

Review of the Manuscript Number: essd-2025-473: Title: High-resolution spatiotemporal fields of Southern Ocean interior carbonate system parameters integrated from float- and ship-based observations by Wanqin Zhong et al.

See attached document.

Review invitation: 14/9/2025

Review accepted: 14/9/2025

Review sent: 21/9/2025

;;;;;; General comment

In this paper authors present a new dataset of the carbonates system, called SOCOML (Southern Ocean CO<sub>2</sub> Machine Learning), derived from shipboard (GLODAP) and float (Argo) data in the Southern Ocean (here south of 30°S). This is a climatological product that includes aragonite saturation state ( $\Omega_{ar}$ ) and anthropogenic CO<sub>2</sub> concentrations (Cant) for a reference year (2013). Such climatology (for DIC and TA) has been previously developed, based on shipboard data (e.g., Lauvset et al, 2016; Keppler et al 2020, 2023). Like for surface pCO<sub>2</sub> and air-sea CO<sub>2</sub> fluxes products (e.g. SOCOM project, Rödenbeck et al, 2015) successfully used to constraint the estimate of the global carbon budget (Friedlingstein et al, 2025) it is important that different climatology for the ocean interior are available for the community (see also a list of such products in Jiang et al, 2025).

After a clear introduction, authors describe the methodology and uncertainties. Three gridded products are offered (with or without O<sub>2</sub>) at 1x1 degree resolution and 84 levels in the water column down to the abyssal domain. This is especially important in the Southern Ocean where AABW are formed and contain significant Cant concentrations (e.g. Rios et al, 2012; Pardo et al, 2017; Mahieu et al, 2020; Zhang et al 2023). This is also challenging as previous analyses explored the changes of Cant inventories over 0-3000m (Gruber et al, 2019; Müller et al, 2023). Here the product extend to the bottom.

The reconstructed fields for AT, DIC, O<sub>2</sub> and nutrients are used to calculate  $\Omega_{ar}$  and Cant concentrations (here derived from TrOCA method). I suspect this new data-sets could be easily used to estimate Cant using other methods. The results (climatology of TA, DIC, and Cant concentrations) are also important to validate OBGCM and ESM models that suffer to reproduce seasonal to multi-decadal DIC and Cant variability. The results will be also probably useful for paleo-oceanography studies (e.g. using pre-industrial DIC profiles deduced from the data presented in this work when calculate DIC-Cant).

Interestingly, through a comparison of different results, authors indicate that the bias in DIC and Cant depend on the dataset used for the training, highlighting the need of maintaining regular update of the dataset such as GLODAP. This is especially true in region where data are relatively sparse such as near coastal Antarctica and in the seasonal ice zone during austral winter. By the way, I was wondering how the sea-ice is taken into account in the method (or if it should be taken into account).

The manuscript is clear, tables and figures adapted. The dataset will be certainly useful for many studies including validation of models. I recommend publication after some clarifications. Below are listed specific and minor comments.

;;;;;;;; Specific comments:

C-01: Title: "High-resolution spatiotemporal fields of Southern Ocean interior carbonate system parameters integrated from float- and ship-based observations". The products are at spatial scale of

1 x 1 degree (not really high-resolution) for a reference year and include anthropogenic CO<sub>2</sub> (Cant) so I would suggest change the title: "Climatological fields of Southern Ocean interior carbonate system parameters and anthropogenic CO<sub>2</sub> integrated from float- and ship-based observations".

C-02: Line 68: « while the Global Ocean Data Analysis Project version 2 (GLODAPv2, Olsen et al., 2016) offers quality-controlled data product from the surface into the ocean interior includes TA and DIC." It also offered climatology of TA, DIC in the interior ocean (Lauvset et al, 2016).

C-03: Line 70: Maybe also refer here to the last RECCAP-2 story for the SO (Hauck et al, 2023).

