Integration of satellite and in situ data to measure CO₂ fluxes in the Mediterranean Sea

Outline:

- Carbon cycle
- Objectives
- In situ pCO₂ and CO₂ fluxes
- Satellite algorithms
- Results and discussion
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Carbon cycle – brief overview

Atmospheric CO_2 concentration increased from about 280 ppm in pre-industrial times to the actual value of about 420 ppm due to antropogenic activities





Sellers, P. J. et al., Observing carbon cycle–climate feedbacks from space. *Proceedings of the National Academy of Sciences of the United States of America*. National Academy of Sciences. <u>https://doi.org/10.1073pnas.1716613115</u>, 2018

22/11/24

Carbon cycle – brief overview

- Ocean interaction with CO₂ has a great spatio-temporal variability not fully characterised with complex dependencies on phisycal, biological and chemical properties of the ocean
- CO₂ absorption leads to the acidification of ocean waters which can trigger negative feedbacks on absorption efficency
- Climate feedbacks are unknown
- Lack of continuous in situ measurements
- Ocean CO₂ absorption efficiency is strongly related with climate evolution

Monitoring atmosphere-ocean exchanges is crucial

Carbon cycle – ocean-atmosphere fluxes

 $F = K_{wa} KH (\Delta pCO_2)_{sea-atm}$

- $K_{wa} = 0.251 < U^2 > (Sc/660)^{-0.5}$ is the Gas Transfer Velocity
- Sc = A + B*SST + C*SST² + D*SST³ + E*SST⁴ is the Schmidt Number
- $\ln(KH) = A_1 + A_2^{*}(100/SST) + A_3^{*}\ln(SST/100) + SSS^{*}[B_1 + B_2^{*}(SST/100) + B_3^{*}(SST/100)^2]$ is the gas solubility
- Sea pCO₂ can be measured or derived
- Air pCO₂ can be measured or derived

Wanninkhof, R., Relationship between wind speed and gas exchange over the ocean revisited, *Limnol. Oceanogr. Methods*, 12, doi:10.4319/lom.2014.12.351, 2014

- Current monitoring mainly rely on model-based estimates of pCO₂ and CO₂ fluxes
- Works on satellite-based estimates of pCO₂







K. V. Krishna, P. Shanmugam and P. V. Nagamani, "A Multiparametric Nonlinear Regression Approach for the Estimation of Global Surface Ocean pCO2 Using Satellite Oceanographic Data," in *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 13, pp. 6220-6235, 2020, doi: 10.1109/JSTARS.2020.3026363.

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- Current monitoring mainly rely on model-based estimates of pCO₂ and CO₂ fluxes
- Works on satellite-based estimates of pCO₂
- Sparse in situ continuos and naval occasional measurements
- Carbon global monitoring projects and datasets:
 - Global carbon budget
 (https://www.globalcarbonproject.org/)
 - Surface Ocean CO₂ atlas (https://socat.info/)





Still missing estimates, including large portion of marginal seas

K. Lee, C.L. Sabine, T. Tanhua, T.W. Kim, R.A. Feely, and H.C. Kim. Roles of marginal seas in absorbing and storing fossil fuel CO2. Energy & Environmental Science, 4:1133–1146, 2011. doi: https://doi.org/10.1039/C0EE00663G.

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Thesis objectives

- Characterization of the Central Mediterranean carbon cycle using in situ data
- Satellite pCO₂ estimates using proxies for spatial monitoring
- CO₂ fluxes estimates merging satellite, model and in situ data



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Mediterranean Sea

- Climate hotspot
- Semi-enclosed basin under environmental stress
- Few carbon in situ measurements
- Few studies on basin-wide carbon cycle
- Suffering long and intense marine heatwaves (2022-2023; 2023-2024)

Marullo, S., Serva, F., Iacono, R., Napolitano, E., di Sarra, A., Meloni, D., . . . Santoleri, R. (2023). Record-breaking persistence of the 2022/23 marine heatwave in the Mediterranean Sea. Environmental Research Letters, 18 (11), 114041. https://doi.org/10.1088/1748-9326/ad02ae

