

Response to Referee's Comments

Referee 2: At present, there are many data products in marine physics, such as temperature and salinity products, but there are few data products in marine chemistry. I support the publication of more marine chemistry data products.

Authors: We thank Referee 2 for his/her interest in marine chemistry data products and comments/suggestions on our study. We will reply to each comment in the following. Throughout this document, the referee's comments are in bold.

1 The author reconstructed surface ocean $p\text{CO}_2$ based on FFNN with region divided by latitudes and similar predictors with previous researches was used, which is not novel.

With the proposed ensemble-based mapping method, statistics, and keys findings presented in the manuscript, we believe that our study is novel and would be a valuable contribution for the marine science community. However, we admit that the first version of the manuscript missed part of discussions on the comparison among the existing methods, and thus the novelty of this study was not easy to interpret. We consider this Referee's feedback important and have revised the manuscript in such a way that our three main contributions are elaborated and highlighted.

First, we propose an ensemble of 100 feed forward neural network (FFNN) models to reproduce and intensively analyse spatially and temporally varying surface $p\text{CO}_2$ fields, air-sea CO_2 fluxes, and their associated uncertainties over the global ocean. At the first glance, this FFNN-based approach looks similar to the other mapping methods proposed in previous studies (e.g., Rödenbeck et al., 2013; Landschützer et al., 2016; Denvil-Sommer et al., 2019; Gregor et al., 2019) since all have used statistical approaches (e.g., interpolation, clustering, classical regression, neural networks) to pursue the same target. Nevertheless, our model design and implementation are different from the others'. The mapping method developed in this study is based on a Monte Carlo approach wherein each model is trained and validated on sub-samples randomly drawn from the monthly gridded SOCATv2020 data and available data of predictors. Besides, the exclusion of p gridded SOCAT data of the reconstructed month itself in model training and validation allows to reduce model over-fitting and to leave much more independent data for model evaluation possibly than the previous studies. Despite leaving a large volume of evaluation data, results obtained are in line with the other reconstructions (see e.g., Friedlingstein et al., 2020, and references therein). The proposed approach is both an extension and an improvement of the first version developed by Denvil-Sommer et al. (2019) at the same laboratory (see quality assessments comparing these two model versions in Chau et al., 2020). Furthermore, the ensemble of FFNN models is framed such that strengths of the existing statistical models have been taken into account and mapping uncertainties can be reduced. That latter are systematically induced by, for instance, discrete boundaries in the two-step clustering-regression by Landschützer et al. (2016); Gregor et al. (2019) or the two-step FFNN-based reconstruction of $p\text{CO}_2$ climatologies and anomalies by Denvil-Sommer et al. (2019) .

Second, we quantify model best estimates (ensemble mean) and uncertainties (ensemble standard deviation) based on the ensembles of 100 model outputs of surface $p\text{CO}_2$ and air-sea CO_2 fluxes, and evaluate these estimates with independent SOCAT data and in situ observations. It is noteworthy that there exist other ensemble-based approaches (Gregor et al., 2019; Rödenbeck et al., 2015; Friedlingstein et al., 2020) but with a small ensemble size (less than 20) and with different concepts and objectives (see in the revised text of the Introduction below for further details). Additionally, in the preceding studies, misfits between the reconstructed and observational data (e.g., the root-mean-square deviation, RMSD) are used to evaluate product quality and infer uncertainty estimates of the reconstructed $p\text{CO}_2$. Reconstruction errors of $p\text{CO}_2$ are then propagated to get uncertainty estimates of the reconstructed CO_2 fluxes (see in Landschützer et al., 2014, for instance). By construction, such uncertainty estimates are restricted to oceanic regions and periods when observations are available (Lebehot et al., 2019; Hauck et al., 2020), and the uncertainty quantification of an averaged $p\text{CO}_2$ or an integrated flux is under low confidence due to sparse data density. As an advantage of our approach, an ensemble of 100 model outputs of $p\text{CO}_2$ and CO_2 fluxes is available at each $1^\circ \times 1^\circ$ ocean grid cell of the globe for each month in the period 1985–2019. The ensemble asset facilitates the quantification of model uncertainty of $p\text{CO}_2$ and CO_2 fluxes averaged or integrated over space and time of interest (see for instance Figures 5 and 9 in the manuscript and Figures RP2.0, RP2.1, RP2.2, and RP2.3 in this document). This is expected to provide more robust estimates than the ones based on reconstruction errors.