C-04: Line 99: "TA, DIC, pH (total scale), nitrate (NO<sub>3</sub>), phosphate (PO<sub>4</sub>) and silicate (SiO<sub>4</sub>) are obtained through neural networks". Add also O<sub>2</sub> in this list as this is used for Cant calculation ?

C-05: Line 100-101: « And Cant is estimated using TrOCA method (refs doing the same with TrOCA in Sothern Ocean). » Missing words and references in the sentence ? Also typo: Southern Ocean.

C-06: Line 110: Authors used GLODAPv2 data (version GLODAPv2.2020). Are you selecting all the TA and DIC data or only samples when nutrients are all available (Nitrates, silicates and phosphates), i.e. samples without phosphates not included. Also, are you using samples with only TA data or with only DIC data ? Please clarify.

C-07: Line 130: Table 1: maybe specify in the caption that data used are in the SO south of 30°S.

C-08: Line 158: "...direct nitrate and pH measurements from Argo floats are excluded from this study." If I understand authors did not used pH and nitrates data from BGC-Argo floats and used only T, S and O<sub>2</sub> from these floats (correct ?). Please clarify. Maybe a table (as Table 1 for GLODAP) would help to know the final selection of data from floats.

C-09: Line 168: typo CDT: ...blue for Argo only with CTD,

C-10: Line 185: Figure 2: In the Box "Step 3", add O<sub>2</sub> in the list of parameters as O<sub>2</sub> is used in TrOCA.

C-11: Line 200: Authors used the TrOCA method to derive Cant concentrations that has been successfully used and/or compared in the SO (e.g. Lo Monaco et al, 2025; Vazquez-Rodriguez et al, 2009; Mahieu et al, 2020; Metzl et al, 2024). Authors refer to Lo Monaco et al (2025) but this is not the correct reference for TrOCA (see reference below). Maybe recall that method is not adapted to estimate Cant in surface layer. How to you extrapolate the Cant concentrations in surface or indicate that climatology is limited to 100m ?

C-12: Line 204:"Finally, the Cant values are scaled to the reference year". It would be useful to specify the reference year, here 2013.

C-13: For Cant did you get any negative value ?

C-14: Line 207: I guess Lewis et al (2021) not listed in references.

C-15: Line 330: "Under the full-parameter pathway, Cant exhibits a slight negative bias relative to shipboard derived values (Cant\_ship\_M)," Curiosity: Is there any change of the bias over time or is it evaluated for the reference year only ?

C-16: Figure 6b: The map is not clear. Is it for surface water, for deep layers ? Please clarify in the caption.

C-17: Line 364: Climatological distribution. Could you recall the period for the climatology presented in Figure 7 and 8; it is a mean for any data spanning 1972-2025 or for a reference year in 2013 ?

C-18: Line 375: when describing the fronts plotted in figure 7 (STF, SAF, PF...), add a reference (Orsi et al 1995, other ?).

C-19: Figures 7 and 8. I think a map is missing: "Abyssal water" listed in the captions.

C-20: Figures 7 and 8. Maybe specify in the caption that the color scales are different for each map.

C-21: Figure 7f,g show high Cant in the SW Atlantic ( $>20 \mu\text{mol/kg}$  ?). This signal is not resolved for the O2-Float-grid (Figure 9a). A comment on this ? Is TrOCA not adapted here or a problem with reconstruction ? (see also comment C-27 below)?

C-22: Figures 9a: Few data show very high Cant in the Pacific and Indian oceans (red points apparently  $> 25 \mu\text{mol/kg}$ ). Are the data correct ? The maps 9a and 9c on top (shipboard) are small and it would be nice to show enlarged maps in Supp Mat.

C-23: Figures 9a and 9c: Could you recall in the caption the layer for the maps in deep layers (2000-4000 db ?)

C-24: Figures 9: the scales at the bottom is not clear (or not fully plotted)

C-25: Figures 9b: would it be possible to change the color for the lines (not clear for GLODAP: green in legend ?).

C-26: Line 417: "The TRACE-derived dataset (purple lines) consistently underestimates Cant relative to the TrOCA-derived values, particularly in intermediate waters." WHY ?