Study site

In situ measurements made at Lampedusa

- Small island with small pollution sources
- Far from land
- Representative for background conditions
- Host observatories (AO, OO, EO) for climate studies and carbon monitoring (within the Integrated Carbon Observation System - ICOS infrastructure)
 - Ocean pCO₂, temperature and salinity are available at 5 m depth from October 2021 at OO
 - Wind speed, atmospheric pressure, atmospheric CO₂ concentration are available at AO



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Variable	Instrument	Accuracy	Height (asl)
Sea pCO ²	ProOceanus CO ² Pro-CV	± 3 ppm	-5m (OO)
SST	CTD SBE16+	±0.005°C	-5m (OO)
SSS	CTD SBE16+	±0.01 PSU	-5m (OO)
Wind speed	Gill windsonic sensor	±2%	10m (OO)
Wind speed	Vaisala WS425	±3%	60m (AO)
Atm. pressure	Vaisala BARO-1	±0.25 hPa	52m (AO)
Atm. CO ² conc.	Picarro G2401	±0.1 ppm	57m (AO)

 pCO_2 issue with the a/d zero measurements between March and July 2022. An empirical correction was applied with an increased associated uncertainty.



22/11/24

Integration of satellite and in situ data to measure CO₂ fluxes in the Mediterranean Sea





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A. Mignot, K. von Schuckmann, P. Landschützer, F. Gasparin, S. van Gennip, C. Perruche, J. Lamouroux, and T. Amm. Decrease in air-sea CO₂ fluxes caused by persistent marine heatwaves. Nature Communications, 13(1):4300, 2022. doi: https://doi.org/10.1038/ s41467-022-31983-0.

- Wind speed significantly influenced the development and persistence of the MHW in the Mediterranean Sea.
- Wind dynamics played a crucial role in reducing CO₂ exchange along the U.S. East Coast.
- A marked shift in wind speed distribution was observed at Lampedusa, with a notable reduction in moderate-to-high wind events.



Edwing, K., Wu, Z., Lu, W., Li, X., Cai, W.-J., & Yan, X.-H. (2024). Impact of marine heatwaves on air-sea CO₂ flux along the US East Coast. Geophysical Research Letters, 51, e2023GL105363. doi: https://doi.org/10.1029/2023GL105363



Pecci et al., Large influence of the 2022-23 marine heatwave on the air-sea CO₂ flux in the Central Mediterranean, in submission to Journal of Geophysical Research: Oceans

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Satellite algorithms

Regional regression algorithms are introduced to estimate pCO_2 with satellite measurable proxies:

Variable	Dataset	Data type	Reference
SST	High Resolution and Ultra High-Resolution L3S SST	Satellite	CMEMS - Mediterranean Sea - High Resolution and Ultra High Resolution L3S Sea Surface Temperature. <u>https://doi.org/10.48670/moi-00171</u>
SSS	Ocean Reanalysis System 5 (ORAS5)	Model	C3S - ORAS5 global ocean reanalysis monthly data from 1958 to present. Copernicus Climate Change Service (C3S) Climate Data Store (CDS). https://doi.org/10.24381/cds.67e8eeb7
Wind Speed	Global Ocean Sea Surface Winds from Scatterometer	Satellite	CMEMS - Global Ocean Daily Gridded Sea Surface Winds from Scatterometer. Retrieved September 2023, from <u>https://doi.org/10.48670/moi-00182</u>
PAR	OLCI – Sentinel-3 satellite	Satellite	Pecci, M. et al. (2024). Validation of photosynthetically active radiation by OLCI on Sentinel-3 against ground-based measurements in the central Mediterranean and possible aerosol effects. <i>European Journal of Remote Sensing</i> , <i>57</i> (1). https://doi.org/10.1080/22797254.2024.2307617
PAR	MODIS – Aqua satellite	Satellite	NASA Ocean Biology Processing Group - Aqua Daily Photosynthetically Active Radiation https://oceancolor.gsfc.nasa.gov/l3/
CHL	Med. Sea, Bio-Geo-Chemical, Satellite Observations	Satellite	CMEMS - Mediterranean Sea, Bio-Geo-Chemical, L3, daily Satellite Observations (1997-ongoing) <u>https://doi.org/10.48670/moi-00299</u>
Atm xCO ₂	In situ data-based fit	In situ-adapted	
Atmospheric pressure	ERA5 hourly reanalysis	Model	Hersbach, H., et al., (2023). ERA5 hourly data on single levels from 1940 to present. Copernicus Climate Change Service (C3S) Climate Data Store (CDS). https://doi.org/10.24381/cds.adbb2d47

