

**Dear Editor,**

**Please find below the point by point answers to the comments provided by both reviewers. In the following text, the comments of the reviewer are in written back and our answers are written in blue. All the modifications suggested by the reviewer have been carefully implemented into the manuscript. This updated version of the manuscript is available with the 'track changes' option at the end of this file, after our answers.**

**On behalf of all co-authors,  
Goulven Laruelle**

Review of bg-2017-64

Global high-resolution monthly pCO<sub>2</sub> climatology for the coastal ocean derived from neural network interpolation by Laruelle et al.

Reviewer: Rik Wanninkhof, NOAA/AOML

This is largely a descriptive paper of procedures to create monthly estimates of coastal pCO<sub>2</sub> levels. As mentioned in the abstract, Laruelle et al. use a modified version of a two-step artificial neural network method (SOM-FFN) to interpolate the pCO<sub>2</sub> data along the continental margins with a spatial resolution of 0.25 degrees and with monthly resolution from 1998 until 2014.

The effort is clearly an impressive one and an important contribution to coastal ocean science. However there are some shortcomings. Many readers will not fully understand the approach and assumptions in SOM-FNN, and this needs more discussion. The manuscript lacks in context and interpretation. Some of the procedural shortcomings that were in the initial global open ocean effort as described in Landschützer et al., (2013; 2015) prevail.

We are grateful for the reviewer's evaluation and his constructive suggestions. Please find below a detailed answer to each comment. All our answers are written in.

On behalf of all co-authors,

Goulven Laruelle

We have introduced a new section to the manuscript, which critically discusses the strength and weaknesses of the approach and its changes since the first open ocean version from Landschützer et al. (2013). This new section permits to better appraise the improvements achieved by tailoring the oceanic set-up for the coastal region and identify the remaining knowledge gaps.

We further understand that one of the main reviewer's concerns relates to the choice of validating the results using a database that largely overlaps with the one used to calibrate the model. Following his recommendation, we modified our approach and, using the latest versions of both SOCAT (i.e. version 4) and LDEO (i.e. v2015), we have now created two entirely independent datasets: one for the calibration (named SOCAT\*) and one for validation (LDEO\*). These two datasets were generated by randomly assigning each measurement common to both original databases to either SOCAT\* or LDEO\* (see comment 3 below for further details on the new approach). Another important suggestion was to further elaborate on the comparison between the simulated pCO<sub>2</sub> field and the validation dataset. We thus created new maps displaying the mean residuals errors between the pCO<sub>2</sub> values generated by the SOM\_FFNN, on the one hand, and those extracted from LDEO\* and SOCAT\*, on the other hand. This representation allows for a more detailed analysis of the performance of the model. As suggested by the reviewer, histograms of residual errors were also computed for each biogeochemical province and will be discussed in the updated manuscript. In addition, we have also introduced a new predictor (wind speed), which helped improve the performances of the SOM\_FFNN compared to those presented in the previous version of the manuscript.

While there are comparisons and validations of the SOM-FNN approach it mostly in terms of a RMSE. It is unclear what impact the RMSE would have on the phenomena investigated. Other means of comparison of how well the approach works should be performed. Rödenbeck et al (2015) present some nice diagnostics that could be applied.

At very least examples of the distribution of errors in pCO<sub>2</sub> should be shown in histograms.

[1] We agree with the reviewer that the assessment of the performance of the model only relied on averaged biases and RMSE calculated for each biogeochemical province. In the updated manuscript, we propose to include maps presenting the average residual errors between the pCO<sub>2</sub> field generated by the model and pCO<sub>2</sub> data extracted from the calibration (SOCAT\*) and validation (LDEO\*) datasets. They are obtained by subtracting the observed values from model output in each grid cell for every month where observations are available. This representation not only allows to assess which regions provide the best match with the observations but also to identify where the simulated pCO<sub>2</sub> overestimates (positive values, in red on the figure below) or underestimates (negative values, in blue on the figure below) the field data. Moreover, as suggested by the reviewer, we introduce a new figure, presenting the distribution of the residual errors between the results of the SOM\_FFN and LDEO\* for each biogeochemical province. This figure reveals nearly Gaussian distributions of the residuals for every biogeochemical province with the exception of province P8, for which the spread is not only the highest (indicating the largest discrepancy between model and observations), but also slightly skewed toward high values, thus revealing a tendency to overestimate the observed pCO<sub>2</sub>.

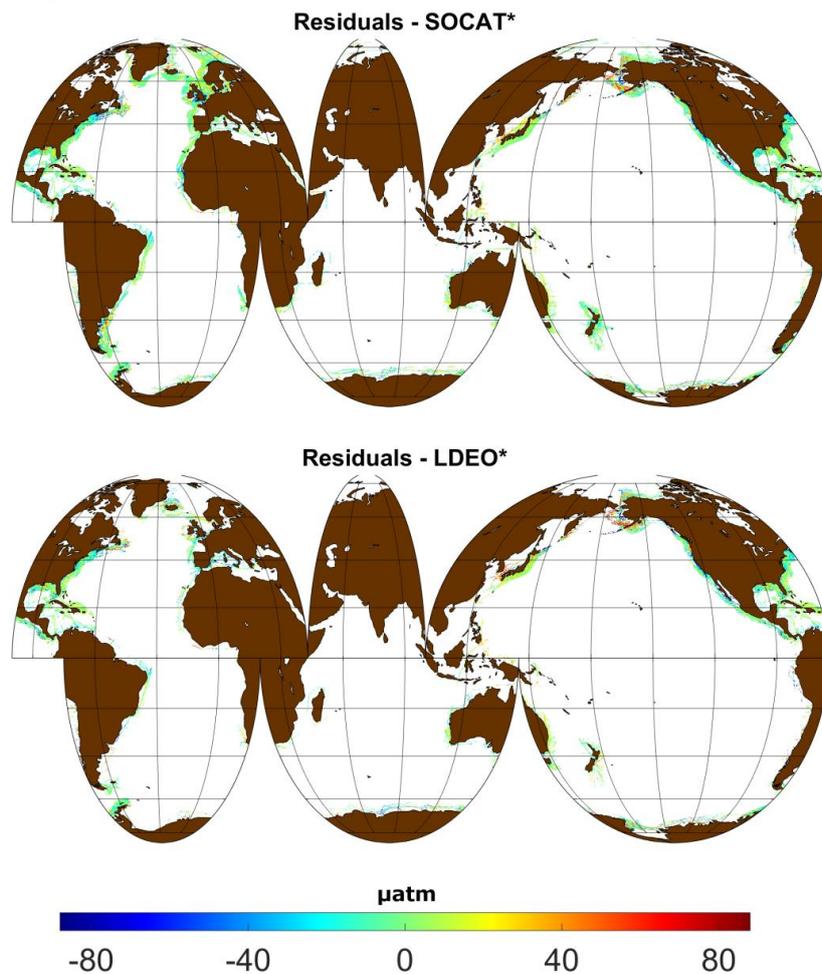


Figure 1: Mean residuals calculated as the difference between the SOM\_FFM pCO<sub>2</sub> outputs and pCO<sub>2</sub> observations from SOCAT\* (top) and LDEO\* (bottom).

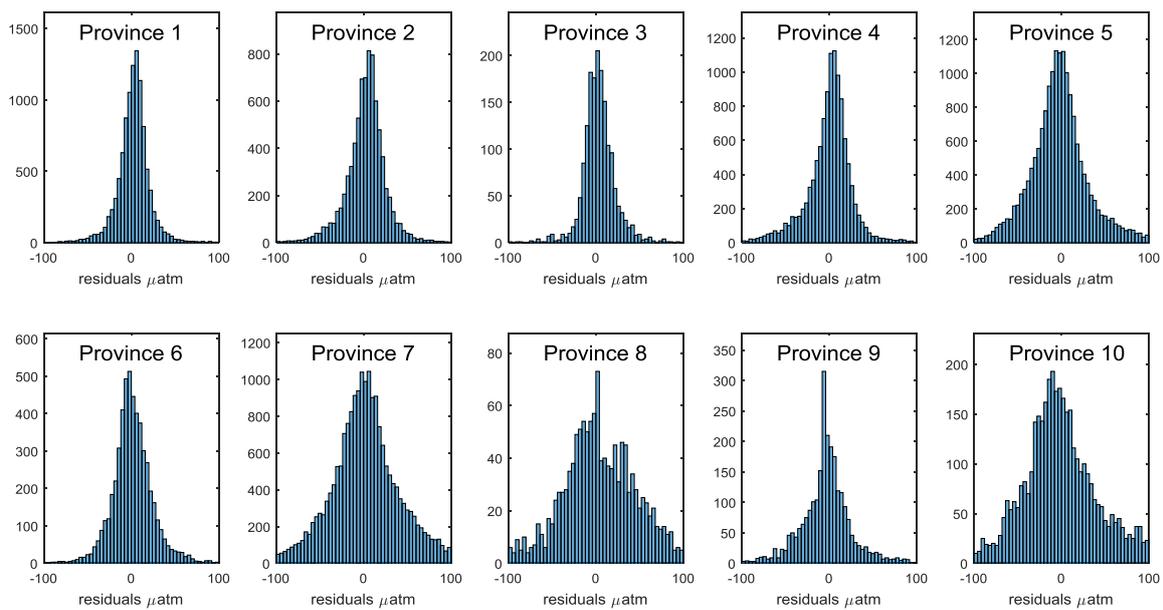


Figure: Histograms reporting the distribution of residuals between observed (LDEO\*) and computed (SOM\_FFNN) pCO<sub>2</sub> in each biogeochemical province.

As the authors indicate, their definition of the coastal realm (200 nm or 1000 m depth) covers a much greater region than commonly viewed as coastal. The outer edge of the domain for much of the ocean can be considered "blue water". Therefore it is surprising that the differences between the coastal SOM-FFNN and open ocean SOM-FFNN in Landschützer et al. are large. A more comprehensive diagnostic comparison should be made as it could suggest some fundamental issues with the approach.

[2] Although both the coastal SOM\_FFNN presented in this study and the oceanic SOM\_FFNN published in Landschützer et al. have a significant overlapping domains, they were not trained with the same datasets. For the most part, the coastal data from SOCAT used here to calibrate our model were not included in the data pool used for the open ocean simulations. In addition, the characteristic ranges of values within which both models are trained are also different for some of the environmental parameters. In particular, the average bathymetry and sea surface salinities are often significantly lower for data used. It is thus not surprising to observe significant differences between the results produced by both models, yet we agree with the reviewer that the magnitude of difference is somewhat interesting and highlights current knowledge gaps regarding the coastal ocean to open ocean transition zone. This certainly deserves some further investigation; however, we do believe that this is beyond the scope of this study. Nevertheless, in the updated manuscript, we will further discuss the differences between coastal and open SOM-FFNN in the transition zone.

The validation approach is weak. There is significant (complete?) overlap between the data in SOCAT and that of Takahashi. The biases in datasets are likely due to different data reduction approaches. More comparisons should be made with actual data not used in the training, and more data should be excluded from the training for validation purposes.

[3] As mentioned by the reviewer, the SOCAT and LDEO databases have a large overlap, and the two datasets cannot be considered independent. In order to provide robust calibration and validation we now created two fully independent datasets based on SOCAT and LDEO, which do not contain any common measurement. We used the latest releases of both databases (i.e. SOCATv4 and LDEOv2015) and filtered out all non-coastal data points, as was already done in the previous version of the manuscript. Under our definition of the coastal zone, SOCATv4 contains  $\sim 8 \cdot 10^6$  data points and LDEO  $\sim 5.6 \cdot 10^6$ , over 70% of which are also part of SOCATv4. We then randomly assigned each of those common data point to either database to insure that each data only belongs to one dataset. In the updated manuscript, the new datasets are renamed SOCAT\* which is used to train the SOM\_FFNN, and LDEO\* which is only used for validation purposes. In the new manuscript, the procedure used to create SOCAT\* and LDEO\* will be detailed in section 2.2 (Data Sources and processing).

The use of a more robust validation did not alter significantly the performances of the SOM\_FFNN and, combined with the inclusion of wind speed as a new predictor, the biases and RMSE generated by the model when compared with LDEO\* are actually slightly lower than those presented in the original simulations (see table below). Also, note that the use of SOCATv4 and LDEOv2015 provides a significant number of data for the year 2015, which motivated us to expend our simulation period from 17 to 18 years.

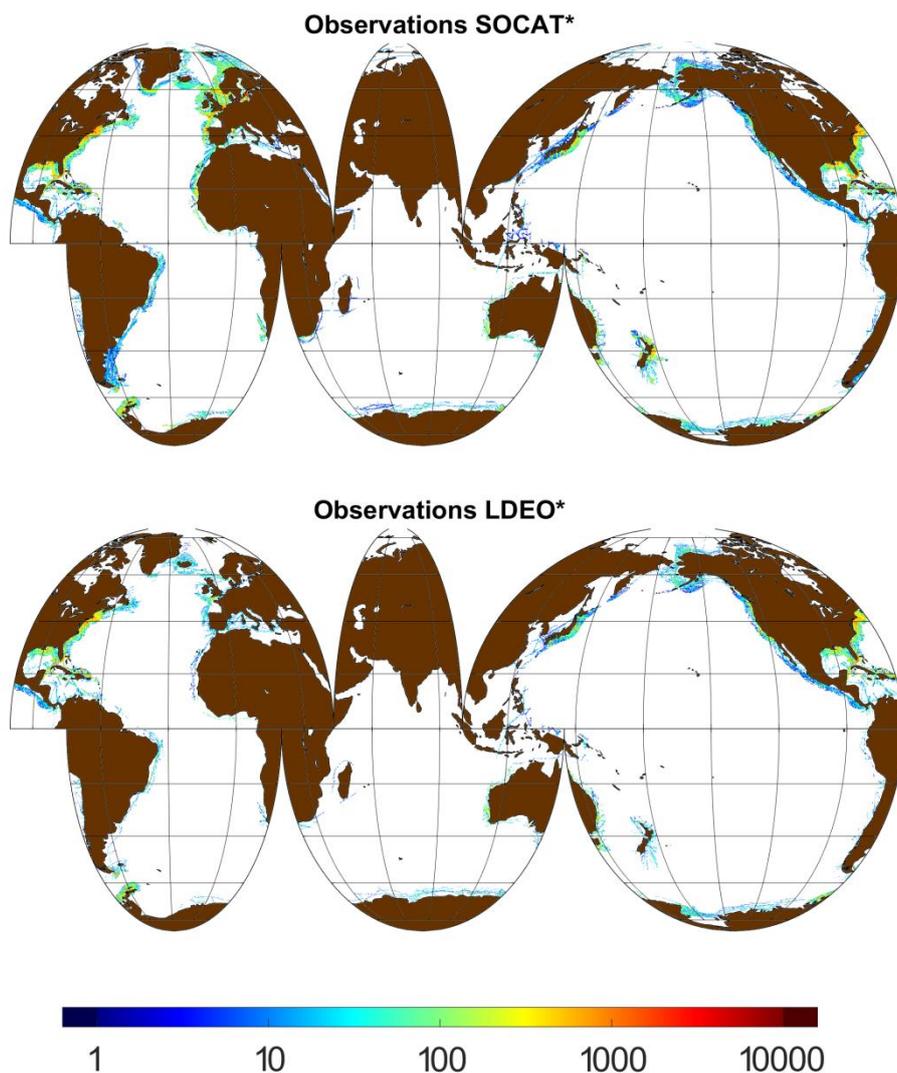


Figure: Number of observations contained in each 0.25° grid cell of the SOCAT\* (top) and LDEO\* (bottom) databases.

Table: Root mean squared error between observed and calculated pCO<sub>2</sub> in the different biogeochemical provinces. The SOM-FFN results are compared to data extracted from the SOCAT\* and the LDEO\* databases.