Another key contribution of this study is a seamless analysis of the reconstructed data and uncertainty estimates over both the open ocean and coastal zones. Interpretations of good or poor reconstructions of surface $p\text{CO}_2$ and air-sea CO_2 fluxes (e.g., data density and distribution, regional to local characteristics of $p\text{CO}_2$ and its potential drivers, model design and resolution) and changes in spatial and seasonal variations of CO_2 fluxes are given. To strengthen our interpretation, we have shown both the temporal and spatial distribution of the reconstructed $p\text{CO}_2$ and CO_2 fluxes fields, model-data misfits, model uncertainty, and linked these materials with their driving mechanisms suggested in previous literature. More importantly, we have made an intercomparison of model reconstruction ability between regions, identified oceanic sectors where the model does not fit the data well, and suggested further improvements on the data reconstruction based on the proposed space-time varying uncertainty fields. Note that oceanic regions divided by latitude bands are only used for this analysis of our results, FFNN models themselves do not follow oceanic regions or biomes in clustering before training as proposed in Landschützer et al. (2016); Gregor et al. (2019). The Referee's comment "**The author reconstructed surface ocean $p\text{CO}_2$ based on FFNN with region divided by latitudes**" seems to be misleading.

These three main points are now elaborate in Section Introduction. Precisely, the two new paragraphs replacing the ones in Lines 37-55 of the manuscript are as follows.

Revised text:

Various data-based approaches have been proposed to infer gridded maps of surface ocean $p\text{CO}_2$ from the sparse set of observational data. They have been successful in obtaining similarly low misfits between the reconstructed and evaluation data and reasonable estimates of air-sea CO_2 fluxes (see in Rödenbeck et al., 2015; Gregor et al., 2019; Friedlingstein et al., 2020) although model design and implementation are quite different (e.g., proportion of SOCAT data used in model fitting and evaluation). Aside from data reconstruction built on a single model mapping $p\text{CO}_2$ data with machine learning, classical regression, or mixed layer schemes (see Rödenbeck et al., 2013; Landschützer et al., 2016, for a few), ensemble-based approaches have recently emerged but with their own concepts and objectives. For example, Denvil-Sommer et al. (2019) designed a two-step reconstruction of $p\text{CO}_2$ climatologies and anomalies based on five neural network models and selected the one that reproduced the $p\text{CO}_2$ field with the smallest model-data misfit. Gregor et al. (2019) and Gregor and Gruber (2021) introduced machine-learning ensembles with six to sixteen different two-step clustering-regression models mapping surface $p\text{CO}_2$ and suggest that the use of their ensemble mean is better than each member estimate. In a broader context, Rödenbeck et al. (2015) presented an intercomparison of fourteen mapping methods targeting the identification of common or distinguishable features of different products in long-term mean, regional and temporal variations. Hauck et al. (2020) and Friedlingstein et al. (2020) also synthesized $p\text{CO}_2$ mapping products and take an ensemble of their observation-based estimates of air-sea CO_2 fluxes as a benchmark to compare with the one derived from ocean biogeochemical models. Despite positive conclusions overall, statistical data reconstructions are still subject to further improvements. In Rödenbeck et al. (2015), Hauck et al. (2020), Bushinsky et al. (2019), and Denvil-Sommer et al. (2021), the authors explain that substantial extensions of surface ocean observational network systems are essential to better determine $p\text{CO}_2$ and fluxes at finer scales and reduce mapping uncertainties. So far mapping uncertainties have been estimated by using misfits between the model outputs and SOCAT data (e.g., the root-mean-square deviation, RMSD). By construction, such uncertainty estimates are restricted to oceanic regions and periods when observations are available (Rödenbeck et al., 2015; Lebehot et al., 2019; Gregor et al., 2019) and the uncertainty quantification of an averaged $p\text{CO}_2$ or an integrated flux over space and time of interest is under low confidence due to sparse data density. Furthermore, most of the previous mapping methods target $p\text{CO}_2$ data and evaluate their estimates solely over the open ocean, with the coastal data excluded or not fully qualified. In Laruelle et al. (2014, 2017) the authors present spatial distribution of air-sea flux density and estimates of total coastal C sink while a recent study (Landschützer et al., 2020) limits their estimation to monthly climatologies of $p\text{CO}_2$ over the global ocean including the coastal regions.

