

Response to the Editor's comments on the manuscript:

CMEMS-LSCE: A global 0.25-degree, monthly reconstruction of the surface ocean carbonate system

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The authors thank the editor and the two reviewers for their contributions to enhance this study. Further, we appreciate your positive evaluation and that our manuscript has been accepted for publication in Earth Science System Data subject to technical corrections. Please kindly find our replies to the editor's comments (EC) below.

EC1. *I fully agree with both reviewers on the relevance of the generated product and the quality of the work and the paper itself.*

However, I also agree with reviewers comments on the needs of keeping $f\text{CO}_2$ together with its measurement temperatures. Figure GC1.3 shows a perfect unbiased fit between CMEMS and SOCAT SST but significant scatter is also present, with many values outside the $\pm 1^\circ\text{C}$ range, so significance in terms of $p\text{CO}_2$ that recommends at least 0.02°C precision on Temperature (Dickson 2007). A plot of diffs can show this better than the property vs property. However, I can also agree with authors that an extra NN step to fit this would add complexity and probably noise.

In my opinion, the manuscript accuracy would be greatly improved by just re-scaling the $f\text{CO}_2$ inputs at SOCAT temperatures to CMEMS temperatures according Wanninkhof et al., (2022) or using the MCS equations.

A basic conversion recipe (matlab):
`co2=CO2SYSv3(400,2300,5,1,35,20,21,0,0,10,1,0,0,1,10,1,2,2); fCO2_out=co2(:,23)`
or (python): `fCO2_out = pyco2.sys(par1=400, par1_type=5, temperature=20, temperature_out=21)['fCO2_out']` for example, for converting from 20°C to 21°C would be preferable to no conversion at all.

Authors:

We thank the Editor for his suggestions to « re-scale the $f\text{CO}_2$ inputs at SOCAT temperatures to CMEMS temperatures ». We would like to take advantage of this reply to reemphasize the importance of homogeneity in predictor data during training, validation, and reconstruction. Please note that we use the gridded version of the SOCAT $f\text{CO}_2$ throughout the process.

SOCAT accepts SST data with a precision of 0.05°C for flags A and B and 0.2°C for flags C and D (Lauvset et al., 2019). These values are substantially higher than the precision of 0.02°C recommended by Dickson et al., (2007). Furthermore, SST data are not associated with SOCAT quality control (QC) flags for $f\text{CO}_2$ (WOCE). SST-based adjustments will add large uncertainty to $f\text{CO}_2$ reconstructions if its input data are not fully qualified or have high sampling uncertainty. These data are next interpolated on the $1^\circ \times 1^\circ$ grid along with corresponding $f\text{CO}_2$ data and yield the gridded version of SOCAT. This is a major source of uncertainty.

We don't intend to downplay the problem which is well recognized by the community and has been addressed in recent publications (e.g. Woolf et al., 2019; Watson et al., 2020). A simple rescaling of SOCAT temperatures to CMEMS temperatures would, however, not solve it. In Wanninkhof et al., (2022), the authors mention in Section Introduction (4th-paragraph) that adjustments with differences in SST falling out of $\pm 1^\circ\text{C}$ are proposed with the available A_T and C_T data (the same requirement holds for $f\text{CO}_2$ rescaling by using the MCS equations). However, SOCAT does not provide data for these two variables. One would have to rely on GLODAP subsurface measurements, co-locating them on the SOCAT $1^\circ \times 1^\circ$ and correcting them for surface temperatures and salinity. Resulting values of A_T and C_T would carry substantial uncertainty making them of only limited use to constrain $f\text{CO}_2$.

We hope that the preceding convinces the editor that there is no straightforward (simple) solution to the problem. It is our opinion that the topic should be addressed by the SOCAT and SOCCOM communities in order to propose an approach common to all mapping methods.

EC2. *Another detail that I missed on the manuscript is the proper statement on the sets of constants used in the MCS, as well as the pH Scale and conditions. Including those details is a key point for solving the MCS thermodynamics, and so, key for future usage and proper understanding of the dataset. This is particularly needed when computing one parameter from a pair, as you do with pH from $f\text{CO}_2$, AT pairs. Apart from the Lewis and so cites that you use, it's convenient to cite the actual toolbox and exact version you are using, be CO2SYS (ven Heuven), v2 (Orr) or v3 (Sharp), or python (Humphreys), as implementations vary. The matlab example in the paragraph above uses CO2SYS v3.2.1, K1&K2 from Lueker, KSO4 from Dickson, KF of Perez and Fraga and TB from Lee, which can be considered the preferred default set to many authors for common oceanic waters right now (but differs from the default set in python version)*

Authors:

Knowing the necessity of providing the information on constants and conditions used in the CO2SYS speciation for this study, we have thoroughly presented these elements in "**Section 3.3 Carbonate system speciation**" - see **Lines 262-273** in the previous revision (quoted in blue below). For pH, data have been reported on *total scale* (see for instance Section Results). We however admit that this information should be stated starting from Section Introduction (please find our correction in the new revised manuscript). In addition to this revision, we cite correctly the Matlab version of CO2SYS used in this study: **CO2SYS.v2** (Orr et al., 2018).

Lines 262-273 in the previous revision:

"The FFNN best estimate (ensemble mean) of $p\text{CO}_2$ reconstructions (Sect. 3.1) and the LIAR outputs of A_T (Sect. 3.2) are used as the prior inputs of the CO2SYS at each grid cell for every month in the period 1985-2021. We take the same data products of SST, SSS, and nutrient concentrations as for the previous reconstructions (Table 1). Pressure (P) is assumed to be 0

dbar at the ocean surface. For equilibrium constants, we choose the best empirical values recommended by Dickson et al. (2007) and Dickson (2010). These settings include (1) the dissociation constants K_1 and K_2 from Lueker et al. (2000) and K_{HSO_4} from Dickson (1990) in combination with the total boron-ratio-salinity formulation by Uppstrom (1974).

The uncertainty of the CO2SYS variables is estimated by error propagation (Orr et al., 2018). Inputs for the CO2SYS error propagation include the reconstruction uncertainty of $p\text{CO}_2$ (FFNN ensemble standard deviation) and of A_T (LIAR error propagation). The uncertainty of SST, SSS, and nutrient concentrations are set to the same values as in the previous section (Sect. 3.2). Equilibrium constants' standard errors are default values (see Table 1, Orr et al., 2018). As for FFNN and LIAR, uncertainty values of each carbonate system variable are computed for each month in 1985-2021 and at each 0.25° -grid box over the global surface ocean."

EC3. *And just as final remark, I ask you to review the notation on symbols. Whether the IUPAC would encourage to use of $p\text{H}$, $p\text{CO}_2$, $f\text{CO}_2$, A_T , C_T , SSS, T ,.. i.e. the first in italics and the later straight except for common abbreviations, it's also common the usage of A_T , C_T , $p\text{CO}_2$,... but is quite unusual to read $p\text{H}$ or A_T as I've seen in the manuscript. It's also preferable to use just only acronym for a specific parameter, say C_T or DIC, but not both in same manuscript.*

Authors:

We have corrected the acronyms of $p\text{H}$ and A_T following the Editor's comments. For dissolved inorganic carbon, we now denote this variable as C_T consistently throughout the text.

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