C-27: Line 426: "Notably, we identify a hotspot of high Cant concentrations in the southwestern Atlantic Ocean near the SAF and PF (Figure 9a), potentially linked to AABW outflow from the Weddell Sea". Intriguing signal (see comment C-21). If the selected depth for Figure 9a is 2000-4000db, would the signal linked to waters above the AABW (e.g. WSDW) or other origin (see for example Gruber, 1998; Ríos et al, 2012). Note also that Müller et al (2023) identified a relatively high increase of the Cant inventory in this region between 2004 and 2014 (for the layer 0-3000m). It would be interesting to show a section of Cant (Lat/depth) crossing this region in the Appendix. See for example figure R1 in this review. Would that anomaly in the SW Atlantic help to check the data or the methods ?

C-28: Line 453: "Although our approach may underestimate uncertainty due to potential representativity error, our dataset offers a significant improvement in both accuracy and spatial representativeness over previous gap-filling approaches". Maybe also recall that your product is extended to the bottom whereas previous analyses were mainly limited to the layer 0-3000m (e.g. Gruber et al, 2019).

C-29: Figure A6: For the abyssal water, the maps are not clear. Why there are so few data. Also change the code for the panels (a), (b), (c), (d) and (e). (not (f)) . As this layer is rather new compared to previous products I think this should be highlighted (move A6 to the main text ?). Are the front useful in these maps ?

C-30: Figures A8 and A9: Missing units for these maps.

;;;;; in references:

C-31: Line 607: Clement and Gruber (2018) not listed in the manuscript.

C-32: Line 656: Change the reference:

Lo Monaco C., C. Goyet, N. Metzl, A. Poisson and F. Touratier, 2005. Distribution and inventory of anthropogenic CO<sub>2</sub> in the Southern Ocean : comparison of three data-based methods. *Journal Geophys. Res.* . 110, C09S02, doi:10.1029/2004JC002571.

;;;;; Reference added in this review not listed in the Manuscript:

Gruber, N., 1998. Anthropogenic CO<sub>2</sub> in the Atlantic Ocean. *Global Biogeochem. Cycles*, 12, 165–191.

Jiang, L.-Q., et al.,: Synthesis of data products for ocean carbonate chemistry, *Earth Syst. Sci. Data Discuss.* [preprint], <https://doi.org/10.5194/essd-2025-255>, in review, 2025.

Keppler, L., Landschützer, P., Gruber, N., Lauvset, S. K., and Stemmler, I.: Seasonal carbon dynamics in the near-global ocean, *Global Biogeochemical Cycles*, 34(12), e2020GB006571, <https://doi.org/10.1029/2020GB006571>, 2020.

Keppler, L., Landschützer, P., Lauvset, S. K., and Gruber, N.: Recent trends and variability in the oceanic storage of dissolved inorganic carbon, *Global Biogeochemical Cycles*, 37(5), <https://doi.org/10.1029/2022gb007677>, 2023.

Lauvset, S. K, R. M. Key, A. Olsen, S. van Heuven, A. Velo, X. Lin, C. Schirnick, A. Kozyr, T. Tanhua, M. Hoppema, S. Jutterström, R. Steinfeldt, E. Jeansson, M. Ishii, F. F. Pérez, T. Suzuki & S. Watelet, 2016. A new global interior ocean mapped climatology: the 1°x1° GLODAP version 2. *Earth Syst. Sci. Data*, 8, 325–340, doi:10.5194/essd-8-325-2016.

Lo Monaco C., C. Goyet, N. Metzl, A. Poisson and F. Touratier, 2005. Distribution and inventory of anthropogenic CO<sub>2</sub> in the Southern Ocean : comparison of three data-based methods. *Journal Geophys. Res.* . 110, C09S02, doi:10.1029/2004JC002571.