In this work, we propose a new inference strategy for reconstructing the monthly $p\text{CO}_2$ fields and the contemporary air-sea fluxes over the period 1985–2019 with a spatial resolution of $1^\circ \times 1^\circ$. It is based on a Monte Carlo approach, an ensemble of 100 neural network models mapping sub-samples drawn from the monthly gridded SOCATv2020 data and available data of predictors. This ensemble approach was developed at the Laboratoire des Sciences du Climat et de l'Environnement (LSCE) as both an extension and an improvement of the first version (LSCE-FFNN-v1, Denvil-Sommer et al., 2019). In the following

sections, we first present the ensemble of neural networks designed with the aim of leaving aside the issue of discrete boundaries in the existing two-step clustering-regressions (see further discussion in Gregor and Gruber, 2021) and reducing the mapping uncertainties induced by the two-step reconstruction of the $p\text{CO}_2$ fields (Denvil-Sommer et al., 2019) or by an ensemble-based reconstruction with a small ensemble size. In addition, each FFNN model follows a leave-p-out cross-validation approach, i.e., the exclusion of p gridded SOCAT data of the reconstructed month itself in model training and validation. This allows to reduce model over-fitting and to leave much more independent data for model evaluation than the previous studies. Mean and standard deviation computed from the ensemble of 100 model outputs are defined as estimates of the mean state and uncertainty of the carbon fields. As one of the novel key findings of this study compared to the existing ones, we compute and analyze the estimates of $p\text{CO}_2$ and air-sea fluxes, model errors, and model uncertainties for different time scales (e.g., monthly, yearly, and multi-decadal) and spatial scales (e.g., grid cells, sub-basins, and the global ocean). We then suggest the use of an indicator map built on the space-time varying uncertainty fields instead of model-data misfits for identifying regions that should be prioritized for future observational programs and model development in order to improve the data reconstruction. Last but not least, the model best estimates and uncertainty of $p\text{CO}_2$ and air-sea fluxes are analysed seamlessly over the open ocean to the coastal zone. Potential drivers of the spatio-temporal distribution and the magnitude of open ocean and coastal CO_2 fluxes are discussed with the aim to better identify underlying processes and to detect potential focus regions for further studies on the evolution of oceanic CO_2 sources and sinks.

In this work, we propose a new inference strategy for reconstructing the monthly $p\text{CO}_2$ fields and the contemporary air-sea fluxes over the period 1985–2019 with a spatial resolution of $1^\circ \times 1^\circ$. It is based on a Monte Carlo approach, an ensemble of 100 neural network models mapping sub-samples drawn from the monthly gridded SOCATv2020 data and available data of predictors. This ensemble approach was developed at the Laboratoire des Sciences du Climat et de l'Environnement (LSCE) as both an extension and an improvement of the first version (LSCE-FFNN-v1, Denvil-Sommer et al., 2019). In the following sections, we first present the ensemble of neural networks designed with the aim of leaving aside the issue of discrete boundaries in the existing two-step clustering-regressions (see further discussion in Gregor and Gruber, 2021) and reducing the mapping uncertainties induced by the two-step reconstruction of the $p\text{CO}_2$ fields (Denvil-Sommer et al., 2019) or by an ensemble-based reconstruction with a small ensemble size. In addition, each FFNN model follows a leave-p-out cross-validation approach, i.e., the exclusion of p gridded SOCAT data of the reconstructed month itself in model training and validation. This allows to reduce model over-fitting and to leave much more independent data for model evaluation than possibly the previous studies. Mean and standard deviation computed from the ensemble of 100 model outputs are defined as estimates of the mean state and uncertainty of the carbon fields. As one of the novel key findings of this study compared to the existing ones, we compute and analyze the estimates of $p\text{CO}_2$ and air-sea fluxes, model errors, and model uncertainties for different time scales (e.g., monthly, yearly, and multi-decadal) and spatial scales (e.g., grid cells, sub-basins, and the global ocean). We then suggest the use of an indicator map built on the space-time varying uncertainty fields instead of model-data misfits for identifying regions that should be prioritized for future observational programs and model development in order to improve the data reconstruction. Last but not least, the model best estimates and uncertainty of $p\text{CO}_2$ and air-sea fluxes are analysed seamlessly over the open ocean to the coastal zone. Potential drivers of the spatio-temporal distribution and the magnitude of open ocean and coastal CO_2 fluxes are discussed with the aim to better identify underlying processes and to detect potential focus regions for further studies on the evolution of oceanic CO_2 sources and sinks.

2 The reconstruction of $p\text{CO}_2$ and sea-air CO_2 flux over global coastal oceans are interesting works but the author needs to do much more works on the validation of coastal results. Because a standard deviation of $41.79 \mu\text{atm}$ between $p\text{CO}_2$ results and SOCAT observations possibly leads to opposite results in the estimate of coastal CO_2 flux.

