

Reviewer 1

The authors developed a new ML approach to reconstruct global surface ocean pCO₂ that considers an impact of different predictors in different ocean regions. Based on Self-Organizing Map method authors defined 11 biogeochemical provinces. A stepwise FFNN regression algorithm was applied to each of these provinces to establish a set of predictors that are highly responsible for pCO₂ variability in considered province. Based on selected predictors and analysis of FFNN size (number of neurons) a monthly 1°x1° surface ocean pCO₂ product from 1992 to 2019 was constructed. The results show a good agreement with validation data and independent observations.

I found this work well-organized and easy to read. It was interesting to see new predictors (phosphate, nitrate, silicate, dissolved oxygen) and their role in pCO₂ variability. The authors presented important results for the Indian Ocean where due to the lack of observations different methods show their disagreements.

Response: Thank you very much for your appreciation and very valuable suggestions to improve the manuscript!

Below, I listed several points that need to be clarified before publication.
Comments:

- **Boundaries between provinces.** In the text we can find “To obtain a smoother distribution, we defined that the grid within 5 1x1 grids of province borders belong to all provinces adjacent to the nearest province border. Samples in these grids were involved in the FFNN training process of multiple provinces, but only counted once in the validation.” Please could you clarify what you mean by “only counted once in the validation”? Is only an output from one province used in the validation? If yes, how do you chose a province from which you take an output?

Response: Thank you for pointing out this unclear description. Due to the definition of new boundaries, in each province additional samples were added, which was outside the original boundary, referred as ‘boundary sample’ here. Now each province contains two types of samples: original samples and boundary samples. The boundary samples were only involved in the training process and were not set as validation samples in the province that it was defines as boundary samples. For one sample near the boundary, it is a ‘original sample’ in only one province and is a ‘boundary sample’ in other provinces. Thus, the sample was involved in the validation of only one province, and was involved in the training process in other provinces as ‘boundary sample’. The

text was modified as “To obtain a smoother distribution, we extended the boundaries of all provinces 5 1°×1° grids outside and divided the samples inside and outside the original boundary of each province into ‘original sample’ and ‘boundary sample’. For one sample near the boundary, it is a ‘original sample’ in only one province and is a ‘boundary sample’ in other provinces. Thus, the sample was involved in the validation of only one province, and was involved in the training process in other provinces as ‘boundary sample’.”

- **Independent observations.** Please could you provide geographical positions and period of stations used as independent observations?

Response: The HOT station is located in 22° 45'N, 158° 00'W and observations started since October 1988. The BATS station is located in 31°50'N, 64°10'W and observations are from October 1988 to December 2019. The ESTOC station is located in 29°10'N, 15°30'W and observations from 1995 to 2009 were used. The information above was added in the validation section.

- **Set of selected predictors.** In table 3 authors presented two sets for most of the regions that depends on the availability CHL-a data. Please could you present more explicitly that the final product is built on two FFNNs, one trained for the period 1992-2001 based on one predictors set and another – for 2002-2019 based on the second predictors set?

Response: Thanks for your suggestion. A description was added in the section 2.4 pCO₂ product as “Then the final product was built based on two FFNNs, one trained for the period 2002-2019 using one predictor set including CHL-a or CHL-a anom, and the second one for the 1992-2001 using the second predictor set without CHL-a and CHL-a anom.”

- **More explicit figures’ captions.** Please provide more explicit figures’ captions, period of presented results, or results averaged over xxxx-xxxx, what are horizontal lines in Fig.6b?

Response: Thanks for your suggestion. The horizontal line was the average pCO₂ growth rate over each decade (1992-2000, 2001-2010 and 2011-2019).

- **Not correct conclusion.** On page 15 lines 375-379 authors concluded that the difference between FNN1 and FFNN3 is relatively small, because predictors used in FFNN1 and FFNN3 were related to main drivers of pCO₂, such as CHL-a, xCO₂ and MLD. However, same drivers are used in FFNN2. Thus, it cannot explain why FFNN2 shows higher differences with observations.

Response: Thank you for pointing out this mistake. After reconsidering this issue, I think the application of latitude and longitude as predictors of pCO₂ may be the reason why FFNN2 shows higher MAE and other validation groups shows relatively closer results. For example, in the province P10 that latitude and longitude were considered not good predictors by the stepwise FFNN algorithm, the three validation groups show significant closer results than that in other provinces. While in other provinces, latitude and longitude were used as predictors in the FFNN1 and FFNN3, decreasing the MAE and RMSE. The text was corrected as “The MAE and RMSE difference between FFNN1 and FFNN3 in some provinces were relatively small. The reason for higher MAE and RMSE showed by the FFNN2 may be the application of latitudes and longitudes as predictors in both the FFNN1 and FFNN3 but not in the FFNN2. In the province P10, latitudes and longitudes were considered not good predictors by the stepwise FFNN algorithm and the results of three validation groups were extremely close.”.

- **On page 18 line 430 authors said that the pattern of reconstructed pCO₂ climatology was close to SOCAT in the Indian Ocean. I would say that it is not so close to mention it in this sentence.**

Response: Thanks for your suggestion. The inaccurate description was now removed.

- **Page 10 lines 298-300: For better structure of paragraph the sentence “In the province P1 located in the Arctic, the silicate concentration and temperature were considered as the most crucial predictor of pCO₂.” could be moved at the end of paragraph where authors mentioned the phosphate, nitrate, silicate, etc.**

Response: Thanks for your suggestion. The sentence was now moved at the end.

- **Page 13 lines 336-337: The sentence about results in the Indian Ocean can be removed if you put the Indian Ocean in the previous sentence, or please add “Also” at the beginning of the sentence dedicated to results in the Indian Ocean.**

Response: At the beginning of the sentence “Also” has been added now.

- **Page 16 lines 390-392: Please could you reformulate this sentence (“The interannual variability and seasonal pattern..”) as it is difficult to read?**

Response: The sentence was modified as “Compared with the independent

observations from the HOT station, the three validation groups both show close results, which were also similar with each other in the seasonal and interannual variability of pCO₂".

- **Page 18 lines 432-436: two sentence can be combined: "Compared with previous climatology product (Landschuster et al., 2020), the global distribution pattern of surface ocean pCO₂ was basically well consistent: inconsistent spatial distribution also existed in the Arctic and parts of the Southern Ocean near the Antarctic continent."**

Response: Thanks for your suggestion. The two sentences now have been combined.

Typo:

Page 2 line 41: "surface ocean pCO₂" should be replaced by "Surface ocean pCO₂".

Page 9 line 261: "validation group" should be replaced by "Validation group".

Page 13 line 332: "Based the K-fold" should be replaced by "based on the K-fold".

Page 20 line 459: "based improved FFNN size" should be replaced by "based on improved FFNN size".

Response: Thank you for pointing out these mistakes. These mistakes have been corrected now.