Province	SOCAT*		LDEO*	
	Bias (µatm)	RMSE (µatm)	Bias (µatm)	RMSE (µatm)
<b>P1</b>	0.0	19.1	2.0	20.5
<b>P2</b>	0.2	24.7	1.3	27.2
<b>P3</b>	-0.3	16.1	2.3	22.7
<b>P4</b>	-0.2	31.2	-1.6	33.0
<b>P5</b>	0.0	34.2	-1.4	38.0
<b>P6</b>	0.0	24.3	1.3	27.9
<b>P7</b>	0.1	37.2	-0.2	52.5
<b>P8</b>	0.2	46.8	3.9	51.4
<b>P9</b>	-0.1	23.0	-2.5	33.4
<b>P10</b>	0.0	35.7	1.6	53.1
<b>Global</b>	0.0	32.9	0.0	39.2

It is unclear how the change in surface water over time is dealt with. Are the pCO<sub>2</sub> data normalized like in the Takahashi monthly climatology? SST and SSS from the WOA are used but are these monthly climatologies that do not reflect change over time. This exercise provides monthly maps from 1998-2014 and it is clear how this is done. Also, the product is referred to as a climatology but it sounds like it is a monthly time series. That is, climatology mostly refers to a (multi) decadal average.

[4] During the training of the SOM\_FFNN, all pCO<sub>2</sub> data from SOCAT\* are associated to a set of environmental conditions corresponding to the location and moment in time when the pCO<sub>2</sub> was measured. The relationships linking pCO<sub>2</sub> to environmental conditions as established by the FFNN are then applied in each cell of the simulation domain for each of the 216 month of the simulation period. The inputs used for these calculations are 3 dimensional fields (latitude, longitude and time) containing values for each grid cell at every monthly time step. We will make sure to clarify this procedure in the updated manuscript. All the data used as inputs for both SOM and FFNN are thus monthly times series and no normalization was applied to the data as was performed in Takahashi et al. (2009).

We realize that our frequent use of the word climatology may be misleading as to what our product really is. In the updated manuscript and the abstract, we will state more clearly that our calculations are performed for every month of the simulation period and thus produce monthly maps for each of the years simulated. Only then, a monthly climatology is derived from those results.

Also note that, in the new simulations, SST and SSS data are not taken from the World Ocean Atlas anymore but from the Met Office's EN4: quality controlled subsurface ocean temperature and salinity profiles and objective analyses (Good et al., 2009). This change was implemented following a comment from reviewer #2 regarding mismatches in spatial resolution of some datasets (the new SST/SSS datasets are at the spatial resolution of 0.25 degree as opposed to WOA which only provides values at 1 degree).

The grouping of provinces such that a coastal region can include an inshore and open ocean province is odd. Perhaps limit the coastal area to just one province

[5] The biogeochemical provinces generated by the Self Organizing Maps regroup ensembles of cells together because of similarities in their environmental characteristics. Within each biogeochemical province, however, some variability can be found and, while bathymetry may significantly contribute to the grouping of cells within a given province, so do the other environmental parameters (i.e. SSS, SST, wind speed and sea ice). As a consequence, some provinces have an extension that includes nearshore and more open waters but for which the range of temperature for example might be limited (see figure below displaying the spatial extent of the updated biogeochemical provinces). The choice to use the SOM and divide the coastal ocean into several provinces as was done for the open ocean in Landschützer et al. (2013) was motivated by the large variety of environmental settings that can be found in the coastal ocean. The current number of 10 provinces was selected as the optimal number during the calibration phase. When developing the model, several simulations were performed with the SOM using increasing numbers of biogeochemical provinces (from 6 to 20) and 10 was the number of biogeochemical provinces yielding the best results in terms of RMSE when compared with both SOCAT and LDEO databases. This number of biogeochemical provinces also guarantees that sufficient data will be located in each biogeochemical province, thus insuring both a proper training of the algorithm and the possibility of a validation against a significant number of observations. For instance, the spatio-temporal distribution of the biogeochemical provinces used in our last simulation allows for at least 1000 different grid cells to be used for validation against LDEO\*.

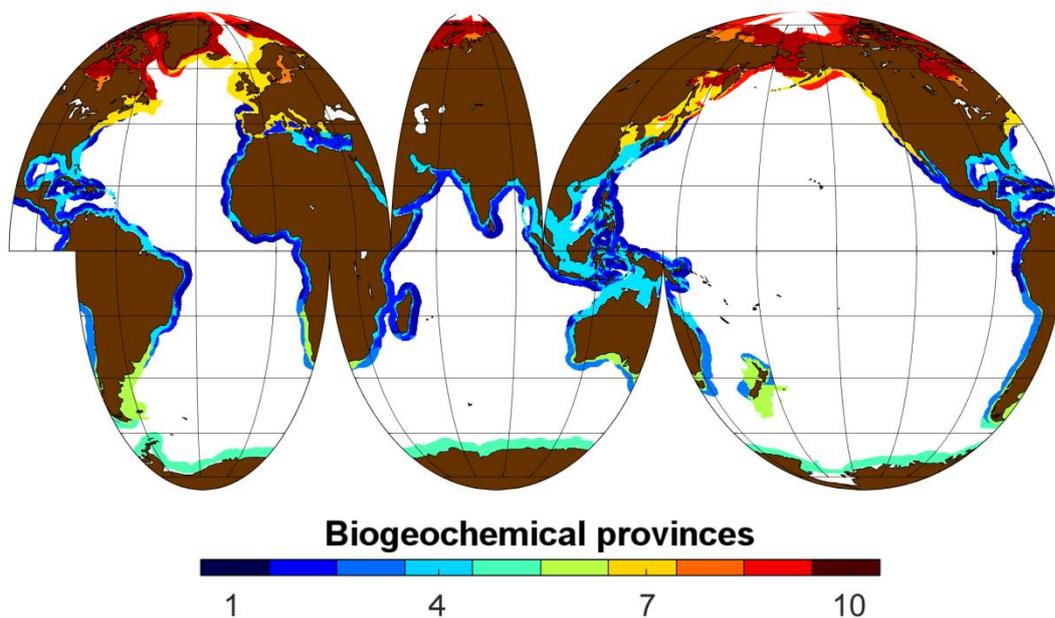


Figure 1: Map of the 10 different biogeochemical provinces generated by the SOM.

It is difficult to assess the data density for the different provinces using as validation or training.

[6] We understand the reviewer's concern and agree that, in the original version of the manuscript, limited information was provided regarding the spatial distribution of the

pCO<sub>2</sub> data used for calibration or validation. In the updated manuscript, a new figure (see comment [3]) now shows the data density of the SOCAT\* and LDEO\* databases for each grid cell of the simulation domain, thus providing a clear view of the amount and spatial distribution of data used both for calibration and validation..

Specific comments often relating to the general observations are below. The referenced text is in italics:

Line 125: "*motivated a number of modifications of the global ocean SOM-FFN method, including a 16 fold increase in spatial resolution from 1 degree to 0.25 degree, the introduction of a second neuron layer in the FFN calculations, the addition of new environmental variables as biogeochemical predictors, and a shortening of the simulation period to the period 1998 through 2014, rate of sea ice SST, SSS, bathymetry, sea-ice concentration and chlorophyll a second artificial neuron layer*". Some more detail on how these modification impact the results would be worthwhile .

[7] As mentioned by both reviewers, the different modifications introduced compared to the original set-up of the global ocean SOM\_FFNN are only mentioned in our method section but not discussed in details in our results. In the updated manuscript, we discuss the impact of those modifications (i.e. resolution and new predictors such as sea ice and wind speed). For instance, the added value of performing our simulations at the spatial resolution of 0.25° is discussed using examples such as the ability of our model to capture the plumes of larges rivers such as the Amazon, which produces an area located North of its river mouth characterized by pCO<sub>2</sub> values significantly lower than those of the surrounding waters (Cooley et al., 2007; Ibanez et al., 2015). The new discussion will also involve the addition of results from simulations performed only using SST, SSS, bathymetry and chlorophyll as predictors (as suggested by reviewer #2). The results of those simulations are presented in the table below and allow quantifying how the addition of new predictors affects the performance of the model. For instance, it can be noticed that, overall, the global RMSE increase significantly (from 39.2 to 48 µatm in the comparison with LDEO\* when chlorophyll, sea ice and wind speed are not taken into account and from 39.2 to 45 µatm when only sea ice and wind speed are not taken into account). This deterioration of the performance of the model, however, is not evenly affecting all provinces and it can be observed in particular that provinces located at high latitudes (i.e. P8, P9 and P10) perform significantly worse without the inclusion of wind speed and sea ice.

Table: Biases and root mean squared error (RMSE) between observed and calculated pCO<sub>2</sub> using only SST, SSS and bathymetry (STB) or SST, SSS, bathymetry and chlorophyll (STBC) as predictors.

Province	SOCAT*		LDEO*					
	Bias (µatm)		RMSE (µatm)		Bias (µatm)		RMSE (µatm)	
	STB	STBC	STB	STBC	STB	STBC	STB	STBC
<b>P1</b>	0.0	-0.2	20.8	21.0	2.4	2.0	21.7	21.5
<b>P2</b>	-0.1	0.1	26.9	27.8	0.5	0.8	29.0	29.6
<b>P3</b>	0.0	-0.5	22.7	21.3	3.0	2.3	27.1	26.8
<b>P4</b>	0.0	-0.2	33.0	33.0	-1.7	-2.3	33.8	33.8
<b>P5</b>	0.2	0.1	52.7	42.2	-1.7	-0.9	56.9	44.5
<b>P6</b>	0.0	0.1	26.8	26.5	-0.5	0.6	28.9	28.0
<b>P7</b>	0.4	0.3	44.3	44.1	1.2	0.3	59.3	58.8

<b>P8</b>	0.1	0.4	82.6	80.0	9.1	9.0	56.3	58.5
<b>P9</b>	0.1	0.9	34.7	36.5	-2.6	-2.8	39.8	41.8
<b>P10</b>	-0.3	0.7	49.8	49.5	-3.9	-3.0	76.5	75.4
<b>Global</b>	0.1	0.2	43.9	42.4	0.0	0.0	48.0	45.0

Line 175: "*SOM-FFN from generating negative values.*" This suggests that there are issues with the original setup. Adding a second neuron layer to prevent negative values certainly is unorthodox.

[8] The SOM-FFN method is some form of a non-linear regression model, which in cases of bad conditioning also produces out of range values. We point here that the negative values do not suggest issues with the model as a whole, but rather issues with the setup of the model. While we did not face the problem of negative values using a standard hidden layer in the open ocean, the added complexity combined with little data in certain province can cause this behaviour in coastal seas. For instance, there exist very few measurements for shallows waters with very low salinity and high sea ice coverage. Faced with conditions for which it was not trained, the SOM\_FFNN does not perform ideally and may generate unrealistic values. In our original manuscript we solved this by introducing a second hidden layer of neurons, however, we found a more stable solution in terms of negative values, i.e we replaced the second neuron layer with the use of a sigmoid activation function bounded between 0 and 1 (normalized pCO<sub>2</sub> units) in the hidden layer. This means that per definition our results are bound to stay above 0. The implementation of this solution did not deteriorate the overall results but prevented the SOM\_FFNN from generating negative pCO<sub>2</sub> values. The new simulations for the revised manuscript were thus carried out with this new setting, which now only uses a single neuron layer.

Line 193: "*All the datasets used in our calculations were converted from their original spatial resolutions to a regular 0.25 degree resolution grid.*" Specify what the original resolution was for each dataset.

[9] A more thorough description of the datasets used in the study will be included into section 2.2 (Data Sources and processing). This description explicitly states the original temporal and spatial resolution of each dataset used. This information will be compiled in the new table reported below. In addition, for the sake of reproducibility, a link toward all datasets used will be provided in the 'Data Availability' section at the end of the manuscript. Note that, as already reported in comment 4, all our products have now an original resolution of 0.25° or finer.

Table: Datasets used to create the environmental forcing files. The original spatial and temporal resolution and the main manipulations applied for their use in the SOM\_FFNN are also reported.

<b>Predictor</b>	<b>dataset</b>	<b>resolution</b>	<b>reference</b>	<b>Manipulation</b>
SST	EN4	0.25°, daily	Good et al., 2013	Monthly average
SSS	EN4	0.25°, daily	Good et al., 2013	Monthly average
Bathymetry	ETOPO2	2 minutes	US Department of Commerce,	Aggregation to 0.25°

Sea ice	NSIDC	0.25°, monthly	2006 Cavalieri et al., 1996	Monthly rate of change in sea ice coverage
Chlorophyll a	SeaWifs, MODIS	9km, monthly	NASA, 2016	Aggregation to 0.25°
Wind speed	ERA	0.25°, 6hours	Dee et al., 2011	Monthly average

Line 196: "*SST and SSS maps were taken from the World Ocean Atlas (Antonov et al., 2010 for SST and Locarnini et al., 2010 for SSS).*" Are these monthly climatologies or monthly time series? If the former it is unclear how the time element from 1998-2014 is incorporated.

[10] The new simulations do not use SST and SSS from the World Ocean Atlas anymore but from the Met Office's EN4: quality controlled subsurface ocean temperature and salinity profiles and objective analyses (Good et al., 2009). Those data are time series and contain individual values in each grid cell of the simulation domain for each of the 216 month of the simulation period. Additional information regarding the incorporation of the time element in our calculation is included in answer [4] and the updated manuscript will be more explicit with respect to the way our calculations are performed.

Line 203 and beyond: "*validation are extracted from the LDEOv2014 database The coastal SOM-FFN results are validated through a comparison with the LDEOv2014 data (Takahashi et al., 2016).*" This is not independent data and not a proper validation in statistical sense.

[11] As discussed in the answer to reviewer's comment [3], we fully agree that the original validation was significantly weakened by the large overlap between SOCAT and LDEO. Now that we created two entirely independent datasets to train the model (SOCAT\*) and evaluate its performances (LDEO\*), we believe that the term "validation" is now appropriate for the updated manuscript.

Line 280: "*Considering these complexities, the achieved RMSE is quite good.*" Two issues here. How are the complexities determined? That is, we know the coastal region is complex but it is unclear if the complexity is incorporated into the analysis using T, S, chl-a and sea ice. And, based on what criteria is the RMSE quite good.

[12] It is true that the coastal region is known to be a complex environment and that was the main message of this sentence. Whether our analysis capture the intricate complexity of the coastal zone has to be indeed better discussed in the revised manuscript. We will thus further develop the section dedicated to the discussion and quantification of the effects induced by modifications in SOM\_FFNN configuration on its performance (see answer to comment [7]). With respect to the RMSE, our criteria to consider the performance of our model 'quite good' is the comparison with the RMSE reported in regional studies . This is further discussed in the answer [13] below.

Line 306: "which compares with the most robust pCO<sub>2</sub> regional coastal estimates from the literature (Chen et al., 2016)". Chen et al. 2016 use a crude remote sensing approach. These are by no means "most robust".

[13] The paper by Chen et al. (2016) indeed presents pCO<sub>2</sub> fields for the Western Florida shelf generated using remote sensing. Such methodology certainly is different and arguably less sophisticated than the method described in our study. However, we did not mean to directly compare the performance of our model with those of Chen et al. (2016). Our aim was to find as many recent studies as possible to compare our results and to gain some confidence in our estimates. Their study reports (table 1, page 12) a list of regional coastal models generating pCO<sub>2</sub> fields derived from other environmental factors. Although the methods used in this list varies greatly (including Multiple Linear Regressions, Mechanistic semi analytical models and Self Organizing Maps), we believe it was relevant to confront the performance of our model applied globally with those of other coastal models, which are only applied at regional scale in well covered areas. What we meant to say is that there exist a body of literature using various methodological approaches to generate pCO<sub>2</sub> fields and the article by Chen was mostly used for his table. Nevertheless, following the reviewer's comment, we will tone down our statement that our results compare with the most robust estimates from the literature. Rather, we'll state that the RMSE calculated in our best constrained biogeochemical provinces (i.e. in the 20-30  $\mu\text{atm}$  range for P1, P2, P3 and P6) can be compared with those obtained by regional models applied in well monitored areas.