We will add in the revised manuscript results comparing the reconstructed data and independent in-situ data of $p\text{CO}_2$ (part in the coastal regions) proposed by Sutton et al. (2019) (see Figures RP2.0, RP2.1, RP2.2, and RP2.3 attached below). The results confirm a reasonably good reconstruction of the proposed approach that fits observational data well at these locations. Also shown in these figures, the reconstructed timeseries cover the full period 1985-2019 while observations are still sparse

and almost distributed in the last two decades. Thus, the reconstructed timeseries would be favored to provide robust estimates of long-term trends and variations of surface pressure of CO₂ and ultimately the corresponding air-sea fluxes.

Referee 2 explains that **a standard deviation of 41.79 μatm between $p\text{CO}_2$ results and SOCAT observations possibly leads to opposite results in the estimate of coastal CO₂ flux**. This seems to be misleading. Indeed, we have written in the manuscript (Lines 126-130):

The reconstructed $p\text{CO}_2$ field matches SOCAT data well: both are normally distributed with the same mean of 361.3 μatm (Fig. 3a) and a high agreement for all percentiles (Fig. 3b) is seen. The slight under- or overestimation at high and low percentiles implies that the model is slightly biased towards the mean value, as is expected when predictor variables do not fully explain predictand variables in the training dataset. This reduced variability is also reflected in the difference between the data standard deviation based on SOCAT $p\text{CO}_2$ (41.79 μatm) and the one based on CMEMS-LSCE-FFNN (36.30 μatm).

In our context, 41.79 μatm is the standard deviation of SOCAT data itself, it is not the standard deviation of differences between the reconstructed and SOCAT observational data.

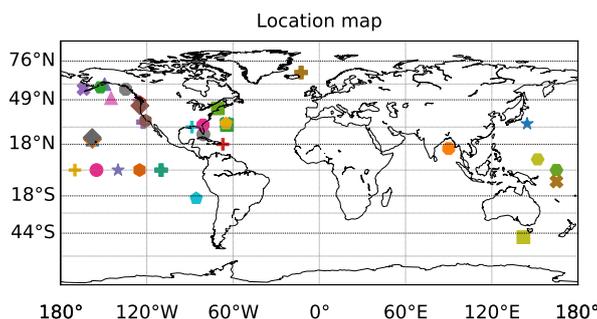


Figure RP2.0. Location map of in situ measurements of ocean surface $p\text{CO}_2$ (Sutton et al., 2019).

3 The CHL data used was only from 1992 to 2019, and was not available in the Arctic and the Southern Ocean in winter, the details about how the reconstruction was carried out when CHL was not available should be declared clearly in the method section.

We will provide this information in the method section. To be precise, climatologies based on all available CHL data (1998-2019) were used as predictors for data unavailable before 1998. We set CHL approximately to 0 mg m^{-3} as its data is missing in the Arctic and the Southern Ocean in winter. These suggestions can also be found in previous studies (e.g., Landschützer et al., 2016; Denvil-Sommer et al., 2019).

4 The subskin temperature correction (Watson et al., 2020) should be considered in the estimate of sea-air CO₂ flux.

Watson et al. (2020) proposed a double correction to the SOCAT data and to the computation of the CO₂ flux in order to remove some aliasing caused by the temperature vertical gradient within the marine boundary layer. However, the Watson et al. (2020) adjustment, if applied here, would add roughly 0.9 PgCyr^{-1} to the global ocean sink estimate based on observations. The adjusted ocean sink estimate would thus surpass the land sink and result in a large carbon budget imbalance. More evidence of their genericity are needed to apply skin and subskin corrections (Friedlingstein et al., 2020).