Satellite algorithms

Traditional regression algorithms to estimate pCO₂ with satellite measurable proxies:

- Use of least-squares method
- Use of different functional forms, including **multiple parameters and non-linear terms**
- Training and test on in situ **daily** datasets
- Use of **seasonal regression** to exploit the pCO₂ hysteresis
- Best performing models applied to satellite data



Satellite algorithms

Machine learning approach to estimate pCO_2 with satellite measurable proxies:

- Use of eXtreme Gradient Boosting (XGBoost) algorithm
- Trained on **bi-hourly** data and tested on daily data
- Use of default and **cross-validated** settings
- Best performing models applied to satellite data

Training and test set

The entire dataset spans from December 2021 to June 2023 (18 months):

- Single regression for the whole dataset («Annual models»)
 - Training set is composed of 12 months of data (Dec21 to Dec22)
 - Test set is composed of 6 months of data (Jan23-June23)

Dataset	Bi-hourly	Daily
Training set	2400 data pairs	200 data pairs
Test set	/	130 data pairs

Training and test set

- Traditional regression models divided to follow the branches of the hysteresis (**«Seasonal models**»):
 - Summer models (Mar-Aug)
 - Training set: Mar22-Aug22
 - Test set: Mar23-Aug23
 - Winter models (Aug-Mar)
 - Training set: Dec21-Mar22 and Aug22-Dec22
 - Test set: Dec22-Mar23



Dataset	Summer models	Winter Models
Training set	120 data pairs	180 data pairs
Test set	80 data pairs	50 data pairs

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Traditional regression models

Model	Functional Form	$SST\left[\frac{\mu atm}{\circ C}\right]$	$SST^2[\frac{\mu atm}{\circ c^2}]$	$SSS\left[\frac{\mu atm}{PSU}\right]$	$\frac{CHL}{[\frac{\mu a t m \cdot L}{\mu g}]}$	$\frac{PAR}{[\frac{\mu a t m \cdot m^2}{W}]}$	$\frac{Wspd}{[\frac{\mu atm \cdot s}{m}]}$	Const. [µatm]
Mod4	A·SST+B·SSS+C·CHL+ D·PAR+E	9.20	0	10.35	-99.12	0.13	0	-146.36
Mod6	A·SST+B·CHL+C·PAR+ D∙ wspd +E	9.23	0	0	-98.99	0.11	-0.66	247.17
Mod9	A·SST+B·CHL+C·PAR+D	9.28	0	0	-99.99	0.14	0	238.68
Mod4_T2	A·SST+B· SST ² +C·SSS+D·CHL+E·PAR+F	25.31	-0.36	18.06	-66.98	0.06	0	-599.96
Mod6_T2	A·SST+B· SST ² +C·CHL+ D·PAR+E· wspd +F	24.56	-0.34	0	-68.94	0.05	-0.78	90.43

Models functional form and coefficient for the «seasonal summer» models weighted with the reciprocal of the pCO₂ uncertainty

Traditional regression models



«Seasonal models» with MODIS PAR product non weighted regression

22/11/24

Traditional regression models



[«]Annual models» with MODIS PAR product weighted regression

ML models



Model	Input variables
Mod1	SST
Mod3	SST, SSS, CHL
Mod5	SST, SSS, CHL, PAR, WSPD
Mod6	SST, CHL, PAR, WSPD
Mod9	T, CHL, PAR

	Model	\overline{R}^2	RMSD [µatm]	Bias [µatm]
D	Mod1	0.76	25.0 (6%)	-1.4 (< 1%)
	Mod3	0.30	37.0 (8%)	26.1 (6%)
	Mod5	0.33	34.2 (8%)	24.3 (5%)
	Mod6	0.51	31.4 (7%)	18.8 (4%)
	Mod9	0.49	32.4 (7%)	19.9 (4%)
cv	Mod1	0.76	25.0 (6%)	-1.7 (<1%)
	Mod3	0.35	37.4 (8%)	27.1 (6%)
	Mod5	0.48	31.4 (7%)	23.5 (5%)
	Mod6	0.61	28.7 (7%)	18.4 (4%)
	Mod9	0.54	31.3 (7%)	17.9 (4%)