Line 349: "highlight the current knowledge gap regarding the mean state and variability of the transition zone." It is unclear if this highlights a knowledge gap or highlights issues with the SOM\_FNN approach. This warrants some discussion

[14] We agree with the reviewer's comment (as well as similar concerns' raised by reviewer 2) and recognise that the original version of the manuscript only briefly compared the results of the updated coastal SOM\_FFN with those of the original oceanic model. In the updated manuscript, a more in depth comparison with the results of the open ocean configuration will be provided. This will allow better identifying the added value of the modifications done to the SOM\_FFN method in our study and help clearly identify remaining knowledge gaps.

Line 358: "Our results indicate that the very nearshore processes controlling the CO<sub>2</sub> dynamics likely" Again the SOM-FNN is a mathematical construct. So I guess what the authors are stating is that the SOM-FNN cannot address adequately nearshore dynamics.

[15] The reviewer is correct; this sentence was meant to stress that, in spite of the improvement provided by the new method, some very nearshore processes still cannot be addressed perfectly. As the reviewer pointed out, the problem does not lie with the mathematical approach used by the spatial resolution required to capture very nearshore processes. The sentence was rephrased as follows:  
**"Overall, the occurrence of large residuals in the shallowest cells of our calculation domain in our results (fig. 2) suggest that the very nearshore processes controlling the CO<sub>2</sub> dynamics likely are the most difficult to reproduce at the global scale."**

Line 429 "2 ". The "n" generally refers to salinity normalization. Perhaps use pCO<sub>2</sub>(SSTmean) .

[16] We will follow the reviewer's suggestion in the updated manuscript and use pCO<sub>2</sub>(SSTmean) instead of npCO<sub>2</sub>.

Line 470: "*cells at a 0.25° spatial resolution for each of the 204 month of the simulation period (from January 1998 to December 2014). Climatologically averaged pCO<sub>2</sub> maps for each month are*". The use of the term climatology is ambiguous here.

[17] We agree with the reviewer, the term climatology is ambiguous in this sentence and elsewhere. To avoid any confusion, the paragraph was rephrased as follows:

"The data product associated to this manuscript consists of a netcdf file containing the pCO<sub>2</sub> for ice-free cells at a 0.25° spatial resolution for each of the **216** month of the simulation period (from January 1998 to December **2015**). **12 maps representing mean pCO<sub>2</sub> fields calculated for each month over the simulation period** are also provided."

Line 471: The province names are peculiar "Deep Polar, Polar Very deep Polar"

[18] Our choice of names for the different biogeochemical provinces was only meant to outline their main geographical distribution. Both reviewers commented on the lack of added value of the distributions of the biogeochemical provinces. In the updated manuscript, the biogeochemical provinces will only be referred to as P1, P2 and so on to avoid confusion. Section 3.1 however, will still discuss the spatial extent of the each biogeochemical province.

Table 1 suggests that Ice is a predictor in the tropics?

[19] We agree that the use of Ice as predictor in the tropics is not relevant, however Ice cover in the tropics in our predictor dataset was 0 at all times, and hence it did not influence the neural network. To avoid confusion, in the updated simulation, Ice is only a predictor in provinces P5 to P10, in which at least partial seasonal ice coverage is reported.

Table 2: List of the biogeochemical provinces, their geographic distribution and the environmental predictors used to calculate surface ocean pCO<sub>2</sub>. SSS stands for sea surface salinity, SST for sea surface temperature, Bathy for bathymetry, Ice for sea-ice cover, Chl for chlorophyll concentration **and Wind for wind speed**.

Province	SSS	SST	Bathy	Ice	Chl	Wind
P1	X	X	X		X	X
P2	X	X	X		X	X
P3	X	X	X		X	X
P4	X	X	X		X	X
P5	X	X	X	X	X	X
P6	X	X	X	X	X	X
P7	X	X	X	X	X	X

<b>P8</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
<b>P9</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>
<b>P10</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>	<b>X</b>

Also P3 and P4 appear to have the same "distribution".

[20] In the original simulations, provinces P3 and P4 did not display exactly the same spatio-temporal distribution but were both referred to as "Deep Tropical" which could indeed lead to confusion. Actually, the average water depth of cells included in P4 was deeper than that of those included in P3 and, P4 generally characterized more 'open waters'. As mentioned in answer [5], the updated manuscript will describe and discuss the spatial distributions of the 10 biogeochemical provinces but the restrictive 'distributions' will be removed from table 1.

Figure 1 shows a peculiar extension off of New Zealand. Is this the Chatham Rise and is this considered coastal?

[21] The extension Southward and Eastward of New Zealand are the Campbell Plateau and Chatham Rise, respectively. They are considered coastal following our 'extended' definition of the continental shelf and upper slope because they are characterized by depth shallower than 1000m (our outer limit) and connected to a continental platform.

Figure 2: Perhaps comment on the absence of high pCO<sub>2</sub> in the SOM-FNN for the summer monsoon upwelling region in the Arabian Sea. Data of the Takahashi climatology clearly show this. Figure 2 does not show the high pCO<sub>2</sub> Arabian Sea seasonal (JAS) upwelling off the coast of the Arabian Peninsula.

[22] It is true that high pCO<sub>2</sub> values have been regularly observed along the coast of the Arabian Sea (Sarma et al., 2003) and are considered to be the consequence of monsoon driver upwelling occurring in the region. As noted by the reviewer, the SOM-FFN does not reproduce these oversaturated waters. We now mention and discuss the inability of the SOM\_FFNN to reproduce this known feature of the Arabian shelf in section 3.3.1, which discusses the general spatial patterns of the pCO<sub>2</sub> fields generated by the model.

#### **Literature cited in the responses:**

Cavaliere, D. J., Parkinson, C. L., Gloersen, P., and Zwally, H.: Sea Ice Concentrations from Nimbus-7 SMMR and DMSP SSM/I-SSMIS Passive Microwave Data, years 1990–2011, NASA DAAC at the Natl. Snow and Ice Data Cent., Boulder, Colo. (Updated yearly.), 1996.

Chen, S., Hu, C., Byrne, R. H., Robbins, L. L., and Yang, B.: Remote estimation of surface pCO<sub>2</sub> on the West Florida Shelf, *Continental Shelf Research*, 128, 10–25, 2016.

Cooley, S. R., V. J. Coles, A. Subramaniam, and P. L. Yager (2007), Seasonal variations in the Amazon plume-related atmospheric carbon sink, *Global Biogeochem. Cycles*, 21, GB3014, doi:10.1029/2006GB002831.

Dee, D. P., Uppala, S. M., Simmons, A. J., Berrisford, P., Poli, P., Kobayashi, S., Andrae, U., Balmaseda, M. A., Balsamo, G., Bauer, P., Bechtold, P., Beljaars, A. C. M., van de Berg, L., Bidlot, J., Bormann, N., Delsol, C., Dragani, R., Fuentes, M., Geer, A. J., Haimberger, L., Healy, S. B., Hersbach, H., Hòlm, E. V., Isaksen, L., Kallberg, P., Köhler, M., Matricardi, M., McNally, A. P., Monge-Sanz, B. M., Morcrette, J. J., Park, B. K., Peubey, C., de Rosnay, P., Tavolato, C., Thépaut, J. N. and Vitart, F.: The ERA-Interim reanalysis: Configuration and performance of the data assimilation system, *Q. J. R. Meteorol. Soc.*, 137(656), 553–597, doi:10.1002/qj.828, 2011.

Good, S. A., M. J. Martin and N. A. Rayner, 2013. EN4: quality controlled ocean temperature and salinity profiles and monthly objective analyses with uncertainty estimates, *Journal of Geophysical Research: Oceans*, 118, 6704–6716, doi:10.1002/2013JC009067

Ibánhez, J. S. P., D. Diverrès, M. Araujo, and N. Lefèvre (2015), Seasonal and interannual variability of sea-air CO<sub>2</sub> fluxes in the tropical Atlantic affected by the Amazon River plume, *Global Biogeochem. Cycles*, 29, 1640–1655, doi:10.1002/2015GB005110.

Landschützer, P., Gruber, N., Bakker, D. C. E., Schuster, U., Nakaoka, S., Payne, M. R., Sasse, T., and Zeng, J.: A neural network-based estimate of the seasonal to inter-annual variability of the Atlantic Ocean carbon sink, *Biogeosciences*, 10, 7793–7815, doi:10.5194/bg-10-7793-2013, 2013.

NASA Goddard Space Flight Center, Ocean Ecology Laboratory, Ocean Biology Processing Group; (Dataset Release 2016): MODIS-Aqua chlorophyll Data; NASA Goddard Space Flight Center, Ocean Ecology Laboratory, Ocean Biology Processing Group, 2016.

Sarma, V. V. S. S., Monthly variability in surface pCO<sub>2</sub> and net air-sea CO<sub>2</sub> flux in the Arabian Sea, *J. Geophys. Res.*, 108 (C8), 3255, doi:10.1029/2001JC001062, 2003.

Takahashi, T., S. C. Sutherland, R. Wanninkhof, C. Sweeney, R. A. Feely, D. W. Chipman, B. Hales, G. Friederich, F. Chavez, A. Watson, D. C. E. Bakker, U. Schuster, N. Metzl, H. Yoshikawa-Inoue, M. Ishii, T. Midorikawa, Y. Nojiri, C. Sabine, J. Olafsson, Th. S. Arnarson, B. Tilbrook, T. Johannessen, A. Olsen, Richard Bellerby, A. Körtzinger, T. Steinhoff, M. Hoppema, H. J. W. de Baar, C. S. Wong, Bruno Delille and N. R. Bates (2009). Climatological mean and decadal changes in surface ocean pCO<sub>2</sub>, and net sea-air CO<sub>2</sub> flux over the global oceans. *Deep-Sea Res. II*, 56, 554–577

U.S. Department of Commerce, National Oceanic and Atmospheric Administration, National Geophysical Data Center. 2006. 2-minute Gridded Global Relief Data (ETOPO2v2). <http://www.ngdc.noaa.gov/mgg/fliers/06mgg01.html>. Accessed 21 May 2017.

Review of bg-2017-64 “Global high-resolution monthly pCO<sub>2</sub> climatology for the coastal ocean derived from neural network interpolation” by Laruelle et al.

This manuscript proposed a modified two-step artificial neural network method for deriving pCO<sub>2</sub> (SOM-FFN, Landschützer et al., 2013), and focused on shelf seas. The most important modifications are (1) much higher resolution as 0.25 degree; (2) inclusion of sea-ice as a predictor of pCO<sub>2</sub>. From this effort, the authors may present a fine scale coastal sea pCO<sub>2</sub> globally, as Fig. 2 in the manuscript shown. This is certainly of value. However, there are some major issues. The method is not new, rather an interpolation of the open ocean model.

We are pleased to see that the reviewer values our coastal pCO<sub>2</sub> maps and are grateful for his constructive remarks and suggestions. We understand that the reviewer is not fully convinced by the novelty of the method and the added value our manuscript under its current form. As explained in answers, we do not concur with the statement that our model only is an extension or interpolation of the previously existing oceanic model. Instead, we believe that it is a significantly modified version, specifically tailored to reconstruct the complex coastal pCO<sub>2</sub> cycle. In the updated manuscript, we propose to put more emphasis on the modifications of the original SOM\_FFNN and compare our coastal set up with the open ocean one. Further attention will also be given to better quantifying the improvements resulting from the modification of the open ocean set-up from Landschützer et al. (2013) and identifying the remaining knowledge gaps (see also replies to comments 2, 7, 14 of reviewer 1).

The reviewer was also concerned by the weakness of the validation of our results performed using a database that largely overlaps with the database used to calibrate the model. Following both reviewer’s recommendations, we modified our approach and, using the latest versions of both SOCAT (i.e. version 4) and LDEO (i.e. v2015), we created two entirely independent datasets, named SOCAT\* for the calibration and LDEO\* for the validation. These two datasets were generated by randomly assigning each measurement common to both original databases to either SOCAT\* or LDEO\* (see comment 2 below for further details on the new approach). In addition, we have also introduced a new predictor (wind speed), which helped improve the performances of the SOM\_FFNN compared to those presented in the previous version of the manuscript.

Please find below a detailed answer to each comment. All our answers are written in blue and the modifications within the text are highlighted in bold and italic.

On behalf of all co-authors,

Goulven Laruelle

It was said that all data were converted to 0.25 degree from their original resolution.

Then please indicate clearly original resolution of each data, for example, SSS, SST and depth. At least for SST and SSS from the World Ocean Atlas, I wonder if the resolution is fine in the shelf seas (sorry I do not

check, my memory is 1 degree). If it is true, I do not think such an interpolation of SST and SSS would help in deriving really high resolution pCO<sub>2</sub> (i.e. the final result might be close to a simple interpolation of modeling pCO<sub>2</sub> of 1 degree resolution).

[1] The spatial resolution of SST and SSS from the World Ocean Atlas is indeed only 1 degree. In response to the reviewer’s comment, we now apply 0.25° resolution datasets

for SSS and SST by using Met Office’s EN4: quality controlled subsurface ocean temperature and salinity profiles and objective analyses (Good et al., 2009). By doing so, all predictors used for the calculation of the SOM\_FFNN have now resolution of 0.25° or higher. We also propose the inclusion of the table below, which lists the selected datasets used, their purpose (i.e. calibration, validation...) and original spatio-temporal resolution.

We reiterate here that we disagree with the notion that our model is a mere interpolation of the global oceanic model developed by Landschützer et al. (2013). Although both the coastal SOM\_FFNN presented in this study and the oceanic SOM\_FFNN published in Landschützer et al. (2013) share common methodologies, they were not trained with the same datasets. For the most part, the coastal data from SOCAT used here for calibration and validation was not included in the data pool used for the open ocean simulations. In addition, the ranges of values (within which both models are trained) are also different for some of the environmental parameters. In particular, the average bathymetry and sea surface salinities are often significantly lower in coastal regions than in the open ocean. We thus believe that the important physical and biogeochemical differences between coastal and open oceanic waters fully justify careful retraining of the SOM\_FFNN. In addition, the typical spatial scales of physical and biogeochemical gradients in nearshore waters are often smaller than 1 degree and justify the implementation of the SOM\_FFNN at a higher resolution. Nevertheless, to better demonstrate the value of our approach, we follow the comment of the reviewer and discuss in more details the comparison between open and coastal ocean models in the revised manuscript.

Table 1: Datasets used to create the environmental forcing files. The original spatial and temporal resolution and the main manipulations applied for their use in the SOM\_FFNN are also reported.

<b>Predictor</b>	<b>dataset</b>	<b>resolution</b>	<b>reference</b>	<b>Manipulation</b>
SST	EN4	0.25°, daily	Good et al., 2013	Monthly average
SSS	EN4	0.25°, daily	Good et al., 2013	Monthly average
Bathymetry	ETOPO2	2 minutes	US Department of Commerce, 2006	Aggregation to 0.25°
Sea ice	NSIDC	0.25°, daily	Cavalieri et al., 1996	Monthly rate of change in sea ice coverage
Chlorophyll a	SeaWifs, MODIS	9km, monthly	NASA, 2016	Aggregation to 0.25°
Wind speed	ERA	0.25°, 6hours	Dee et al., 2011	Monthly average

SOCAT was used for tuning the model and LDEO was used for validation, while the two dataset was largely overlapped. This is not allowed for developing a sound and solid approach. Randomly picking data from SOCAT for calibration, and then removing those data at the same location when picking the LDEO data for validation, would not be too hard to do.

[2] As mentioned by the reviewer, the SOCAT and LDEO databases have a large overlap, and the two datasets cannot be considered independent. In order to remedy to this problem, we followed the reviewer suggestion and created two datasets based on SOCAT and LDEO which do not contain any common measurements. We used the latest releases of both databases (i.e. SOCATv4 and LDEOv2015) and filtered out all non-coastal data points, as it was already done in the previous version of the manuscript. Under our definition of the coastal zone, SOCATv4 contains  $\sim 8 \cdot 10^6$  data points and LDEO  $\sim 5.6 \cdot 10^6$ , over 70% of which are also part of SOCATv4. We then randomly assigned each of those common data points to either database, thus insuring that each data only belongs to one dataset. In the updated manuscript, the new datasets are then called SOCAT\* which is used to train the SOM\_FFNN, and LDEO\* which is only used for validation purposes. In the new manuscript, the procedure used to create SOCAT\* and LDEO\* will be detailed in section 2.2 (Data Sources and processing).