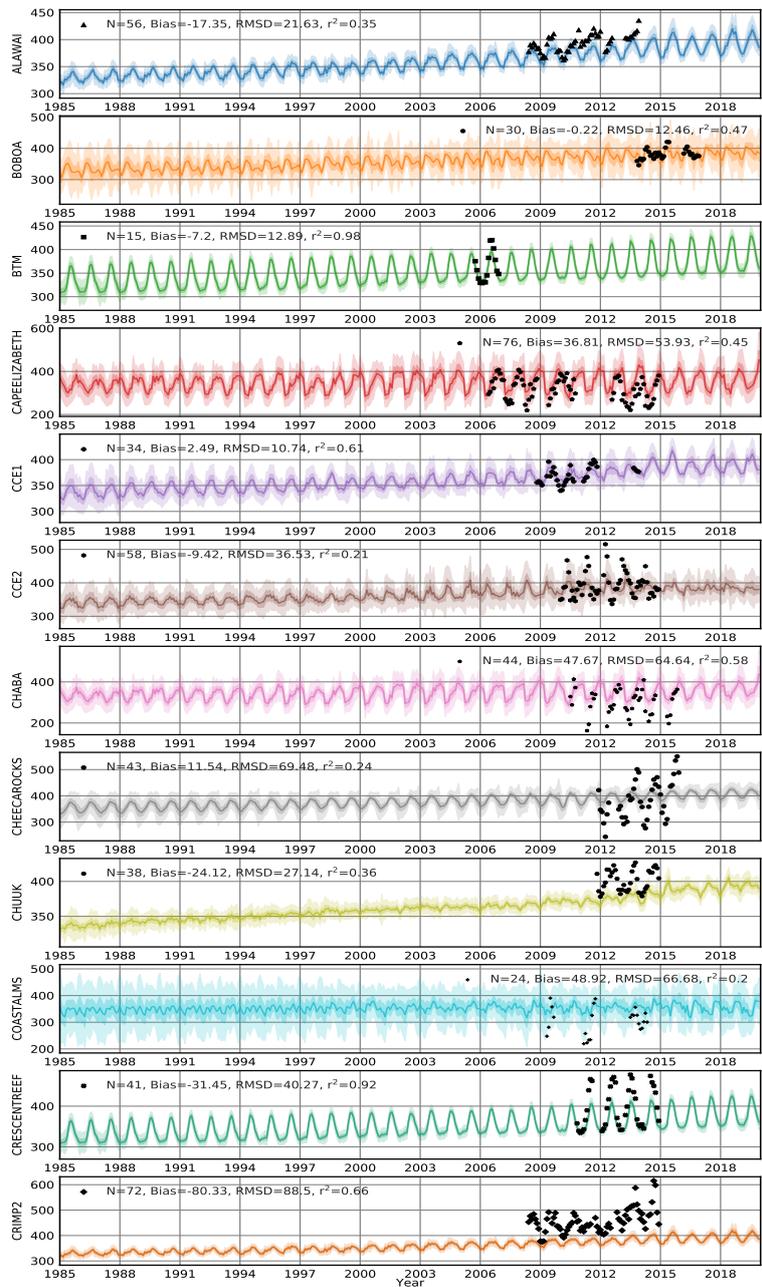


Figure RP2.1. Time series of ocean surface $p\text{CO}_2$ at different stations- part 1 (see in Location map RP2.0). Measurements at each station (Sutton et al., 2019) are monthly averaged, the ensemble mean and ensemble spread are computed from reconstructed data at the four nearest neighbors of that location. Number of observations (N), Bias, RMSD, and model-data correlation (r^2) have been computed on these monthly interpolated data. In each subplot, dots stand for observational data and the coloured line with shaded areas stand for the mean and uncertainty envelopes computed from the CMEMS-LSCE- FFNN 100-member ensemble (dark: 68% confidence interval, i.e. mean \pm 1std; light: 99% confidence interval, t.e. mean \pm 3std).