Mahieu, L., Lo Monaco, C., Metzl, N., Fin, J., and Mignon, C.: Variability and stability of anthropogenic CO<sub>2</sub> in Antarctic Bottom Water observed in the Indian sector of the Southern Ocean, 1978–2018, *Ocean Sci.*, 16, 1559–1576, <https://doi.org/10.5194/os-16-1559-2020>, 2020.

Metzl, N., et al: Anthropogenic CO<sub>2</sub>, air–sea CO<sub>2</sub> fluxes, and acidification in the Southern Ocean: results from a time-series analysis at station OISO-KERFIX (51° S–68° E), *Ocean Sci.*, 20, 725–758, <https://doi.org/10.5194/os-20-725-2024>, 2024.

Müller, J. D. , N. Gruber, B. Carter, R. Feely, M. Ishii, N. Lange, S. K. Lauvset, A. Murata, A. Olsen, F. F. Pérez, C. Sabine, T. Tanhua, R. Wanninkhof, D. Zhu, Decadal trends in the oceanic storage of anthropogenic carbon from 1994 to 2014. *AGU Adv.* 4, e2023AV000875 (2023).

Orsi, A. H., T. Whitworth III, and W. D. Nowlin Jr., On the meridional extent and fronts of the Antarctic Circumpolar Current, *Deep Sea Res., Part I*, 42, 641–673, 1995.

Pardo, P. C., et al.: Carbon uptake and biogeochemical change in the Southern Ocean, south of Tasmania. *Biogeosciences*, 14(22), 5217–5237. <https://doi.org/10.5194/bg-14-5217-2017>, 2017

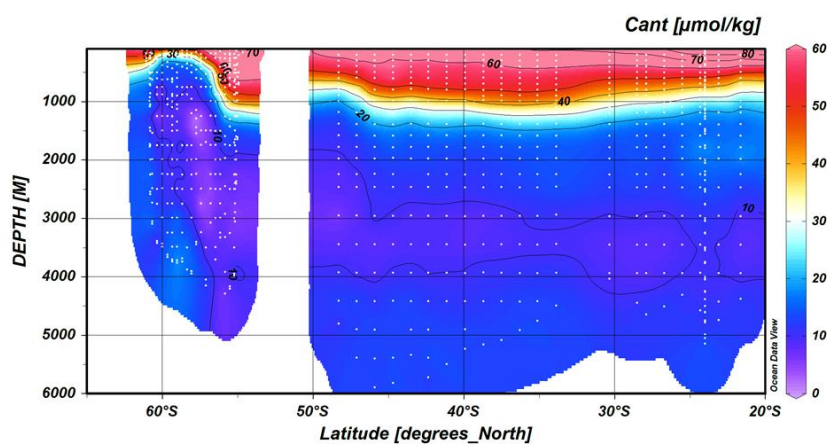
Ríos, A. F., Velo, A., Pardo, P. C., Hoppema, M., and Pérez, F. F.: An update of anthropogenic CO<sub>2</sub> storage rates in the western South Atlantic basin and the role of Antarctic Bottom Water, *J. Mar. Syst.*, 94, 197–203, <https://doi.org/10.1016/j.jmarsys.2011.11.023>, 2012.

Rödenbeck, C., et al, 2015. Data-based estimates of the ocean carbon sink variability – First results of the Surface Ocean pCO<sub>2</sub> Mapping intercomparison (SOCOM). Biogeosciences 12: 7251-7278. doi:10.5194/bg-12-7251-2015..

Vazquez-Rodriguez, M., et al, 2009. Anthropogenic Carbon Distributions in the Atlantic Ocean: data-based estimates from the Arctic to the Antarctic. Biogeosciences, 6, 439-451. <https://doi.org/10.5194/bg-6-439-2009>

;;;;;;;;;; Figure for review

Figure R1; Section of Cant ( $\mu\text{mol/kg}$ ) along cruises in the South-Western Atlantic (GLODAP data in 2018-2019, Expocode: 29HE20190406 and 74JC20181103). In deep layers, below 1500m, there is no concentration higher than 20  $\mu\text{mol/kg}$  as suggested in Figure 7 f,g.



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