The use of a more robust validation did not alter significantly the performances of the SOM\_FFNN and, combined with the inclusion of wind speed as a new predictor, the biases and RMSE generated by the model when compared with LDEO\* are actually slightly lower than those presented in the original simulations (see table below). Also, note that the use of SOCATv4 and LDEOv2015 provides a significant number of data for the year 2015, which motivated us to expend our simulation period from 17 year to 18.

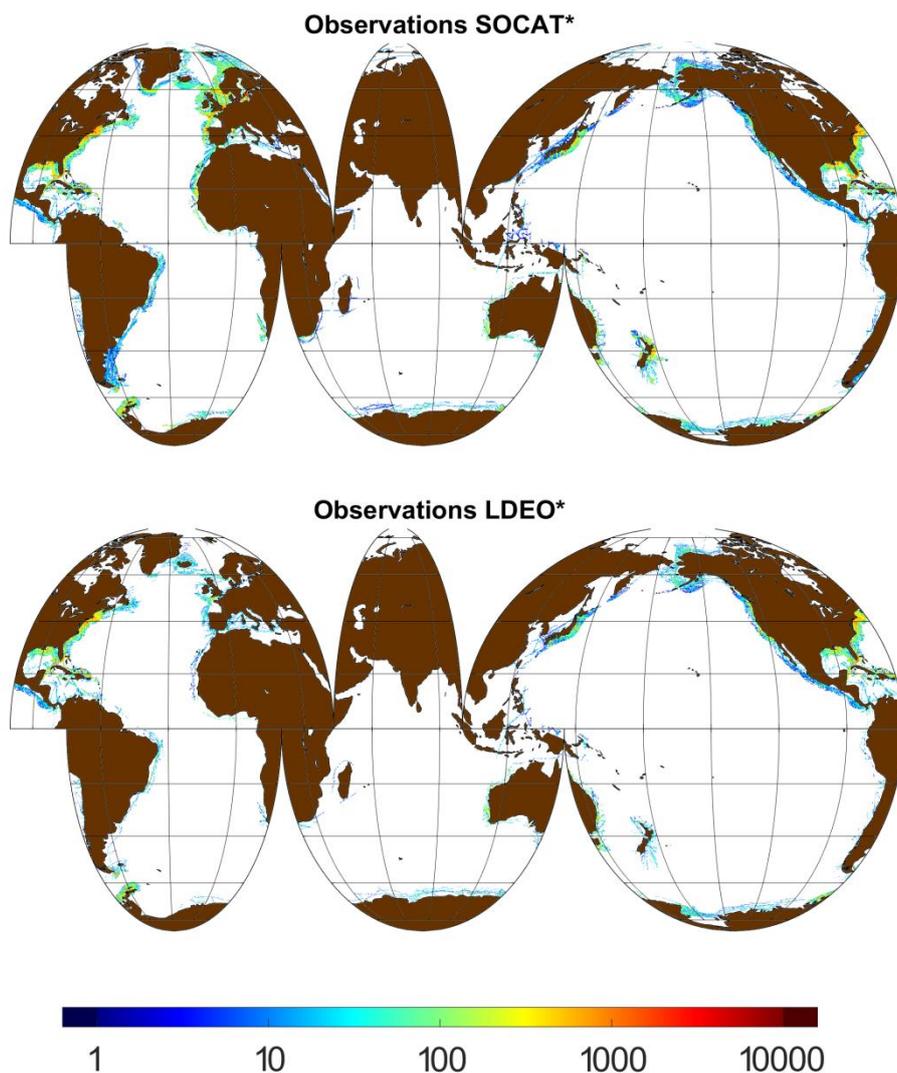


Figure: Number of observations contained in each 0.25° grid cell of the SOCAT\* (top) and LDEO\* (bottom) databases.

“Table: Root mean squared error between observed and calculated pCO<sub>2</sub> in the different biogeochemical provinces. The SOM-FFN results are compared to data extracted from the SOCAT\* and the LDEO\* databases.

Province	SOCAT*		LDEO*	
	Bias (µatm)	RMSE (µatm)	Bias (µatm)	RMSE (µatm)
<b>P1</b>	0.0	19.1	2.0	20.5
<b>P2</b>	0.2	24.7	1.3	27.2
<b>P3</b>	-0.3	16.1	2.3	22.7
<b>P4</b>	-0.2	31.2	-1.6	33.0
<b>P5</b>	0.0	34.2	-1.4	38.0
<b>P6</b>	0.0	24.3	1.3	27.9
<b>P7</b>	0.1	37.2	-0.2	52.5
<b>P8</b>	0.2	46.8	3.9	51.4
<b>P9</b>	-0.1	23.0	-2.5	33.4
<b>P10</b>	0.0	35.7	1.6	53.1
<b>Global</b>	0.0	32.9	0.0	39.2

The target of this manuscript is not clear. Based on the title, it looks that it is talking about a new product. As to the text, methods and validation are vague, while the authors are still eager to describe the seasonality and spatial distribution, but with no way to go into depth. And maybe because of no full confidence in the results, they frequently warned “considered with caution”. I would suggest the authors focusing on method and validation, teasing each detail carefully, which would raise the merit of this study. Because one of the most important changes is to include ice, the authors need to show that by including ice, what was improved? What more was acquired/learned?

[3] The manuscript presents monthly pCO<sub>2</sub> fields for the coastal ocean generated by a statistical method that was never applied in such environment. Obviously, a large part of the manuscript is dedicated to presenting the methods (i.e. the modifications of the open ocean set up in order to better capture the dynamics of continental shelves) and we agree with the reviewer that each critical point of the method should be discussed thoroughly. Following his recommendation, we now discuss results obtained with our model ignoring our new predictors (wind speed and sea ice cover) to better quantify their contribution to the accuracy of our results. Similarly, the added value of performing our simulations at the spatial resolution of 0.25° is also discussed using examples such as the ability of our model to capture the plumes of larges rivers such as the Amazon, which produces an area located North of its river mouth characterized by pCO<sub>2</sub> values significantly lower than those of the surrounding waters (Cooley et al., 2007; Ibanez et al., 2015). We believe that this discussion will clearly allow the reader to understand the added value of our approach. In addition, the validation of our results is now much more developed by including maps of mean residuals obtained when comparing the pCO<sub>2</sub> field generated by the SOM\_FFNN with data from LDEO\* and histograms of the distribution of these residuals with each biogeochemical province (see figures below).

However, we also believe that it is useful to thoroughly describe our results in terms of spatial and seasonal trends and not restrict our analysis to comparison against

validation data. One of the main values of our data product is the resolution of the seasonal variations of pCO<sub>2</sub> in regions of the continental shelf that were largely under sampled until now. We thus believe that, although the main purpose of our manuscript is to describe a new coastal pCO<sub>2</sub> data product, dedicating a significant fraction of our results and discussion to the emerging spatial and temporal patterns in the coastal pCO<sub>2</sub> field is justified and relevant. As for our warning that results in certain regions should be “considered with caution”: Despite the increasing number of observations collected and the methodological advancements, there are still regions, such as the Siberian shelves, where only few observations exist and our process understanding is limited. Limited observations mean on the one hand limited information to train our model but on the other hand also only limited means to validate our results. This should not be misinterpreted as us having a lack of confidence, but rather us having limited means of validating our results for some areas of the global coastal ocean. With this statement, we wanted to highlight these limitations and help the reader to critically reflect on our results.

Table: Biases and root mean squared error (RMSE) between observed and calculated pCO<sub>2</sub> using only SST, SSS and bathymetry (STB) or SST, SSS, bathymetry and chlorophyll (STBC) as predictors.

Province	SOCAT*				LDEO*			
	Bias (μatm)		RMSE (μatm)		Bias (μatm)		RMSE (μatm)	
	STB	STBC	STB	STBC	STB	STBC	STB	STBC
<b>P1</b>	0.0	-0.2	20.8	21.0	2.4	2.0	21.7	21.5
<b>P2</b>	-0.1	0.1	26.9	27.8	0.5	0.8	29.0	29.6
<b>P3</b>	0.0	-0.5	22.7	21.3	3.0	2.3	27.1	26.8
<b>P4</b>	0.0	-0.2	33.0	33.0	-1.7	-2.3	33.8	33.8
<b>P5</b>	0.2	0.1	52.7	42.2	-1.7	-0.9	56.9	44.5
<b>P6</b>	0.0	0.1	26.8	26.5	-0.5	0.6	28.9	28.0
<b>P7</b>	0.4	0.3	44.3	44.1	1.2	0.3	59.3	58.8
<b>P8</b>	0.1	0.4	82.6	80.0	9.1	9.0	56.3	58.5
<b>P9</b>	0.1	0.9	34.7	36.5	-2.6	-2.8	39.8	41.8
<b>P10</b>	-0.3	0.7	49.8	49.5	-3.9	-3.0	76.5	75.4
<b>Global</b>	0.1	0.2	43.9	42.4	0.0	0.0	48.0	45.0

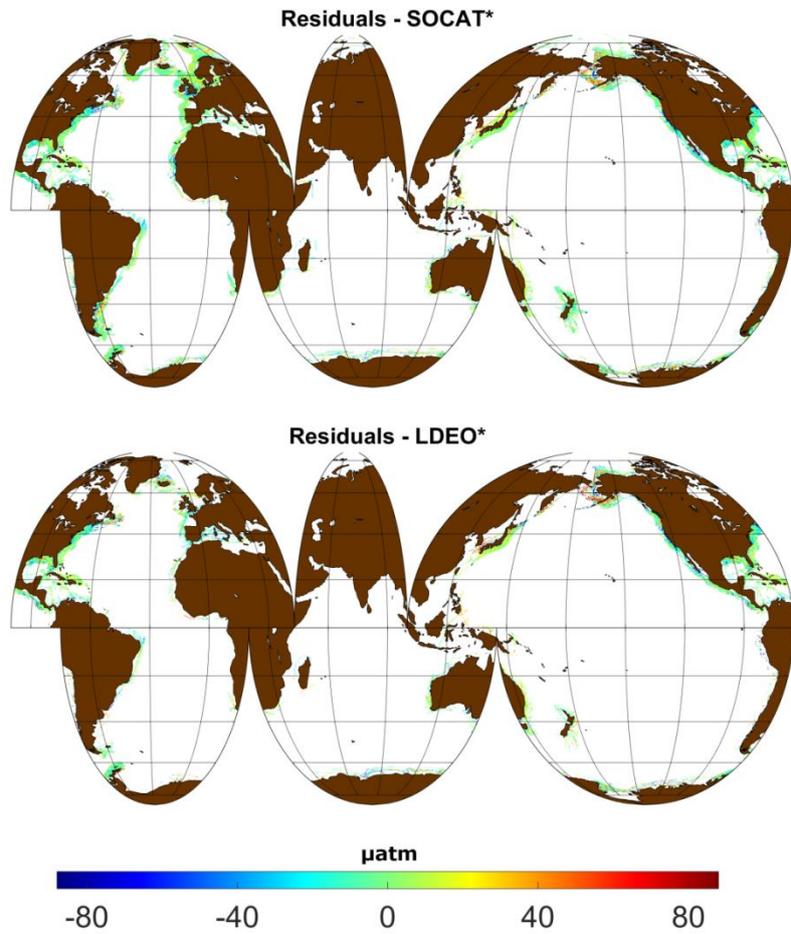


Figure 1: Mean residuals calculated as the difference between the SOM\_FFM  $\text{pCO}_2$  outputs and  $\text{pCO}_2$  observations from SOCAT\* (top) and LDEO\* (bottom).

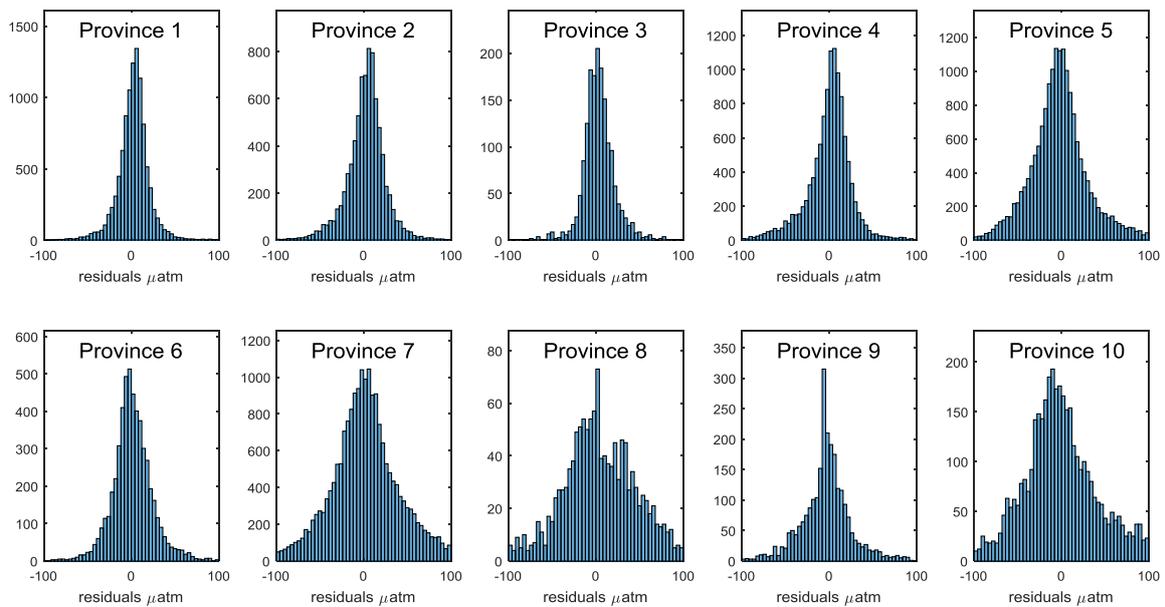


Figure: Histograms reporting the distribution of residuals between observed (LDEO\*) and computed (SOM\_FFN)  $\text{pCO}_2$  in each biogeochemical province.

Specific comments: Abstract- Writing of the abstract needs to be improved. A very clear point should be delivered. People want to know by modifying an established algorithm, what has been acquired/improved and how good it is. Now the authors just say it is assessed using two datasets. Meridional distribution is confirmed. And then talking about seasonality produced from this dataset, which people do not know if it is true or not. If spatial and temporal variability are what the authors concerned, the title should be changed correspondingly.

[4] As mentioned in answer [3], the updated manuscript now dedicates more effort to better identifying what was improved and learned with each of the modification introduced to the SOM\_FFNN compared to its open ocean set up. Also, we now implemented a more robust validation of our results (following several suggestions of both reviewers), including a revised comparison with monthly climatological cycles extracted from LDEO\* at 40 locations (see figure below). We thus do not agree with the reviewer when he suggests that our discussion regarding the seasonality of pCO<sub>2</sub> in coastal waters is unsubstantiated. We not only think that these seasonal signals are supported by our validation but also that the discussion of the seasonal dynamics of the coastal pCO<sub>2</sub> is very relevant to the manuscript and the wider research community. We agree however that the original abstract was not specific enough (especially with respect to seasonal variability) and we will make sure that the updated abstract better reflects the novelty of our approach.