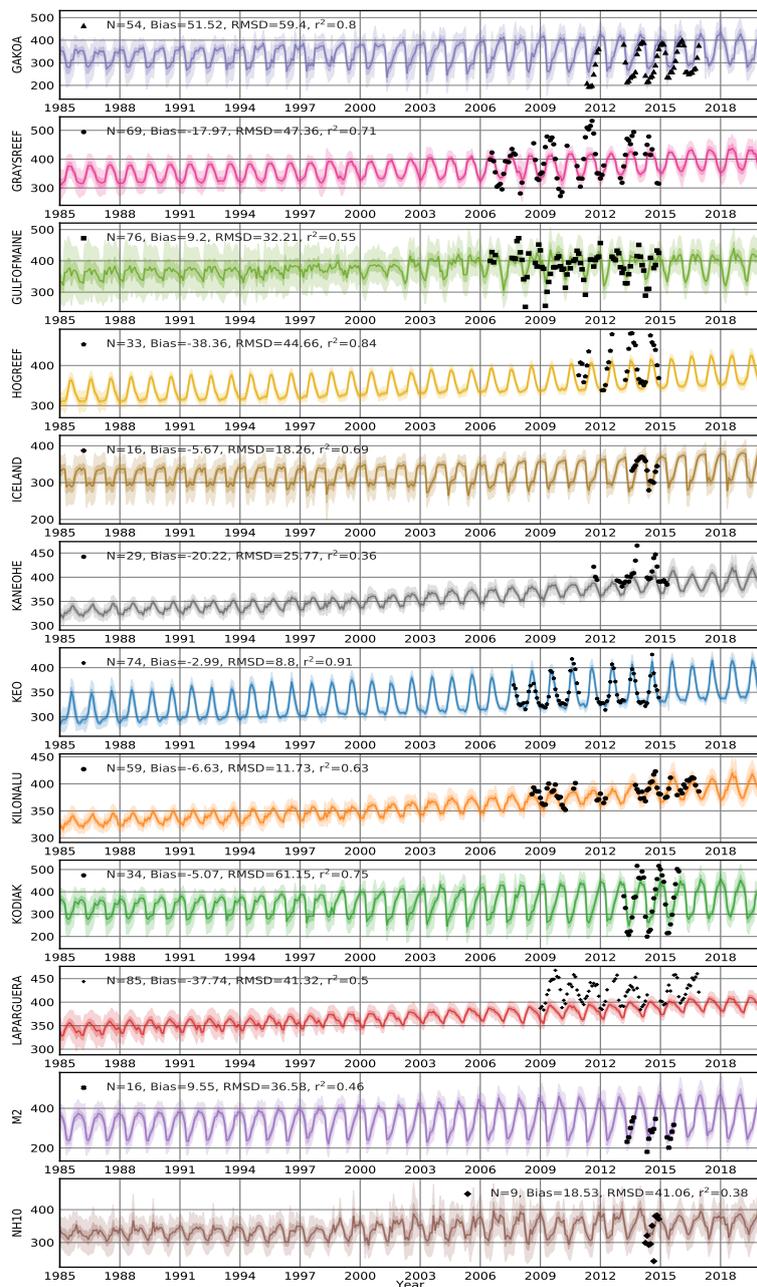


Figure RP2.2. Time series of ocean surface $p\text{CO}_2$ at different stations- part 2 (see in Location map RP2.0). Measurements at each station (Sutton et al., 2019) are monthly averaged, the ensemble mean and ensemble spread are computed from reconstructed data at the four nearest neighbors of that location. Number of observations (N), Bias, RMSD, and model-data correlation (r^2) have been computed on these monthly interpolated data. In each subplot, dots stand for observational data and the coloured line with shaded areas stand for the mean and uncertainty envelopes computed from the CMEMS-LSCE- FFNN 100-member ensemble (dark: 68% confidence interval, i.e. mean \pm 1std; light: 99% confidence interval, t.e. mean \pm 3std).