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Performance summary



Fluxes estimates

- Fluxes computed using satellite-estimated pCO₂ and satellite/model-based ancillary quantities
- The need of simultaneous data from different dataset leads to a reduced dataset (approximately 100 data pairs for the MODIS-based dataset and 50 for the OLCI-based dataset)



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Conclusion and next steps

- Observed data of pCO₂ and CO₂ fluxes show a net sink effect
- Strong MHW impact on the magnitude of the exchanges
- The use of regional regression algorithms improve the agreement between estimated and observed pCO₂ values (with traditional regressions performing better than ML, probably due to the small dataset)
- CO₂ fluxes estimates using satellite-based pCO₂ and ancillary quantities show a good agreement with fluxes computed using observed data

Dataset	Bias	RMSD	R ²
CMEMS pCO ₂	28.4 [µatm] (7%)	40.0 [µatm] (10%)	0.91
MPNR algorithm	-7.4 [µatm] (2%)	31.9 [µatm] (7%)	0.59
Mod6_T2	4.4 [µatm] (1%)	13.0[µatm] (3%)	0.94
CMEMS Fluxes	$9.8 \cdot 10^{-10} \left[\frac{kg}{m^2 s} \right]$ (86%)	$3.1 \cdot 10^{-9} \left[\frac{kg}{m^2 s}\right]$ (270%)	0.22
Mod9	1.0· $10^{-12} \left[\frac{kg}{m^2s}\right]$ (<< 1%)	1.3· $10^{-9} \left[\frac{kg}{m^2s}\right]$ (110%)	0.75

Conclusion and next steps

- Despite being promising, a larger dataset is needed for a more robust statistics:
 - Use of different satellite input (CMEMS L4 salinity, ERA5 or CCMP wind speed, SEVIRI daily PAR) to increase the dataset size for pCO₂ and fluxes estimates
- Carry on the monitoring with a special focus on the SST and MHW impact on ocean absorption efficiency
- Extend the pCO_2 and CO_2 fluxes estimates to a broader area
- Compare the estimates with other Mediterranean carbon datasets (e.g., Integrated Carbon Observation System stations)

Thanks for the attention!

ntegration of satellite and in situ data to measure CO fluxes in the Mediterranean Sea

Performance metrics

Bias =
$$\frac{1}{N} \sum_{i} (y_i - x_i)$$

$$\text{RMSD} = \sqrt{\frac{1}{N} \sum_{i} (y_i - x_i)^2}$$

$$R^{2} = 1 - \frac{\sum_{i} (y_{i} - x_{i})^{2}}{\sum_{i} (y_{i} - \bar{y})^{2}}$$

$$\bar{R}^2 = 1 - (1 - R^2) \frac{n-1}{n-k-1}$$

Where

- y is the predicted values
- x is the observed value
- n is the dataset size
- k is the number of parameters used in the regression

pCO₂ hysteresis



22/11/24

• Current monitoring mainly rely on model-based estimates of pCO₂ and CO₂ fluxes

Dataset	Bias	RMSD	R ²
CMEMS pCO ₂	28.4 [µatm] (7%)	40.0 [µatm] (10%)	0.91
CMEMS Fluxes	$9.8 \cdot 10^{-10} \left[\frac{kg}{m^2 s}\right]$ (86%)	$3.1 \cdot 10^{-9} \left[\frac{kg}{m^2 s}\right]$ (280%)	0.22



Mediterranean Sea Biogeochemistry Analysis and Forecast - https://doi.org/10.25423/cmcc/medsea_analysisforecast_bgc_006_014_medbfm3

22/	′11	/24

- Current monitoring mainly rely on model-based estimates of pCO₂ and CO₂ fluxes
- Works on satellite-based estimates of pCO₂

Dataset	Bias	RMSD	R ²
MPNR algorithm global data	/	5.35-8.77 [μatm]	0.82-0.93
MPNR algorithm on Med	-7.4 [µatm] (2%)	31.9 [µatm] (8%)	0.59



K. V. Krishna, P. Shanmugam and P. V. Nagamani, "A Multiparametric Nonlinear Regression Approach for the Estimation of Global Surface Ocean pCO2 Using Satellite Oceanographic Data," in *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 13, pp. 6220-6235, 2020, doi: 10.1109/JSTARS.2020.3026363.