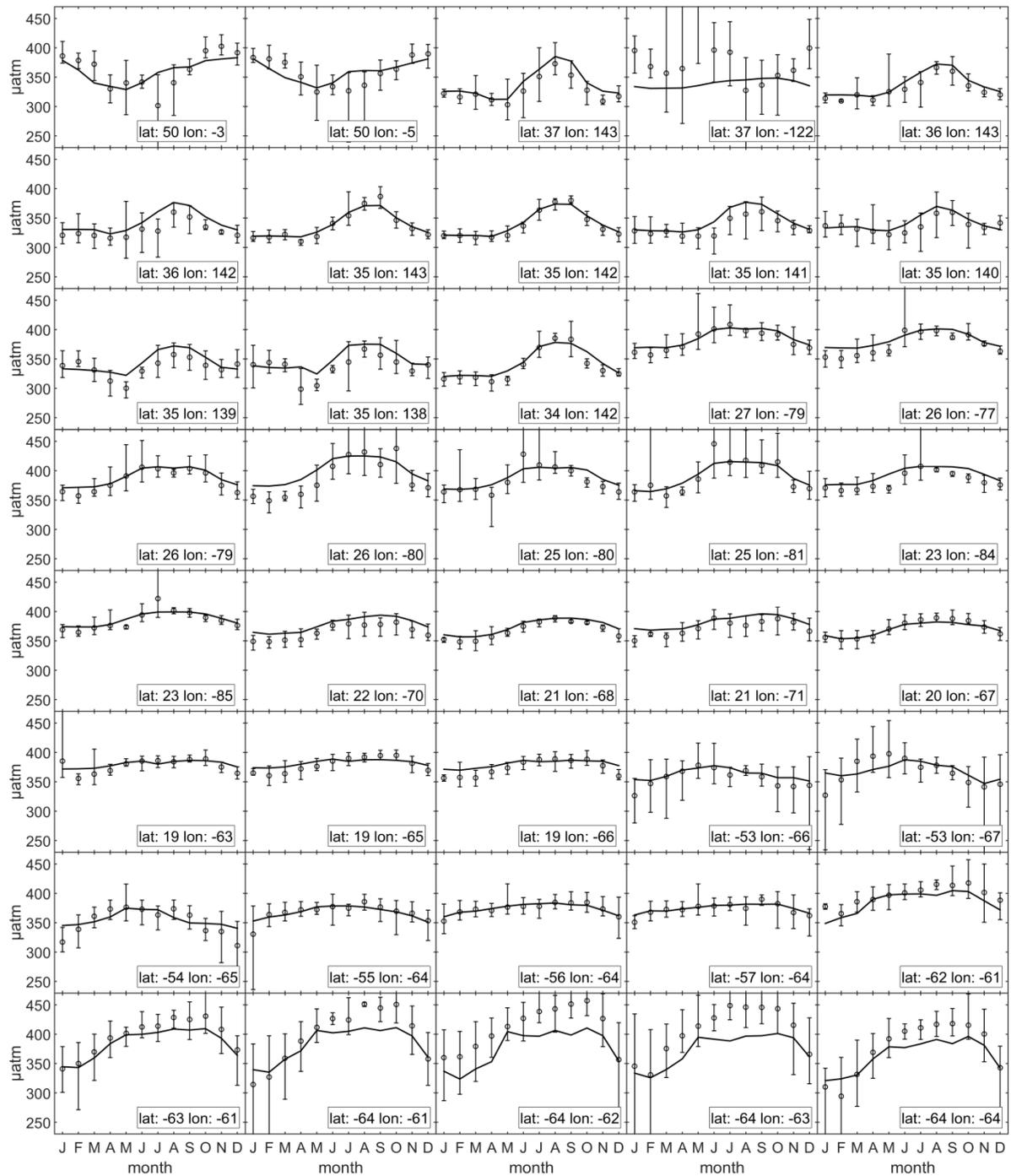


Figure: Climatological monthly mean pCO<sub>2</sub> extracted from the LDEO\* database (points) and generated by the artificial neural network (lines) for grid cells having more than 40 months of data. The error bars associated with the data represent the inter-annual variability, reported as the highest and lowest recorded values for a given month at a given location.

Line 36-39, "Overall, the seasonality in shelf pCO<sub>2</sub> cannot solely be explained by temperature-induced changes in solubility, but are also the result of seasonal changes in circulation, mixing, and biological productivity."

This should be well known by everybody. I wonder what it adds to place this sentence in the abstract. It is not clear if it is to explain the seasonality the model produced is not satisfied, or simply to explain the seasonality. One may guess that in the model only temperature was included, so the modeling seasonality can't be explained. But in fact salinity, chlorophyll and sea-ice were all included as predictors in the model, with circulation, mixing, and biological productivity all considered in addition to temperature-induced changes in solubility.

[5] We agree with the reviewer that all readers familiar with the dynamics of carbon in coastal waters will be aware that the seasonal changes of pCO<sub>2</sub> are not only driven by temperature variations but also hydrodynamics, planktonic productivity etc... The purpose of this sentence was to refer to our analysis of the effect of temperature change on the seasonal cycle of pCO<sub>2</sub> presented at the end of section 3 but we agree that the phrasing was too generic and did not report any new finding. In the updated manuscript, the abstract will be more specific and the outcome of our seasonal analysis more clearly presented (i.e. in which regions of the world, is temperature the dominant driver of the seasonal change in coastal pCO<sub>2</sub>, see also answer [4]).

Line 118, it is Landschützer et al. 2015? Should it be 2014?

[6] Indeed, the SOM FFN method is only briefly described in Landschützer et al. (2015) and the reference will be replaced by Landschützer et al. (2014) in the updated manuscript.

Line 141-144, "This approach facilitates future integration with existing global ocean data products (e.g., Landschützer et al., 2016; Rödenbeck et al., 2015) and model outputs, which typically struggle to represent the shallowest parts of the ocean (Bourgeois et al., 2016)". Can you explain what the inner boundary of the global ocean data products is, where they are still confident? I do not think 500 m depth would still be too shallow to struggle. I would think that using 500 m depth as the outer boundary of shelf model would be more than enough (You used 1000 m depth as the outer boundary).

[7] Unfortunately, there is no such thing as a universally accepted inner boundary for ocean data products and models but the extension of their simulation domain varies from one study to the other. The 200m isobaths are commonly used as limit between the open ocean and continental shelves but this limit is somewhat artificial (Walsh et al., 1988, Laruelle et al., 2013). The purpose of extending our outer limit for coastal water as far as 1000m depth is to insure an overlap between coastal and oceanic data product to prevent some regions of the world to remain untreated by either approaches.

Line 152-156, chlorophyll was not included to define biogeochemical provinces using SOM?

[8] Indeed, chlorophyll was not included to define the biogeochemical provinces using SOM, due to the fact that the data coverage is incomplete in the high latitudes in winter due to e.g. cloud coverage. This is the same reason Chl a is excluded from the calculations of provinces P8, P9 and P10 during the Feed Forward Network step. This will be clarified in the text.

Line 185-189, SeaWiFS extends to 2014? Please double-check. To my knowledge, it ends in 2010. By the way, normally people write it as SeaWiFS, not SeaWIFS.

[9] As pointed out by the reviewer, SeaWiFS data do not extend past 2010. The data used later than this date and all the way to December 2015 are taken for MODIS. Also, SeaWiFS will be written as suggested by the reviewer throughout the updated manuscript. This reply will be used to clarify the manuscript and details will be included in the table listing all data sources (see answer [1]).

Line 186, should it be “one of the environmental drivers”?

[10] The sentence will be corrected as suggested.

Section 2.2, it would be better if to appear before the model. Then no need to ask readers to “see below” in Line 164 and 168.

[11] Following the reviewer’s suggestion, the sections 2.1 and 2.2 of the manuscript will be inverted, in order to present the datasets used and their processing, before describing the modifications performed to the SOM\_FFNN.

Line 198, why ice was recalculated? And what kind of recalculation?

[12] The original spatial resolution of the sea ice coverage is days and monthly averages had to be calculated from the original data as well as monthly rates of change in sea ice coverage. This is now explained more clearly in the updated manuscript. In addition, the new table 2 listing all the original spatial and temporal resolutions of all datasets and the manipulations performed with them will help make the data processing more transparent.

Line 211-222 is not evaluation. It is the model training.

[13] Following the reviewer’s suggestion, this subsection has been renamed ‘model training’.

Line 216, do you mean you used chlorophyll in FFNN but not in SOM? Why?

[14] Indeed chlorophyll was used in FFNN but not in SOM as justified in answer [8].

I would say that the entire data and method section is really confusing. A cartoon, with input and out clearly indicated, and calibration (training) and validation clearly separated, would help. Also, why twice FFNN? The rationale to do this is not clear.

[15] We agree with the reviewer that the different steps and datasets required by our approach may be confusing to the reader and we now improved the clarity of the method in the updated manuscript. In particular, the suggestion of the reviewer to use a conceptual scheme detailing the different steps of the method will be included in the revised ms.

As for the choice of using twice the FFNN, it is true that such choice is uncommon and generally not required in a Feedforward Network. Following the remarks of both reviewers regarding this modification, another solution was considered to replace the second neuron layer with the use of a sigmoid activation function bounded between 0 and 1 in the hidden layer. The implementation of this solution did not deteriorate the overall results. The new simulations were thus carried out with this new setting which only uses a single neuron layer.

Line 353-359, this explanation is confusing. There is no reason why results from the global open ocean model can be so different from the coastal model in the overlapped

cells. The only critical changes are higher resolution (actually it is an interpolation) and sea ice. Have you tried giving up ice, let other conditions be the same, see what it will be?

[16] As mentioned in answer [1], we do not agree with the notion that our results are just an interpolation of the oceanic model. Other than the spatial resolution and the choice of environmental predictors, both oceanic and coastal models were trained on fundamentally different datasets – the open ocean model was trained with open ocean pCO<sub>2</sub> measurements and the coastal model was trained with coastal pCO<sub>2</sub> measurements. Therefore, we are not surprised that the 2 estimates differ in overlapping areas. However, we do agree that the magnitude of disagreement is somewhat larger than one would expect, highlighting on the one hand current knowledge gaps regarding the coastal to open ocean continuum and on the other hand that more research is needed to close this knowledge gap. The suggestion from the reviewer to perform simulations without the new coastal predictors to quantify their effect is now also included in the updated manuscript, as already discussed in answer [3].

Fig. 2, suggest to use other color, say brown for lands. It is now not easy to tell ice cover from the land.

[17] The suggestion of the reviewer has been implemented in the new version of the manuscript. As an example, all the maps presented in these replies already use a brown colour to represent land.

#### **Literature cited in the responses:**

Cavalieri, D. J., Parkinson, C. L., Gloersen, P., and Zwally, H.: Sea Ice Concentrations from Nimbus-7 SMMR and DMSP SSM/I-SSMIS Passive Microwave Data, years 1990–2011, NASA DAAC at the Natl. Snow and Ice Data Cent., Boulder, Colo. (Updated yearly.), 1996.

Cooley, S. R., V. J. Coles, A. Subramaniam, and P. L. Yager (2007), Seasonal variations in the Amazon plume-related atmospheric carbon sink, *Global Biogeochem. Cycles*, 21, GB3014, doi:10.1029/2006GB002831.

Dee, D. P., Uppala, S. M., Simmons, A. J., Berrisford, P., Poli, P., Kobayashi, S., Andrae, U., Balmaseda, M. A., Balsamo, G., Bauer, P., Bechtold, P., Beljaars, A. C. M., van de Berg, L., Bidlot, J., Bormann, N., Delsol, C., Dragani, R., Fuentes, M., Geer, A. J., Haimberger, L., Healy, S. B., Hersbach, H., Hølm, E. V., Isaksen, L., Kallberg, P., Köhler, M., Matricardi, M., McNally, A. P., Monge-Sanz, B. M., Morcrette, J. J., Park, B. K., Peubey, C., de Rosnay, P., Tavolato, C., Thépaut, J. N. and Vitart, F.: The ERA-Interim reanalysis: Configuration and performance of the data assimilation system, *Q. J. R. Meteorol. Soc.*, 137(656), 553–597, doi:10.1002/qj.828, 2011.

Good, S. A., M. J. Martin and N. A. Rayner, 2013. EN4: quality controlled ocean temperature and salinity profiles and monthly objective analyses with uncertainty estimates, *Journal of Geophysical Research: Oceans*, 118, 6704-6716, doi:10.1002/2013JC009067

Ibáñez, J. S. P., D. Diverrès, M. Araujo, and N. Lefèvre (2015), Seasonal and interannual variability of sea-air CO<sub>2</sub> fluxes in the tropical Atlantic affected by the Amazon River plume, *Global Biogeochem. Cycles*, 29, 1640–1655, doi:10.1002/2015GB005110.

Landschützer, P., Gruber, N., Bakker, D. C. E., Schuster, U., Nakaoka, S., Payne, M. R., Sasse, T., and Zeng, J.: A neural network-based estimate of the seasonal to inter-annual variability of the Atlantic Ocean carbon sink, *Biogeosciences*, 10, 7793-7815, doi:10.5194/bg-10-7793-2013, 2013.

Landschützer, P., Gruber, N., Bakker, D. C. E., and Schuster, U.: Recent variability of the global ocean carbon sink, *Global Biogeochemical Cycles*, 28, 927–949, doi:10.1002/2014GB004853, 2014.

Landschützer, P., Gruber, N., Haumann, F. A. Rödenbeck, C. Bakker, D.C.E. , van Heuven, S. Hoppema, M., Metzl, N., Sweeney, C., Takahashi, T., Tilbrook, B. and Wanninkhof, R.: The reinvigoration of the Southern Ocean carbon sink, *Science*, 349, 1221-1224. doi: 10.1126/science.aab2620, 2015.

Laruelle, G. G., Dürr, H. H., Lauerwald, R., Hartmann, J., Slomp, C. P., Goossens, N., and Regnier, P. A. G.: Global multi-scale segmentation of continental and coastal waters from the watersheds to the continental margins, *Hydrol. Earth Syst. Sci.*, 17, 2029-2051, doi:10.5194/hess-17-2029-2013, 2013.

NASA Goddard Space Flight Center, Ocean Ecology Laboratory, Ocean Biology Processing Group; (Dataset Release 2016): MODIS-Aqua chlorophyll Data; NASA Goddard Space Flight Center, Ocean Ecology Laboratory, Ocean Biology Processing Group, 2016.

U.S. Department of Commerce, National Oceanic and Atmospheric Administration, National Geophysical Data Center. 2006. 2-minute Gridded Global Relief Data (ETOPO2v2). <http://www.ngdc.noaa.gov/mgg/fliers/06mgg01.html>. Accessed 21 May 2017.

Walsh, J. J.: On the nature of continental shelves, Academic Press, San Diego, New York, Berkeley, Boston, London, Sydney, Tokyo, Toronto, 1988.