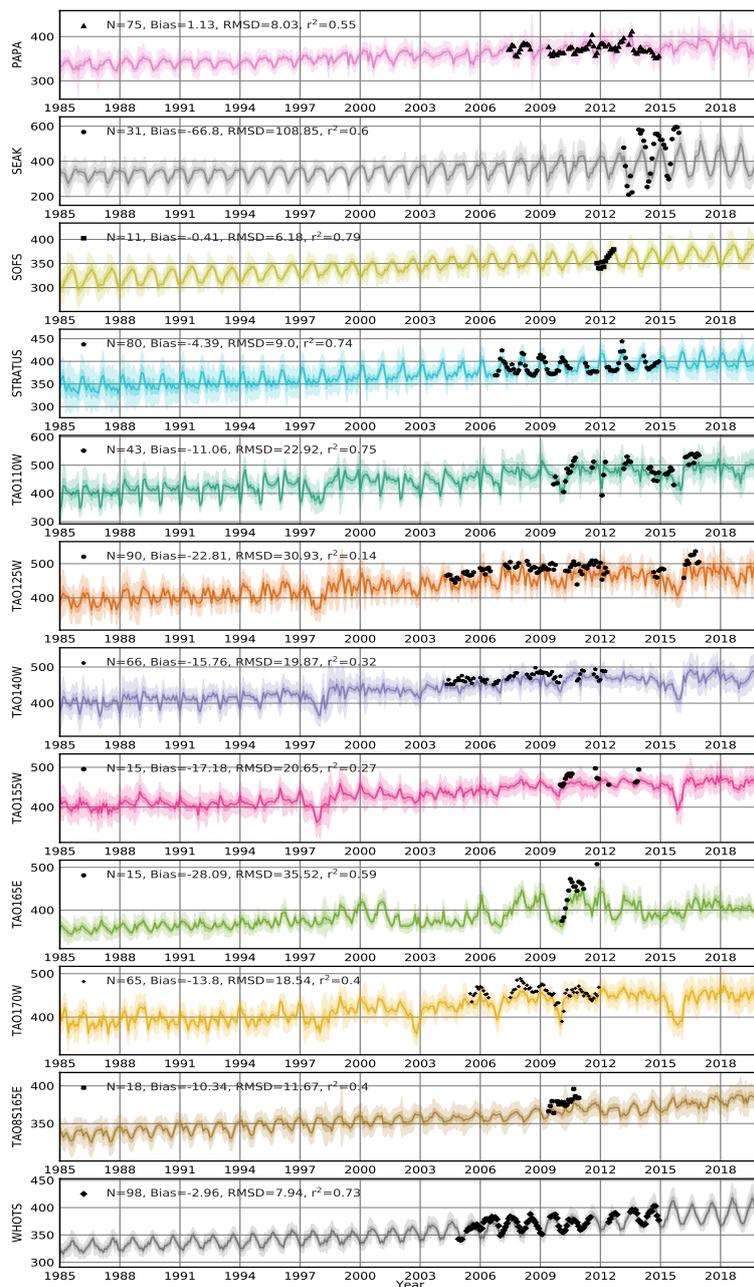


Figure RP2.3. Time series of ocean surface $p\text{CO}_2$ at different stations- part 3 (see in Location map RP2.0). Measurements at each station (Sutton et al., 2019) are monthly averaged, the ensemble mean and ensemble spread are computed from reconstructed data at the four nearest neighbors of that location. Number of observations (N), Bias, RMSD, and model-data correlation (r^2) have been computed on these monthly interpolated data. In each subplot, dots stand for observational data and the coloured line with shaded areas stand for the mean and uncertainty envelopes computed from the CMEMS-LSCE- FFNN 100-member ensemble (dark: 68% confidence interval, i.e. mean \pm 1std; light: 99% confidence interval, t.e. mean \pm 3std).

5 The author should reconsider the topic of this manuscript. If the author want focus on the CO₂ flux of global open oceans, additional work was necessary rather than only discussing spatial distribution or interannual variability, because the reconstruction method in this manuscript and the results was not novel. If the author want focus on the CO₂ flux of global coastal oceans, which was still a research gap, much more works are needed to make the result convince.

As mentioned in our response to Referee's comment 1, the manuscript presents three main contributions:

- i. Our data reconstruction is based on a new model design - an ensemble of 100 neural network models.
- ii. We quantify and evaluate model best estimates and uncertainties based on the ensemble asset. For the first time, the space-time varying uncertainty estimates (see for instance Figures 5 and 9 in the manuscript and Figures RP2.0, RP2.1, RP2.2, and RP2.3 in this document) derived from the ensemble of model outputs are presented and analysed. We promote the use of the proposed uncertainty fields which would be more informative than the RMSD-based uncertainty fields (e.g., proposed in Landschützer et al., 2014) in identifying oceanic sectors where further improvements on the data reconstruction will be needed.
- iii. More importantly, the manuscript presents seamless analysis of the reconstructed data and uncertainty estimates over the open ocean and coastal zones. Furthermore, the open ocean estimates are considered as references for the coastal data assessment.

We believe that the ensemble-based approach and analysis therein are novel and the Introduction section has been changed to better highlight these contributions. However, we agree with the referee that the reconstructed data need to be evaluated with independent in situ observations. In the revised version of the manuscript we propose to add Figures RP2.0, RP2.1, RP2.2, and RP2.3 and an interpretation of these results (see also in our reply to Referee's comment 2).

6 Line 76: "An ensemble of 100 FFNNs was used to reconstruct monthly $p\text{CO}_2$ fields.....", How are these 100 models built? Why did you do that? How are the results of 100 models selected? Line 84-85: "The random extraction and the FFNN training were repeated 100 times so that 100 versions of the monthly FFNNs have been obtained", Why is it the "100 times"? How is the "100 times" determined? Does it converge after 100 iterations?

The description of the construction of the ensemble approach is given in the manuscript (Lines 81-89) as follows (Figure 1 is used to illustrate a neural network model mapping the target $p\text{CO}_2$ and predictor variables).

To reconstruct the $p\text{CO}_2$ fields over the global ocean for each target month over the 1985–2019 period, all the available SOCAT data and the co-located predictors have been collected for the month before and the month after the target month. We randomly extracted two thirds of each one of these datasets to make training datasets for the FFNNs, leaving the remaining third to be corresponding test datasets. The FFNNs were then trained for each target month.

Our ensemble approach comprises multiple network models, each trained and validated on resampled data of SOCAT $p\text{CO}_2$ and predictors. In statistics, it belongs to the classes of bootstrapping and Monte Carlo methods. Theoretically, the number of samples or the ensemble size must be substantially large to get a convergence. However, it was demonstrated in the literature (e.g., Goodhue et al., 2012; Efron et al., 2015) that with the ensemble size of 50 the model estimation is likely stable and with the ensemble size over 100 the improvement in standard errors between model outputs and evaluation data is negligible. It was also tested in the first phase of our model development. Figure RP2.4 shows an illustration of the reconstruction skill with respect to the ensemble size. For each ensemble of N model outputs of $p\text{CO}_2$ ($N \in \{5, 10, 20, 50, 75, 100\}$), RMSD is computed between the ensemble mean (our best model estimate) and SOCAT data over the period 1985-2019. As seen in this figure, the reconstruction starts to stabilize with $N = 50$. In this study, we have exploited a large but realistic amount of computing resources to run an ensemble of 100 neural network models.

