

In situ dataset for initialization and validation of the Copernicus Med-MFC biogeochemical model system (MedBGCins)

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The biogeochemical model system in use by the Mediterranean Monitoring Forecasting Centre (Med-MFC) of the EU Copernicus Marine Service requires several observational datasets for data assimilation and model initialization and validation (Coppini et al., 2023; Cossarini et al., 2021; Salon et al., 2019). The present MedBGCins dataset consists of the in situ measurements, coming from selected platforms, on which the initialization and validation of the biogeochemical model system are built.

The MedBGCins dataset collects in situ measurements along the Mediterranean Sea water column and during the 1995-2023 time period for nutrients (i.e., nitrate, nitrite, phosphate, silicate, ammonium), dissolved oxygen, dissolved inorganic carbon, total alkalinity, total scale pH at 25°C. The dataset also provides pCO₂ and total scale pH at in situ conditions, reconstructed by using the PyCO₂SYS Python toolbox (Humpreys et al., 2024). The complete list of variables is indicated in Table 1.

The largest subset of the original data are from EMODnet Chemistry Mediterranean Sea - Eutrophication and Acidity aggregated datasets 1911/2022 v2023 (reference in Table 2), including both profiles and time series, plus other documented cruises (same table), and are filtered according to:

- selected measurement platforms, defined according to the SeaDataNet and MarineXML Vocabulary (<http://vocab.nerc.ac.uk/collection/L06/current/>): 'man-powered small boat (3A)', 'offshore structure (16)', 'ship (30)', 'research vessel (31)', 'vessel of opportunity (32)', 'self-propelled small boat (33)', 'vessel at fixed position (34)', 'vessel of opportunity on fixed route (35)', 'fishing vessel (36)', 'self-propelled boat (37)', 'man-powered boat (38)', 'naval vessel (39)', 'moored surface buoy (41)', 'subsurface mooring (43)', 'fixed subsurface vertical profiler (45)', 'mooring (48)';
- sampling frequency, requiring a number of measurements lower than number of days of sampling for the time series (otherwise the station data were neglected);
- average vertical distance of profile samples, larger than 2 m;
- range of minimum and maximum values for the variables, indicated in Table 3.

PyCO₂SYS parametrizations

The toolkit in use is Version v1.8.3 (doi:10.5281/zenodo.10671397). The adopted parametrizations include:

- equilibrium constant parameterisations to use to model carbonic acid dissociation taken from Mehrbach et al. (1973) as refitted by Dickson and Millero (1987), corresponding to $\text{opt_k_carbonic} = 4$ ($2 < T < 35$ °C, $20 < S < 40$, Seawater scale, real seawater);

- equilibrium constant parameterisation to use to model bisulfate ion dissociation taken from Dickson (1990), corresponding to `opt_k_bisulfate` = 1;
- ratio of total boron to salinity to use to estimate total borate taken from Upström (1974), corresponding to `opt_total_borate` = 1;
- equilibrium constant parameterisation to use for hydrogen fluoride dissociation taken from Dickson and Riley (1979), corresponding to `opt_k_fluoride` = 1.

The reconstruction of the missing carbonatic variables, starting from a couple of observed variables (i.e., total alkalinity and dissolved inorganic carbon, total alkalinity and pH at the total scale, dissolved inorganic carbon and pH at the total scale), has been conducted only in presence of simultaneous measurements of temperature and salinity. The reconstruction also included phosphate and silicate concentrations, both observed or prescribed (i.e., equal to 0.2×10^{-5} mol kg⁻¹, respectively).

Files and variables included in the dataset

The MedBGCins dataset is composed by two separate sets of variables:

- MedBGCins_nut: including nutrients and dissolved oxygen;
- MedBGCins_carb: including carbonatic system variables and variables in support of the reconstruction;

each of them released in two file formats: NetCDF4 and parquet.

The list of variables and corresponding units of measurements are included in Table 1. The “flag” variable only includes values equal to 1, standing for “EMODnet-derived”, or 2, “other datasets”, referring to the original source of data. A text file for the identification of the cruise from its number (included in the “id_cruise” variable) and original source of data (“flag”) is also provided for each set of variables: MedBGCins_nut_cruises.txt and MedBGCins_carb_cruises.txt.