1 **Global high resolution monthly pCO<sub>2</sub> climatology for the coastal ocean derived from**  
2 **neural network interpolation**

3 *Running head: Global coastal pCO<sub>2</sub> maps*

4 Goulven G. Laruelle<sup>1</sup>, Peter Landschützer<sup>2</sup>, Nicolas Gruber<sup>3</sup>, Jean-Louis Tison<sup>1</sup>, Bruno  
5 Delille<sup>4</sup>, Pierre Regnier<sup>1</sup>

6 1. Department Geoscience, Environment & Society (DGES), Université Libre de  
7 Bruxelles, Belgium

8 2. Max Planck Institute for Meteorology, Hamburg, Germany

9 3. Environmental Physics, Institute of Biogeochemistry and Pollutant Dynamics, ETH  
10 Zürich, Zürich, Switzerland

11 4. Unité d'Océanographie Chimique, Astrophysics, Geophysics and Oceanography  
12 department, University of Liège, Belgium

13 Corresponding author: Goulven G. Laruelle

14  
15 Revised version of manuscript bg-2017-64 (Minor revisions)

**Deleted:** For submission to  
Biogeosciences

20 **Abstract**

21 In spite of the recent strong increase in the number of measurements of the partial pressure of  
22 CO<sub>2</sub> in the surface ocean (pCO<sub>2</sub>), the air-sea CO<sub>2</sub> balance of the continental shelf seas remains  
23 poorly quantified. This is a consequence of these regions remaining strongly under-sampled  
24 both in time and space, and of surface pCO<sub>2</sub> exhibiting much higher temporal and spatial  
25 variability in these regions compared to the open ocean. Here, we use a modified version of a  
26 two-step artificial neural network method (SOM-FFN, Landschützer et al., 2013) to  
27 interpolate the pCO<sub>2</sub> data along the continental margins with a spatial resolution of 0.25  
28 degrees and with monthly resolution from 1998 until 2015. The most important modifications  
29 compared to the original SOM-FFN method are (i) the much higher spatial resolution, and (ii)  
30 the inclusion of sea-ice and wind speed as predictors of pCO<sub>2</sub>. The SOM-FFN is first trained  
31 with pCO<sub>2</sub> measurements extracted from the SOCATv4.0 data base. Then, the validity of our  
32 interpolation, both in space and time, is assessed by comparing the generated pCO<sub>2</sub> field with  
33 independent data extracted from the LDVEO2015 data base. The new coastal pCO<sub>2</sub> product  
34 confirms a previously suggested general meridional trend of the annual mean pCO<sub>2</sub> in all the  
35 continental shelves with high values in the tropics and dropping to values beneath those of the  
36 atmosphere at higher latitudes. The monthly resolution of our data product permits us to  
37 reveal significant differences in the seasonality of pCO<sub>2</sub> across the ocean basins. The shelves  
38 of the western and northern Pacific, as well as the shelves in the temperate North Atlantic  
39 display particularly pronounced seasonal variations in pCO<sub>2</sub>, while the shelves in the  
40 southeastern Atlantic and in the South Pacific reveal a much smaller seasonality. The  
41 calculation of temperature normalized pCO<sub>2</sub> for several latitudes in different oceanic basins  
42 confirms that the seasonality in shelf pCO<sub>2</sub> cannot solely be explained by

**Deleted:** 4

**Deleted:** a

**Deleted:** The validity of our interpolation, both in space and time, is assessed by comparing the SOM-FFN outputs

**Deleted:** SOCATv3

**Formatted:** Subscript

**Deleted:** and

**Deleted:** LDVEO2014

**Deleted:** sets

**Deleted:** But

**Deleted:** allows investigating the seasonal variations in pCO<sub>2</sub> and reveals

**Formatted:** Subscript

**Formatted:** Subscript

**Deleted:** exist

**Deleted:** Overall

**Deleted:** cycles

**Deleted:** ,

**Formatted:** Subscript

59 temperature-induced changes in solubility, but are also the result of seasonal changes in  
60 circulation, mixing, and biological productivity. Our results also reveal that the amplitudes of  
61 both thermal and non-thermal seasonal variations in pCO<sub>2</sub> are significantly larger at high  
62 latitudes. Finally, thanks to this product having been extended to cover open ocean areas as  
63 well, it can be readily merged with existing global open ocean products to produce a true  
64 global perspective of the spatial and temporal variability of surface ocean pCO<sub>2</sub>.

Formatted: Subscript

Formatted: Not Superscript/ Subscript

65

66 **1. Introduction**

67 The quantitative contribution of the coastal ocean to the global oceanic uptake of atmospheric  
68 CO<sub>2</sub> is still being debated (Borges et al., 2005; Chen and Borges, 2009; Cai, 2011;  
69 Wanninkhof et al., 2013; Gruber, 2015), but several recent studies have suggested that the flux  
70 density, or uptake per unit area, is greater over continental shelf seas than over the open ocean  
71 (Chen et al., 2013; Laruelle et al., 2014). Laruelle et al. (2014) used more than 3·10<sup>6</sup> pCO<sub>2</sub>  
72 measurements from the SOCATv2 database (Pfeil et al., 2014 Bakker et al., 2016) to  
73 demonstrate very strong disparities in air-seawater CO<sub>2</sub> exchange at the regional scale as well  
74 as pronounced seasonal variations, especially at temperate latitudes. Furthermore, it was  
75 suggested that, despite the presence of a seasonally varying sea-ice cover, Arctic continental  
76 shelves are a regional hotspot of CO<sub>2</sub> uptake (Bates et al., 2006; Laruelle et al., 2014;  
77 Yasunaka et al., 2016). Yet, even with this much larger dataset compared to previous studies,  
78 large regions of the global coastal ocean remained either void of data or very poorly  
79 monitored in space and time, including the seasonal cycle. These data gaps not only limit our  
80 ability to reduce uncertainties in flux estimates and to unravel whether they differ from the  
81 adjacent open ocean, but also hamper the identification and quantification of the many  
82 processes controlling the source-sink nature of the coastal ocean (Bauer et al., 2013). Laruelle  
83 et al., (2014) attempted to overcome this limitation by combining various upscaling methods  
84 depending on data density in different regions, e.g., resorted to using annual means, wherever  
85 the seasonal coverage was deemed to be insufficient. But they could not overcome the  
86 limitation that the data alone are insufficient to assess whether there are any trends in coastal  
87 fluxes. This is a serious gap when considering that the influence of human activity on coastal  
88 system is increasing rapidly (Doney, 2010; Cai, 2011; Regnier et al., 2013; Gruber, 2015).

Deleted: reports

Deleted: de

Deleted: do

Deleted: underlying

93 In the open ocean, novel statistical methods relying on artificial neural networks (ANNs) have  
94 permitted the generation of a series of high-resolution continuous monthly maps for ocean  
95 surface CO<sub>2</sub> partial pressures (pCO<sub>2</sub>) (e.g., Landschützer et al., 2013; Sasse et al., 2013;  
96 Nakaoka et al., 2013; Zeng et al., 2014). Although differing in their details (see e.g.,  
97 Rödenbeck et al., 2015 for an overview), these products typically have a nominal spatial  
98 resolution of 1-degree and monthly temporal resolution. By filling in the spatial and temporal  
99 gaps, these products greatly facilitate the calculation of the air-sea CO<sub>2</sub> exchange, as they do  
100 not require separate assumptions about the surface ocean pCO<sub>2</sub> in areas lacking data. Such  
101 methods are also well suited to resolve spatial gradients, and they also permit to determine  
102 seasonal and inter-annual variations and trends in pCO<sub>2</sub> (e.g., Landschützer et al., 2014, 2015,  
103 2016; Zeng et al., 2014). Because of the small relative contribution of the coastal ocean to the  
104 total oceanic surface area and the relatively coarse spatial resolution of the ANN-based  
105 surface ocean pCO<sub>2</sub> products so far, they are not well suited to resolve the high  
106 spatio-temporal variations of the surface ocean pCO<sub>2</sub> fields along the shelves.

Deleted: have

107 Reproducing the complex seasonal dynamics of the CO<sub>2</sub> exchange at the air-water interface in  
108 the coastal ocean is of particular importance considering that they often have large  
109 intra-annual variability (Signorini et al., 2013). For instance, in temperate climates, it is  
110 common for continental shelf waters to turn from CO<sub>2</sub> sinks for the atmosphere during spring  
111 to CO<sub>2</sub> sources during summer (Shadwick et al., 2010; Cai, 2011; Laruelle et al., 2014, 2015).  
112 Shelf waters are also typically characterized by small-scale physical features such as coastal  
113 currents, river plumes and eddies inducing sharp biogeochemical fronts (Liu et al., 2010) that  
114 markedly influence the spatial patterns of the pCO<sub>2</sub> fields (e.g., Turi et al., 2014).

Deleted: display

117 To resolve the high spatial and temporal variability in air-sea CO<sub>2</sub> exchange over the global  
118 shelf region, the two step artificial neural network method developed by Landschützer et al.  
119 (2013) is modified here for the specific conditions that prevail in these environments. Our  
120 calculations are performed at a much finer resolution of 0.25 degree and new environmental  
121 drivers such as sea ice cover are used at high latitudes to account for the potentially  
122 significant role of sea-ice in the CO<sub>2</sub> exchange (Bates et al., 2006; Vancoppenolle et al., 2013;  
123 Parmentier et al., 2013; Moreau et al., 2016; Grimm et al., 2016). The definition of the  
124 coastal/open oceanic boundary varies strongly from one study to the other (Walsh, 1988;  
125 Laruelle et al., 2013), with a potentially large impact on the shelf CO<sub>2</sub> budget (Laruelle et al.,  
126 2010). Here, we use a very wide definition for this boundary (i.e., 300km width or 1000m  
127 depth) to secure spatial continuity between our new shelf pCO<sub>2</sub> product and those already  
128 existing for the open ocean (Landschützer et al., 2013, 2016; Rödenbeck et al., 2015). Our  
129 approach leads to the first continuous and monthly resolved pCO<sub>2</sub> maps over the 1998-2015  
130 period across the global shelf region, permitting us to study the seasonal dynamics of these  
131 regions in relationship to that of the adjacent open ocean.

Deleted: significantly

Deleted: climatology

Deleted: (

Deleted: 4

Deleted: )

132

## 133 2. Methods

134 The method used in this study is a modified version of the SOM-FFN method developed by  
135 Landschützer et al. (2013) to calculate monthly-resolved pCO<sub>2</sub> maps of the Atlantic Ocean at  
136 a 1 degree resolution and later applied to the entire global open ocean (Landschützer et al.,  
137 2014). The reconstruction of a continuous pCO<sub>2</sub> field involves establishing numerical  
138 relationships between pCO<sub>2</sub> and a number of independent environmental predictors that are  
139 known to control its variability both in time and space. The first step of the method relies on

145 the use of a neural network clustering algorithm (Self Organizing Map, SOM) to define a  
146 discrete set of biogeochemical provinces characterized by similar relationships between the  
147 independent environmental variables and a monthly resolved pCO<sub>2</sub> field. The second step  
148 consists in deriving non-linear and continuous relationships between pCO<sub>2</sub> and some or all of  
149 the aforementioned independent variables using a feed-forward network (FFN) method,  
150 within each biogeochemical province created by the SOM. The method is extensively  
151 documented in Landschützer et al. (2013, 2014) but the specific modifications introduced in  
152 this study to better simulate the characteristics of the shelves, the choice of environmental  
153 drivers and their data sources as well as the definition of the geographic extent of this analysis  
154 are described in the following sections. Figure 1 summarizes the different steps involved in  
155 the calculations of the SOM-FFN.

Deleted: climatological

Deleted: described

Deleted: 2015

Formatted: Not Highlight

## 157 2.1. Data Sources and processing

Moved (insertion) [1]

Deleted: 2

158 All the datasets used in our calculations were converted from their original spatial resolutions  
159 to a regular 0.25 degree resolution grid. The temporal resolution of all datasets is monthly (i.e.,  
160 216 months over the entire period), except for the bathymetry that is assumed constant over  
161 the course of the simulations and wind speed whose original resolution is 6 hours. For the  
162 latter, monthly averages are calculated for each grid cell to generate monthly values. SST and  
163 SSS maps were taken from the Met Office's EN4, which consists of quality controlled  
164 subsurface ocean temperature and salinity profiles and their objective analyses (Good et al.,  
165 2009). The bathymetry was extracted from the global ETOPO2 database (US Department of  
166 Commerce, 2006). The sea ice concentrations was taken from the global 25 km resolution  
167 monthly data product compiled by the NSIDC (National Snow and Ice Cover Data; Cavalieri

Deleted: 04

Deleted: which

Deleted: :

Deleted: World Ocean Atlas (Antonov et al., 2010 for SST and Locarnini et al., 2010 for SSS)

Deleted: are

Deleted: recalculated

Deleted: extracted

181 et al., 1996). Wind speed data were extracted from ERA-Interim reanalysis (Dee et al., 2011).  
 182 The chlorophyll surface concentrations were extracted from the monthly 9 km resolution  
 183 SeaWIFS data product prior to 2010 and from MODIS for later years (NASA, 2016). The list  
 184 of all data products used in the calculations as well as the transformations applied to produce  
 185 monthly 0.25 degrees resolution forcing files are summarized in table 1.  
 186 Finally, the surface ocean pCO<sub>2</sub> were taken from the gridded SOCATv4 product (Sabine et al.,  
 187 2013; Bakker et al., 2016) while those used for the validation stem from the LDEOv2015  
 188 database (Takahashi et al., 2016). With our definition of the coastal zone, SOCATv4 contains  
 189 ~8 10<sup>6</sup> data points and LDEO ~5.6 10<sup>6</sup>, with over 70% of the data shared with SOCATv4.  
 190 Because of this significant overlap between both data products, we created two entirely  
 191 independent datasets by randomly assigning each of those common data point to either  
 192 database to insure that each data only belongs to one dataset. The resulting datasets are named  
 193 SOCAT\* and LDEO\*, respectively, with the former being used for training and the latter for  
 194 validation. Prior to the creation of both datasets, all data from SOCAT were converted from  
 195 fCO<sub>2</sub> (fugacity of CO<sub>2</sub> in water) to pCO<sub>2</sub> using the formulation reported in Takahashi et al.  
 196 (2012). The data densities of SOCAT\* and LDEO\* are shown on Fig. 2 and reveal a  
 197 heterogeneous spatial coverage. Northern temperate shelves are generally well covered,  
 198 especially in the North Atlantic. In this region, the data density is better in SOCAT\* than  
 199 LDEO\* thanks to the addition of many European cruises in the SOCAT database. On the  
 200 other hand, equatorial regions remain under-sampled, especially in the Indian Ocean. Because  
 201 of the difficulty of sampling in waters seasonally covered in ice, Polar Regions are very  
 202 unevenly represented in SOCAT\* and LDEO\*. Luckily, some areas, such as some parts of

- Deleted: 3
- Deleted: r
- Deleted: m
- Deleted: are extracted
- Deleted: v2014
- Deleted: However
- Deleted: under
- Formatted: Font: 12 pt
- Formatted: Font: 12 pt
- Deleted: of which are also part of
- Formatted: Font: 12 pt, Superscript
- Formatted: Font: 12 pt
- Formatted: Font: 12 pt, Superscript
- Formatted: Font: 12 pt
- Deleted:
- Formatted: Font: 12 pt
- Formatted: Font: 12 pt
- Formatted: Font: 12 pt
- Deleted: ed
- Formatted: Font: 12 pt
- Deleted: were
- Deleted: which was used for calibration and
- Deleted: which was used
- Deleted: in
- Deleted: overall

219 Antarctica and the Bering Sea do contain enough data to train and validate the SOM-FFN.

**Deleted:** calibrate

220 Overall SOCAT\* contains roughly 40% more data than LDEO\*.

**Deleted:** This latter database contains ~ 10.5 million pCO<sub>2</sub> measurements collected between 1957 and 2015. While a large overlap with the SOCAT database is inevitable, LDEOv2014 was compiled independently and is the only other global pCO<sub>2</sub> dataset (of comparable size and coverage to SOCAT) presently available. The data from SOCAT were converted from fCO<sub>2</sub> (fugacity of CO<sub>2</sub> in water) into pCO<sub>2</sub> using the formulation reported in Takahashi et al. (2012).

## 2.2. Modifications of the SOM-FFN method

**Formatted:** Font: Not Bold

223 The specific characteristics of the continental shelves motivated a number of modifications of  
224 the global ocean SOM-FFN method, including a 16-fold increase in spatial resolution from 1  
225 degree to 0.25 degree, the addition of new environmental variables as biogeochemical  
226 predictors, and a shortening of the simulation period to the period 1998 through 2015. All  
227 these modifications are detailed here below.

**Deleted:** 1

**Deleted:**

228 The higher resolution of 0.25°×0.25° results in over 2 million grid cells that help to better  
229 track the global coastline and its complex geomorphological features (Crossland et al., 2005;  
230 Liu, 2010). It is also common along Eastern and Western boundary currents to find  
231 continental shelves as narrow as 10-20 km, i.e., an extension that is significantly smaller than  
232 a single cell at 1-degree resolution. Additionally, biogeochemical fronts associated with river  
233 plumes, coastal currents and upwelling are characterized by spatial scales of the order of tens  
234 of kilometers or even smaller (Wijesekera et al., 2003). The chosen resolution is also identical  
235 to the gridded coastal pCO<sub>2</sub> product from the SOCAT initiative (Sabine et al, 2013, Bakker et  
236 al., 2014).