We will make this information appear in the Method section.

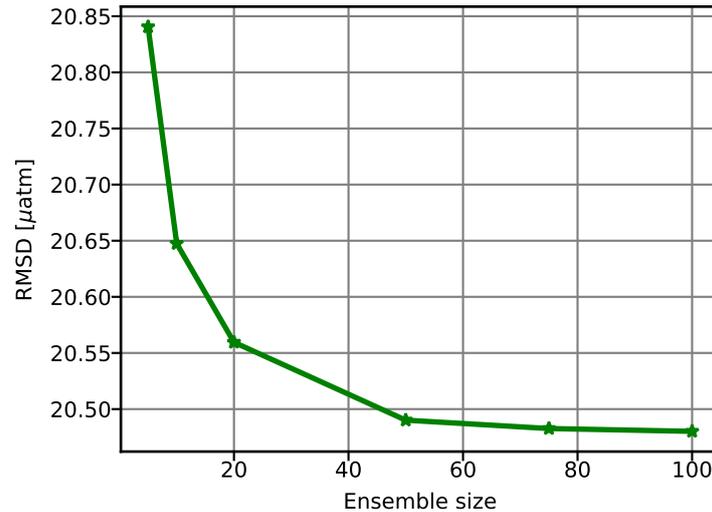


Figure RP2.4. RMSD between a best estimate (ensemble mean) and SOCAT data of ocean surface $p\text{CO}_2$ with respect to the ensemble size in $\{5, 10, 20, 50, 75, 100\}$.

7 Table 2, What is the meaning of two numbers in the rightmost column of Table 2, for example: 0.07 ± 0.04 , 0.30 ± 0.13

The numbers without brackets (e.g., 0.07 ± 0.04 , 0.30 ± 0.13) in the rightmost column of Table 2 in the manuscript refer to the estimates derived from observation-based methods. In the caption of Table 2, we wrote: *In column 'RECCAP1', values in parentheses are the 'best' estimates proposed by RECCAP1 studies, the others are the estimates computed with different methods using $p\text{CO}_2$ observations.* Further information can be found in Lines 438-443:

RECCAP1 best estimates were derived from averages or medians of estimates based on the $p\text{CO}_2$ climatology or $p\text{CO}_2$ diagnostic model, and/or the atmospheric and ocean inversions and GOBM models (see Schuster et al., 2013; Ishii et al., 2014; Sarma et al., 2013; Lenton et al., 2013, and references therein). The observation-based estimates of regional net fluxes reported in these studies were computed from the reconstruction of SOCAT $p\text{CO}_2$ data (only used in Schuster et al., 2013), LDEO data (<https://www.ldeo.columbia.edu/res/pi/CO2/>), and its climatology (Takahashi et al., 2009).

This information will be added to the caption of Table 2 to make it more visible to the readers.

8 Line 444-446: “The global open ocean uptake obtained in this study of $1.344 \pm 0.111 \text{ PgC yr}^{-1}$ lies between the observation based net sink estimate by Wanninkhof et al. (2013) (1.18 PgC yr^{-1}) and the global sum of regional best estimates given in Table 2 (1.8 PgC yr^{-1})”. In table 2, I can’t find the value of 1.8 PgC yr^{-1}

It means that 1.8 PgC yr^{-1} is the sum of all the 'best' estimates (between brackets) given in Table 2.

9 Line 462-463: The discrepancy is possibly due to an overestimation of Arctic $p\text{CO}_2$ by the CMEMS-LSCE-FFNN (see in Sect. 3.1.2) and to the lack of estimates over a large portion of the seasonally sea-ice covered regions. This sentence means that the data in the Arctic are not accurate at present. So the data in the Arctic is not suitable for use at present.

Results shown in Sect. 3.1 in the manuscript confirm that the model reconstruction of $p\text{CO}_2$ over the Arctic does not fit SOCAT data well and is much more uncertain than for other oceanic regions. The factors behind the poor estimates of Arctic $p\text{CO}_2$

have been further discussed in the Discussion section (Lines 460-469). Despite the need for further improvements, our analysis fairly documents the current status and discusses the way forward.

References

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