁻³	monthly	XYZT	3	Total Dissolved Inorganic Phosphorus Concentration

si	mol m ⁻³	monthly	XYZT	3	Total Dissolved Inorganic Silicic Concentration
o2	mol m ⁻³	monthly	XYZT	3	Dissolved Oxygen Concentration

Requirements of the **README**:

- Original study citation and dataset citation if applicable
- Specify explicitly the reported variable w.r.t. the following formulation: $\Delta DIC = \Delta DIC_{ant}^{ss} + \Delta DIC_{ant}^{ns} + \Delta DIC_{nat}^{ns} + \Delta DIC_{nat}^{ns}$
- Other comments or idiosyncrasies in the dataset that will affect global or regional comparison
- Does the estimate include (or try to include) riverine input of DIC? If applicable, information about riverine dissolved organic carbon (DOC) and total alkalinity (TA) input should be added.

File specifications

Grid / Coordinate system

Lon, Lat: 1x1 degree grid (0.5 to 359.5°E longitude, -89.5 to 89.5°N latitude) Lon in °E, Lat: in °N

Depth: positive downwards in meters using. User specified depth levels.

Time: days since Jan 1, 1980, centered on the 15th 00:00:00 of each month.

File naming

File name = <variable_id>__<start-end>_<version_id>.nc

variable_id: e.g. spco2, dissic from tables.

Product name: e.g. CMEMS-FFNN, GLODAPv2

start-end: starting year and end year if applicable

version_id: We suggest to use version numbering of your files, indicating the date of creation as vYYYYMMDD. Please keep track of the submitted versions in your readme file, briefly explaining the differences between versions.

Please create one file for full time-series per 2-D-variable. For 3-D variables, split in chunks as need be, but not more than one variable per file.

Readme files

Products will be stored in a data repository with folder structure reflecting the naming convention. Apart from the data file (.nc), the readme file should sit in the same folder and carry the same name extended by _readme.txt

File tarring/compression

Instructions for data submission through MPI-BGC FTP-server

Uploading data

For RECCAP2-ocean data products, it is recommended to upload zipped or tar files using the FTP:

ftp://ftp.bgc-jena.mpg.de/pub/incoming

For FTP upload, please add a readme file with the file information: owner, version, description that should go in the file metadata (as defined under the product protocols).

Please notify <u>abastos@bgc-jena.mpg.de</u> and <u>jensdaniel.mueller@usys.ethz.ch</u> when uploading files.

For additional **information regarding data upload**, please refer to this document [link] provided by Ana Bastos.

Data access

Data uploaded by various data providers through the MPI-BGC FTP-server, will be further compiled into single files. The compiled files will be made available through the following data portal:

https://www.bgc-jena.mpg.de/geodb/projects/Home.php

The download required authorization and registration. RECCAP2-ocean partners should already be authorized through their email, but still need to register upon first access. For additional information regarding registration, please refer to this document [link] provided by Ana Bastos.

Data policy

We will use the Fair Use Policy of RECCAPv2-oceans (see here)