**Deleted:** the introduction of a second neuron layer in the FFN calculations,

**Deleted:** 2014

**Deleted:** in

**Deleted:** ing

**Deleted:** thus

**Deleted:** to

237 The definition of the geographic extent of the shelf region excludes estuaries and other  
238 inland water bodies, but uses a wide limit for the outer continental shelf that encapsulates all  
239 current definitions of the coastal ocean. This approach facilitates future integration with  
240 existing global ocean data products (e.g., Landschützer et al., 2016; Rödenbeck et al., 2015)  
241 and model outputs, which typically struggle to represent the shallowest parts of the ocean

264 (Bourgeois et al., 2016). The outer limit used here is given by whichever point is the furthest  
265 from the coast: either 300\_km distance from the coastline (which roughly corresponds to the  
266 outer edge of territorial waters (Crossland et al., 2005)) or the 1000\_m isobaths (Laruelle et al.,  
267 2013). The resulting domain (Fig SI\_B) covers 77 million km<sup>2</sup>, more than twice the surface  
268 area generally attributed to the coastal ocean (Walsh et al., 1998; Liu et al., 2010; Laruelle et  
269 al., 2013).

Deleted: 1

270 The predictor variables for the SOM-FFN networks were chosen based on a set of  
271 trial-and-error experiments with the selection criteria being the quality of fit, i.e., the best  
272 reconstruction of the available observations. The first step of the SOM-FFN calculations, i.e.,  
273 the self-organizing map-based clustering (SOM) relies on the assignment of the surface ocean  
274 data to biogeochemical provinces sharing common spatio-temporal patterns of sea-surface  
275 temperature (SST), sea-surface salinity (SSS), bathymetry, rate of change in sea ice coverage,  
276 wind speed and observed pCO<sub>2</sub>. Chlorophyll a is not included in the list of environmental  
277 factors used to generate the biogeochemical provinces because of the incomplete data  
278 coverage at high latitude in winter due to cloud coverage. Both the use of wind speed and the  
279 rate of change in monthly sea ice concentration are novelties compared to the set-up of  
280 Landschützer et al. (2013). The latter is calculated from the gridded monthly sea ice  
281 concentration field of Cavalieri et al. (1996). It allows accounting for the complex processes  
282 occurring in melting and forming sea ice that are known to strongly influence the dynamics of  
283 the carbon within sea-ice covered areas (Parmentier et al., 2013). This first step is performed  
284 without any data normalization of the datasets, as this permits us to give more weight to the  
285 pCO<sub>2</sub> data. Based on a series of simulations using different numbers of biogeochemical  
286 provinces, we found that a clustering of the data into 10 biogeochemical provinces minimized

Deleted:

Deleted:

Deleted: The

Deleted: is a

Deleted: novelty

Deleted: and

Formatted: Subscript

294 the average deviation between simulated and observed pCO<sub>2</sub> (see below) while insuring that  
295 at least 1000 different grid cells can be used for validation against LDEO\* in each province.

296 In the second step of the estimation procedure, i.e., the application of the feed-forward  
297 network method (FFN), SST, SSS, bathymetry, sea-ice concentration and chlorophyll a are  
298 used as predictors to establish the non-linear relationships between these predictors and the  
299 target pCO<sub>2</sub> (for data sources, see below). Similar to the SOM in step one, the selected  
300 variables not only comprise proxies representing the solubility and biological pumps of the  
301 coastal ocean, but also yield the best fit to the data. These calculations are done iteratively  
302 using a sigmoid activation function on an incomplete dataset in order to perform an  
303 assessment on the remaining data after each iteration, until an optimal relationship is found.

304 Additionally, as performed in Landschützer et al. (2015), the output pCO<sub>2</sub> data were smoothed  
305 using the spatial and temporal mean of each point's neighboring pixels both in time and space  
306 within the 3 pixel neighborhood domain. This operation is performed iteratively and does not  
307 significantly alter the results, but it ensures smoother transitions in the pCO<sub>2</sub> field at the  
308 boundaries between the provinces. This smoothing method yielded good results for the open  
309 Southern Ocean where marked pCO<sub>2</sub> fronts are also observed (Landschützer et al., 2015) and  
310 was deemed relevant here due to the potentially strong pCO<sub>2</sub> gradients characterizing the  
311 shelves.

312 Another change from the most recent global ocean SOM-FFN application (Landschützer  
313 et al., 2016) is the different temporal extension of the simulation period, which covers the  
314 period from 1998 through 2015, instead of 1982 through 2011. This overall shortening was  
315 necessary because one of environmental driver, i.e., chlorophyll data derived from SeaWIFS,  
316 only starts in September 1997 (NASA, 2016). Monthly chlorophyll data throughout the entire

**Deleted:** During

**Deleted:** calculation

**Deleted:** This step now includes a second artificial neuron layer that consists, for each iteration, of an additional procedure of optimization of the relationship fitting. This addition significantly increases the calculation time but prevents the SOM-FFN from generating negative values.

**Deleted:** 2014

**Deleted:** only

**Deleted:** the

329 simulation period was preferred here over the use of a monthly climatology as done in  
330 Landschützer et al. (2016) to better capture inter-annual variability. At the same time, we have  
331 been able to extend the coastal product by 4 years to the end of 2015.

### 333 2.3. Model training and evaluation

334 We evaluated the coastal SOM-FFN product using the root mean squared error (RMSE)  
335 metric, calculated as the difference between estimated and observed pCO<sub>2</sub>. During the early  
336 development stage, preliminary simulations were performed using only data from SOCAT  
337 v2.0 (Pfeil et al., 2013, Sabine et al. 2013) to train the FFN algorithm. Each simulation was  
338 carried out using different subsets of environmental predictors extracted from the complete set  
339 (SST, SSS, bathymetry, sea ice concentration and chlorophyll a). The results obtained were  
340 then compared to the more complete dataset of SOCAT\*, which contain 40% more shelf  
341 pCO<sub>2</sub> measurements from 1998 through 2015 (Bakker et al., 2016). This process allowed, for  
342 each province, to calculate the RMSE for several combinations of independent predictor  
343 variables for the pCO<sub>2</sub>. Next, the combinations of predictors displaying the lowest RMSE  
344 were kept for the final simulations, which then used all data from SOCAT\*. Thus, the pCO<sub>2</sub>  
345 calculations in each province potentially rely on a different set of predictors (Table 1).

346 The coastal SOM-FFN results are validated through a comparison with the LDEO\* dataset  
347 through the calculation of residuals and RMSE. Additionally, a model-to-model comparison is  
348 also performed with the global ocean results of Landschützer et al. (2016) in the regions  
349 where the domains overlap. To perform this latter analysis, the coastal high resolution coastal  
350 pCO<sub>2</sub> product generated here was aggregated to a regular monthly 1° resolution to match the  
351 grid used by Landschützer et al. (2016).

Deleted: ¶

Moved up [1]: 2.2. Data Sources and processing¶

All the datasets used in our calculations were converted from their original spatial resolutions to a regular 0.25 degree resolution grid. The temporal resolution of all datasets is monthly (i.e., 204 months over the entire period), except for the bathymetry that is assumed constant over the course of the simulations. SST and SSS maps were taken from the World Ocean Atlas (Antonov et al., 2010 for SST and Locarnini et al., 2010 for SSS). The bathymetry was extracted from the global ETOPO2 database (US Department of Commerce, 2006). The sea ice concentrations are recalculated from the global 25 km resolution monthly data product compiled by the NSIDC (National Snow and Ice Cover Data; Cavalieri et al., 1996). The chlorophyll surface concentrations were extracted from the monthly 9 km resolution SeaWiFS data product (NASA, 2016). Finally, the surface ocean pCO<sub>2</sub> were taken from the gridded SOCATv3 product (Sabine et al., 2013; Bakker et al., 2016) while those used from the validation are extracted from the LDEOv2014 database (Takahashi et al., 2016). This latter database contains ~ 10.5 million pCO<sub>2</sub> measurements collected between 1957 and 2015. While a large overlap with the SOCAT database is inevitable, LDEOv2014 was compiled independently and is the only other global...

Deleted: ¶

¶

Deleted: Evaluation procedures

Deleted: v3.0

Deleted: 2014

Deleted: v3.0

Deleted: v2014

Deleted: base (Takahashi et al., 2016)

437 Finally, the ability of the coastal SOM-FFN to capture seasonal variations is assessed by  
438 comparing the cell-average simulated monthly pCO<sub>2</sub> to monthly means for cells extracted  
439 from the LDEO\* database. The cells retained for this analysis are all those for which the  
440 average for each month could be calculated from measurements performed on at least three  
441 different years.

Deleted: v2014

### 443 3. Results and discussion

#### 444 3.1. Biogeochemical provinces

445 Despite the fact that the SOM is not given any prior knowledge regarding space and time,  
446 the spatial distribution of the 10 biogeochemical provinces is mostly controlled by latitudinal  
447 gradients and distance from the coast (Figure 3; high-resolution monthly maps are also  
448 available in the supplementary information (SI)). Although the exact spatial extent of each  
449 province varies from one month to the other following the seasonal variations of the  
450 environmental forcing parameters, each province roughly corresponds to one type of  
451 climatological setting. Nevertheless, because of these spatial migrations, most cells belong to  
452 different provinces depending on the month (see figure SI B). These seasonal migrations are  
453 mostly driven by changes in temperature, sea-ice cover, pCO<sub>2</sub> and, to a lesser degree, salinity.  
454 P<sub>1</sub>, P<sub>2</sub> (Province 1, etc.) and P<sub>4</sub> are three of the largest provinces, covering a total of 35.7·10<sup>6</sup>  
455 km<sup>2</sup> and representing warm tropical regions with bottoms at shallow to intermediate depths.  
456 During summer, the spatial coverage of P<sub>4</sub> expands north- and southward as a consequence of  
457 warming. P<sub>2</sub> represents tropical regions with deeper bottom depths. P<sub>1</sub> and P<sub>2</sub> display less  
458 seasonal changes in their spatial distribution than P<sub>4</sub> due to weaker seasonal temperature  
459 changes. P<sub>3</sub> and P<sub>6</sub>, which cover a combined 9.2·10<sup>6</sup> km<sup>2</sup>, are found in the Southern

Deleted: 1

Deleted: 1 of

Deleted: and

Formatted: Subscript

Deleted: P1

Deleted: 2

Deleted: the two

Deleted: 26.1

Deleted: 1

Deleted: 3

Deleted: and P4

Deleted: They

Deleted: 1

Deleted: P5

474 Hemisphere and correspond to sub-polar and temperate regions, respectively. Their spatial  
 475 distributions are subject to marked latitudinal migrations throughout the year as a result of the  
 476 large amplitude changes in seasonal temperature observed in mid-latitude coastal waters  
 477 (Laruelle et al., 2014). Similarly, P7, correspond to temperate Northern Hemisphere waters  
 478 and display marked seasonal changes including the shelves of the Norwegian basin in summer  
 479 and most of the Mediterranean Sea in winter. P5, P8, P9 and P10 together cover  $22.7 \cdot 10^6$  km<sup>2</sup>.  
 480 These provinces are partly (seasonally) covered by sea-ice with an average spatial ice cover  
 481 over the study period of 57%, 39%, 54% and 46% for P5, P8, P9 and P10, respectively. P5  
 482 represents the shelves of Antarctica all year round. P8 includes large fractions of the enclosed  
 483 seas at higher northern latitudes such as the Baltic Sea and Hudson Bay while P9 (only  
 484  $2.9 \cdot 10^6$  km<sup>2</sup>) represents permanently deep and cold polar regions. P5 and P10 represent most  
 485 of the polar shelves (P5 for the Antarctic, and P10 for the Arctic) and are covered in sea ice at  
 486 levels of 57% and 46%, respectively. The regions experiencing most notable shifts in province  
 487 allocation during the year include the northern Polar Regions as well as the temperate narrow  
 488 shelves of the Atlantic and Pacific, particularly Western Europe and Eastern North America  
 489 and Eastern Asia (see Fig. SI.B).

Deleted: cover a combined  $14 \cdot 10^6$  km<sup>2</sup>

Deleted: P7,  
 Deleted: 21.3

- Deleted: .1
- Deleted: 8.5
- Deleted: 41
- Deleted: .3
- Deleted: 65
- Deleted: 5.8
- Deleted: P7
- Deleted: P10
- Deleted: P7
- Deleted: P10
- Formatted: Not Highlight
- Deleted: P8 and P9
- Formatted: Not Highlight
- Formatted: Not Highlight
- Deleted: both the
- Formatted: Not Highlight
- Deleted: Arctic and
- Formatted: Not Highlight
- Deleted: 47
- Formatted: Not Highlight
- Deleted: 56
- Formatted: Not Highlight
- Deleted: polar regions
- Deleted: SI1
- Formatted: Not Highlight
- Deleted: 2

491 **3.2. Performance of the coastal SOM-FFN**

492 The mean climatological pCO<sub>2</sub> estimated by the coastal SOM-FFN for annually and  
 493 seasonally averaged conditions are reported in Figure 3. Before briefly analysing the main  
 494 spatial and temporal variability of the pCO<sub>2</sub> fields (section 3.3), we evaluate here the overall  
 495 performance of our interpolation method globally and at the level of each province, including  
 496 its ability to capture the seasonal cycle.

518 **3.2.1. Comparison with training data (SOCAT\*).**

519 Within each province, the pCO<sub>2</sub> simulated by the coastal SOM-FFN are compared to the

520 measurements extracted from SOCAT v4.0 (table 2). Globally, the average difference between

521 observed and simulated pCO<sub>2</sub> is almost null (overall bias = 0.0 μatm) and the absolute bias is

522 lower than 4 μatm in all ten provinces. The average RMSE over all provinces of 32.9 μatm is

523 comparable with those reported for other statistical reconstructions of coastal pCO<sub>2</sub> fields

524 summarized by (Chen et al., 2016), although none of these studies were performed at global

525 scale and many rely on different statistical approaches often using remote sensing data. This

526 RMSE is about twice that achieved for the open ocean (Landschützer et al., 2014) reflecting

527 the larger spatiotemporal variability in the coastal ocean, as well as more complex processes

528 governing that variability. Considering these complexities, achieving at the global scale

529 RMSE in the same range as those reported for regional coastal studies is quite good.

530 Significant variations in both bias and RMSE can be observed between provinces (table 2). P1

531 and P3 have the best fit between simulated and observed pCO<sub>2</sub> with RMSE lower than 20

532 μatm. In 5 provinces that cover a cumulated surface area of 31.2 · 10<sup>6</sup> km<sup>2</sup> (P1, P2, P3, P6 and

533 P9) RMSE's do not exceed 25 μatm. In P8 however, the maximum RMSE is found with a

534 value of 46.8 μatm. Overall, the performance of the SOM-FFN deteriorates for provinces

535 regularly covered by sea-ice ice (P5, P8-10) in which data coverage is relatively low (RMSE >

536 34 μatm). This trend is consistent with the spatial distribution of the average residual errors

537 between the pCO<sub>2</sub> field generated by the model and pCO<sub>2</sub> data extracted SOCAT\* (Fig. 4a).

538 The residuals are obtained by subtracting the observed values from model output in each grid

539 cell for every month where observations are available. Thus, positive values correspond to

540 cells where the simulated pCO<sub>2</sub> overestimates the field data, while negative values represent

- Deleted: SOCAT\*
- Deleted: v3.0 data
- Deleted: 3
- Deleted: +
- Deleted: 1
- Deleted: 6
- Deleted:
- Deleted: (Chen et al., 2016)
- Deleted: the
- Deleted: ed
- Deleted: P2
- Deleted: absolute bias and
- Deleted: 2 μatm and
- Deleted: , respectively
- Deleted: 6
- Deleted: which
- Deleted: 52
- Deleted: .6
- Deleted: P4,
- Deleted: P8
- Deleted: 30
- Deleted: P7
- Deleted: bias and
- Deleted: are maximum
- Deleted: s
- Deleted: 7.4 μatm and 63.4
- Deleted: , respectively
- Deleted: P7
- Deleted: and
- Deleted: and in which R
- Formatted: Not Highlight
- Formatted: Not Highlight
- Formatted: Subscript
- Formatted: Subscript

571 cells where the simulated pCO<sub>2</sub> underestimates the field data. The bulk of the residuals fall in  
 572 the -20 to 20 μatm range in temperate and tropical regions, except for very shallow regions  
 573 tha are under the influence of a large river such as the Mississippi. There, the SOM-FFN often  
 574 underestimates the observed pCO<sub>2</sub>. There also exist coastal areas where the SOM-FFN  
 575 underestimates the observed pCO<sub>2</sub> such as the Nova Scotia, the South Western coast of  
 576 England or the shelves of California and Morpcco. The complex hydrodynamics of those  
 577 regions (some of them being characterized as upwelling regions) may explain the weaker  
 578 performance of the SOM-FFN. At high latitudes, the performance of the model deteriorates  
 579 somewhat. For example, the Bering Sea both contains cells with very high (>50 μatm) and  
 580 very low average residuals (<-50 μatm).