Table 1: List of variables included in the MedBGCins dataset

Set of variables	Variable name	Variable definition	Units
MedBGCins_nut	year	year	/
	month	month	/
	day	day	/
	lat	latitude	degrees_North
	lon	longitude	degrees_East
	depth	depth	m

	nitrate	nitrate concentration	mmol m ⁻³
	nitrite	nitrite concentration	mmol m ⁻³
	ammonium	ammonium concentration	mmol m ⁻³
	phosphate	phosphate concentration	mmol m ⁻³
	silicate	silicate concentration	mmol m ⁻³
	oxygen	dissolved oxygen concentration	mmol m ⁻³
	chlorophyll	chlorophyll concentration	mg m ⁻³
	flag	number of identification for the source of data (1-EMODnet, 2-others)	/
	id_cruise	number of identification for the cruise	/
MedBGCins_carb	year	year	/
	month	month	/
	day	day	/
	lat	latitude	degrees_North
	lon	longitude	degrees_East
	depth	depth	m
	ALK	total alkalinity concentration	μmol kg ⁻¹
	pH_T25	observed pH at total scale, temperature of 25 °C, pressure = 0 dbar	/
	pH_ins	observed pH at total scale, in situ conditions	/
	pH_ins_rec	reconstructed pH at total scale, in situ conditions	/

	pH_ins_merged	merged field of pH_ins and pH_ins_rec when pH_ins is absent	/
	DIC	dissolved inorganic carbon concentration	$\mu\text{mol kg}^{-1}$
	DIC_rec	reconstructed dissolved inorganic carbon concentration	$\mu\text{mol kg}^{-1}$
	DIC_merged	merged field of DIC and DIC_rec when DIC is absent	$\mu\text{mol kg}^{-1}$
	pCO2_rec	reconstructed partial pressure of carbon dioxide, in situ conditions	μatm
	xCO2_rec	reconstructed dry mole fraction of carbon dioxide, in situ conditions	ppm
	temp	temperature	degrees_C
	salinity	salinity	psu
	silicate	silicate concentration	$\mu\text{mol kg}^{-1}$
	phosphate	phosphate concentration	$\mu\text{mol kg}^{-1}$
	flag	number of identification for the source of data (1-EMODnet, 2-others)	/
	id_cruise	number of identification for the cruise	/

Table 2: List of included datasets and references

Source	Reference
EMODnet Chemistry Mediterranean Sea - Eutrophication and Acidity aggregated	Hellenic Centre for Marine Research, Hellenic National Oceanographic Data Centre (HCMR/HNODC) https://doi.org/10.13120/74158cb0-a21f-42ea-8a29-72a96b2a0da2 downloaded at https://emodnet-chemistry.webdav.awi.de/

datasets 1911/2022 v2023	
METEOR51	https://doi.org/10.3334/cdiac/otg.carina_06mt20011018
METEOR84	https://doi.org/10.3334/cdiac/otg.clivar_06mt20110405
PROSOPE	https://doi.org/10.1594/PANGAEA.805265
BOUM 2008	https://doi.org/10.25921/xtgz-jr54
AEGAEO APR, AEGAEO SEPT	https://isramar.ocean.org.il/PERSEUS_Data/CruiseInfo.aspx?cruiseid=4848 https://isramar.ocean.org.il/PERSEUS_Data/CruiseInfo.aspx?cruiseid=4850
REGINA MARIS	https://doi.org/10.25921/qb64-tc92
Garcia del Cid	https://doi.org/10.25921/0w06-rf56
SESAME - ADRIATIC 2008	https://doi.org/10.25921/bzcp-p786 https://doi.org/10.25921/satj-p906
CARBOGIB 1-6	https://doi.org/10.1594/PANGAEA.618900 https://doi.org/10.1594/PANGAEA.618899 https://doi.org/10.1594/PANGAEA.618898 https://doi.org/10.1594/PANGAEA.618897 https://doi.org/10.1594/PANGAEA.618896 https://doi.org/10.1594/PANGAEA.618895
GIFT 1-2	https://doi.org/10.1594/PANGAEA.618916 https://doi.org/10.1594/PANGAEA.618915
MEDSEA 2013	https://doi.org/10.7289/v5n87832
SOMBA	https://doi.org/10.25921/2ka0-nj81
TALPRO	https://doi.org/10.1594/PANGAEA.902293
MEDWAVES	https://doi.org/10.1594/PANGAEA.890197
PEACETIME	https://doi.org/10.17882/75747
MSM72	https://doi.org/10.1594/PANGAEA.905887
ADRI-ACIDIT	https://doi.org/10.1594/PANGAEA.916129
<i>other cruises</i>	Lazzari et al., 2016

Table 3: Range of validity as minimum and maximum values for the main variables

Variable [units]	Min-max range
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nitrate [mmol m ⁻³]	0-150
nitrite [mmol m ⁻³]	0-15
ammonium [mmol m ⁻³]	0-30
phosphate [mmol m ⁻³]	0-10
silicate [mmol m ⁻³]	0-150
dissolved oxygen [mmol m ⁻³]	20-500
chlorophyll [mg m ⁻³]	0-80
total alkalinity [μmol kg ⁻¹]	1000-4000
dissolved inorganic carbon [μmol kg ⁻¹]	1000-4000
total scale pH at in situ conditions []	7-10
pCO ₂ [μatm]	0-800

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