581 —

### 582 3.2.2. Evaluation with LDEO\* data

583 The comparison of our results with the data from LDEO\* yields a global bias of 0.0 μatm  
 584 (calculated as the average difference between observed and SOM-FFN estimated pCO<sub>2</sub>) for  
 585 the entire shelf domain. However, the spread is relatively large with an average RMSE of 39.2  
 586 μatm. This average RMSE is 19% larger than the one obtained when comparing the  
 587 SOM-FFN results with the SOCAT\* dataset, which has been used to train the model. A  
 588 province-based analysis reveals strong differences in the calculated RMSEs, ranging from 20  
 589 μatm to 53 μatm (Table 2, LDEO\*). A review of various statistical models used to generate  
 590 continuous global ocean pCO<sub>2</sub> maps, including some using remote sensing data and  
 591 algorithms, reports RMSE or uncertainties typically varying within the 10-35 μatm range  
 592 (Chen et al., 2016) with outliers as high as 50 μatm in the Mississippi delta (Lohrenz and Cai,  
 593 2006). This report also shows that open ocean estimates generally yields RMSE lower than 17

- Deleted: cells
- Deleted: where
- Formatted: Not Highlight
- Formatted: Not Highlight
- Deleted:
- Formatted: Subscript, Not Highlight
- Formatted: Not Highlight
- Formatted: Subscript
- Deleted: r
- Deleted: s
- Deleted: .
- Deleted: and
- Deleted: f
- Deleted: r
- Deleted: hith
- Deleted: Comparison
- Deleted: v2014
- Deleted: v2014
- Deleted: very small
- Deleted: -2.4
- Deleted: 42
- Deleted: 24
- Deleted: 67

612  $\mu\text{atm}$ , in agreement with Landschützer et al. (2014), whereas coastal estimates are associated  
 613 with much higher uncertainties. This is likely because these coastal regions have complex  
 614 biogeochemical dynamics and high frequency variability that cannot be fully captured with  
 615 the current generation of data interpolation techniques using the limited available predictor  
 616 data.

617 In our simulations, the province averaged biases are larger than those calculated with  
 618 SOCAT\* but their absolute value remains small and never exceed 3.9  $\mu\text{atm}$  (P8). Provinces  
 619 P1, P2, P3 and P6 have RMSE < 30  $\mu\text{atm}$ , which compares with the most robust pCO<sub>2</sub>  
 620 regional coastal estimates from the literature (Chen et al., 2016). Together, these 4 provinces  
 621 account for 37% of our domain. P4, P5 and P9 display RMSE comprised between 33  $\mu\text{atm}$   
 622 and 38  $\mu\text{atm}$  for P4 and P9, respectively. Overall, these 7 provinces covering the entire  
 623 tropical and temperate latitudinal bands as well as some subpolar regions account for >72% of  
 624 the shelf surface area and yield RMSE of less than 38  $\mu\text{atm}$  and absolute biases of less than  
 625 2.3  $\mu\text{atm}$ . Provinces in the polar regions (P5, P7, P8, and P10) overall display larger deviations  
 626 with respect to the LDEO\* dataset, but the absolute value of their biases never exceeds 3.9  
 627  $\mu\text{atm}$ . Their RMSE all fall in the 51-53  $\mu\text{atm}$  range. This suggests a significantly lower  
 628 performance of the SOM-FFN in regions partly covered in sea-ice. This can be attributed to  
 629 the limited number of available data points and their very heterogeneous distribution in time  
 630 and space, as well as to the very limited range of variation of some of the controlling variable  
 631 such as temperature and salinity. The relatively good performance of the model in tropical  
 632 region might be partly attributed to the relatively small seasonal variations in pCO<sub>2</sub> within  
 633 these areas. The residuals calculated by subtracting the SOM-FFN results from LDEO\* are  
 634 very similar to those obtained by subtracting the SOM-FFN results from SOCAT\* (Fig. 4b).

- Deleted: integrated
- Deleted: provinces
- Deleted: P4
- Deleted: negligible biases (with absolute values <0.5  $\mu\text{atm}$ , table 2) and
- Deleted: 3
- Deleted: 44
- Deleted: P3
- Deleted: P5
- Deleted: slightly higher biases of -2.3 and -5.2  $\mu\text{atm}$ , respectively and
- Deleted: of
- Deleted: 44
- Deleted: 67
- Deleted:  $\mu\text{atm}$
- Deleted: 5
- Deleted: 62
- Deleted: 45
- Deleted: 4
- Deleted: sub-polar and
- Deleted: P6
- Deleted: ,
- Deleted: P9
- Deleted: v2014
- Deleted: 10
- Deleted: Except for P8, which displays a
- Deleted: of 35  $\mu\text{atm}$ , all other province...
- Deleted:
- Deleted: ing
- Deleted: 45
- Deleted: 70
- Deleted: s
- Deleted: to
- Deleted: s
- Deleted: to

672 The residual errors have a nearly Gaussian distribution for every biogeochemical province  
673 with the exception of province P8 (Fig. 5). In this case, the distribution has not only the  
674 highest spread, but is also skewed toward high values.

675 In order to evaluate the contribution of the newly added predictors compared to the oceanic  
676 set up of the SOM-FFN (Landschützer et al., 2013), the model was also trained without wind  
677 speed and sea ice cover. The RMSE obtained with those simulations (Table 4) are  
678 significantly higher than those obtained using all predictors (Table 3). However, the overall  
679 bias remain small. The results of those simulations are presented in the table below and allow  
680 to quantify how the addition of new predictors affects the performance of the model. For  
681 instance, it can be noticed that the global RMSE increases significantly (from 39.2 to 48  $\mu\text{atm}$   
682 in the comparison with LDEO\* when chlorophyll, sea ice and wind speed are not taken into  
683 account and from 39.2 to 45  $\mu\text{atm}$  when only sea ice and wind speed are not taken into  
684 account). This deterioration of the performance of the model, however, is not evenly affecting  
685 all provinces. Provinces located at high latitudes (i.e. P8, P9 and P10) perform significantly  
686 worse without the inclusion of wind speed and sea ice.

687 Finally, while the use of residuals and RMSE provide valid quantitative assessment of the  
688 model performance, it does not provide insights regarding its ability to reproduce the seasonal  
689 pCO<sub>2</sub> cycle. To address this issue, Figure 7 displays observed mean monthly pCO<sub>2</sub> extracted  
690 from LDEO\* and calculated by the coastal SOM-FFN for the 40 locations where the LDEO\*  
691 database has the most data (>40 month). The error bars associated with the observations  
692 reflect the inter-annual variability. Overall, the coastal SOM-FFN captures the timing of the  
693 seasonal pCO<sub>2</sub> cycle in most locations well with pCO<sub>2</sub> minima and maxima occurring at the  
694 same time in our results and in the uninterpolated LDEO\* data. The pCO<sub>2</sub> maximum

**Deleted:** distribution of the

**Deleted:** within each biogeochemical province assumes

**Deleted:** s

**Deleted:** of the residuals

**Deleted:** for which the spread is not only the highest (indicating the largest discrepancy between model and observations), but also slightly skewed toward high values, thus revealing a tendency to overestimate the observed pCO<sub>2</sub>.

**Formatted:** Subscript

**Deleted:** T

**Deleted:** , however,

**Deleted:** ing

**Deleted:** , overall,

**Formatted:** English (U.S.)

**Deleted:** s

**Deleted:** and it can be observed in particular that

**Deleted:** p

**Deleted:** ¶

**Deleted:** W

**Deleted:** of

**Deleted:** s

**Deleted:** a

**Deleted:** 3

**Deleted:** v2014

**Deleted:** 53

**Deleted:** v2014

**Deleted:** v2014

**Deleted:** ¶

726 generally taking place in early summer is accurately captured by the coastal SOM-FFN. In  
727 terms of amplitudes in the pCO<sub>2</sub> signal, the coastal SOM-FFN and the LDEO\* data reveal  
728 primarily how different the seasonal pCO<sub>2</sub> cycle is from one region to the other, with very low  
729 amplitude (<40 μatm) in some sub-tropical areas, amplitudes > 100 μatm at high Northern  
730 and Southern latitudes, and sometimes very sharp increases during summer like off the coast  
731 of Japan. In most regions, the SOM-FFN-based reconstructions are able to capture these  
732 variations and predict seasonal amplitudes comparable to those observed in the data. However,  
733 in cells for which the difference between observed and simulated seasonal pCO<sub>2</sub> amplitude is  
734 larger than 20%, the coastal SOM-FFN tends to systematically underestimate the amplitude of  
735 the seasonal pCO<sub>2</sub> cycle. This limitation of our model might result from the often short time  
736 scales associated with the continental influences in near-shore locations, which are not  
737 captured by the environmental predictors used in our calculation. It may also be the result of  
738 very short-term events that are aliased in our monthly average calculations.

Deleted: the most

Deleted: v2014

Deleted: .

Deleted: at

Deleted: s

### 739 3.2.3. Comparison with global SOM-FFN

740 The comparison of our coastal SOM-FFN results with those of Landschützer et al. (2016) for  
741 the overlapping grid cells (Table 3) reveals significant differences between both interpolated  
742 data products with a RMSE between 24 and 32 μatm for most provinces except P7, P9 and  
743 P10 (53, 55 and 37 μatm, respectively). These RMSE values are comparable, but slightly  
744 lower than those obtained for the comparison with the LDEO\* database, in line with those  
745 observed with the SOCAT\* database. The differences (coastal SOM-FFN minus global  
746 SOM-FFN), however, are much larger than those observed between our results and the  
747 LDEO\* database and highlight the current knowledge gap regarding the mean state and

Deleted: 2

Deleted: 20

Deleted: 37

Deleted: P9

Deleted: and

Deleted: \_v2014

Deleted: \_v2014

760 variability of the transition zone. They range from -17.9 to 11.7  $\mu\text{atm}$  from one province to

Deleted: 6

761 the other but only amount to -0.6  $\mu\text{atm}$  when considering the cells from all provinces at once.

Deleted: 8

Deleted: 6

762 The overlapping cells used for the comparison with Landschützer et al. (2016) are mostly

763 located over 100km away from the coastline and therefore the open ocean as well as our new

764 shelf ocean data set are constrained by fairly different data because all the ‘shelf’ cells from

765 the open ocean data product have a  $\text{pCO}_2$  calculated by a model calibrated mostly for

766 conditions representative of the open ocean. Overall, the occurrence of large residuals in the

Deleted:

767 shallowest cells of our calculation domain in our results (Fig. 2) suggest that the very

Deleted: Our

Deleted: indicate

768 nearshore processes controlling the  $\text{CO}_2$  dynamics likely are the most difficult to reproduce at

Deleted: with a global SOM-FFN

769 the global scale. However, the added value of performing our simulations at the spatial

770 resolution of  $0.25^\circ$  is exemplified by the ability of our model to capture the plumes of larges

Deleted: explified

771 rivers such as the Amazon, where  $\text{pCO}_2$  is significantly lower than that of the surrounding

Deleted: which

772 waters (Cooley et al., 2007; Ibanez et al., 2015).

Deleted: produces an area located North of its river mouth characterized by

Formatted: Subscript

Deleted: values

Deleted: those

Deleted:

### 774 3.3. Spatial and temporal variability of the coastal $\text{pCO}_2$

#### 775 3.3.1 Spatial variability

776 Figure 4a presents the annual average  $\text{pCO}_2$  estimated by the coastal SOM-FFN, representing

Deleted: 2a

777 the mean over 1998 through 2015 period (monthly climatological maps are shown in Fig. SI

Deleted: 2014

778 A). High annual mean values of  $\text{pCO}_2$ , close to or above atmospheric levels, are estimated

Deleted: 2

779 around the equator up to the tropics. This is consistent with previous studies that identified

780 tropical and equatorial coastal regions as weak  $\text{CO}_2$  sources for the atmosphere (Borges et al.,

781 2005; Cai, 2011; Laruelle et al., 2010; 2014). A hotspot of very high  $\text{pCO}_2$  emerges from our

782 analysis around the Arabian Peninsula, extending into the eastern Mediterranean Sea as well

Deleted: in the Indian Ocean

Deleted: past the tropic of Cancer

802 as into the Red Sea and the Persian Gulf. These regions are poorly monitored and it remains  
803 difficult to assess if pCO<sub>2</sub> values in excess of 450 μatm are realistic or not, but the limited  
804 body of available literature suggests that very high pCO<sub>2</sub> are indeed observed in these regions  
805 (Ali, 2008; Omer, 2010). The very high temperature and salinity conditions observed in the  
806 Red Sea, in particular, reduce the CO<sub>2</sub> solubility and induce very high pCO<sub>2</sub> conditions.

807 However, these predicted pCO<sub>2</sub> lie outside of the range used for the training of the SOM-FFN  
808 (typically 200–450 μatm) and should thus be considered with caution. Along the oceanic coast  
809 of the Arabian Peninsula, the SOM-FFN predicts pCO<sub>2</sub> ranging from 365 to 390 μatm all year  
810 round and thus does not capture the well-known increase in pCO<sub>2</sub> resulting from the monsoon  
811 driven summer upwelling in the region (Sarma, 2003; Takahashi et al., 2009).

812 In both hemispheres, pCO<sub>2</sub> values in the 325 to 370 μatm range are generally reconstructed at  
813 temperate latitudes, i.e., up to 50°N and 50°S, respectively. The northern high latitudes  
814 generally have very low pCO<sub>2</sub> values, down to 300 μatm and below, a result that is consistent  
815 with the Arctic shelves contributing a large proportion (up to 60%) of the global coastal  
816 carbon sink (Bates and Mathis, 2009; Cai, 2011; Laruelle et al., 2014). Several hotspots of  
817 pCO<sub>2</sub> with values as high as 450 μatm can be observed nevertheless north of 70°N, most

818 notably along the eastern coast of Siberia in winter (see Fig. SI P), which displays a large  
819 zone characterized by pCO<sub>2</sub> > 400 μatm centred on the mouth of the Kolyma River. Such high  
820 pCO<sub>2</sub> values have been punctually observed in Arctic coastal waters (Anderson et al., 2009)

821 and could result from the discharge of highly oversaturated riverine waters. But, overall,  
822 pCO<sub>2</sub> measurements over Siberian shelves are rare. Thus, our results should be considered  
823 with caution in this region because of the scarcity of data to train and validate the coastal  
824 SOM-FFN. It should also be noted that the vast majority of this high pCO<sub>2</sub> region is covered

Deleted: calibration

Formatted: Subscript

Formatted: Subscript

Formatted: Not Superscript/ Subscript

Deleted: 320

Deleted: 360

Deleted: 3

Deleted: around

Deleted: particularly

831 by sea ice (Fig. 4b&c) and, although the model estimates pCO<sub>2</sub> values over the entire domain,  
832 only ice-free (or partially ice-free) cells will contribute to the CO<sub>2</sub> exchange across the air-sea  
833 interface (Bates and Mathis, 2009; Laruelle et al., 2014).

Deleted: 2b

### 834 3.3.2. Temporal variability

835 The reconstructed pCO<sub>2</sub> field is also subject to large seasonal variations (see figures SI P&A).

Deleted: 2

836 To explore these variations further, Figure 8 reports seasonal-mean latitudinal profiles of

Deleted: 3

837 pCO<sub>2</sub> for continental shelves neighbouring the Eastern Pacific, Atlantic, Indian and Western

Deleted: 4

838 Pacific, respectively. The analysis excludes continental shelves at latitudes higher than 65

839 degrees, because a large fraction of these shelves are seasonally covered by sea ice. The

840 latitudinal pCO<sub>2</sub> profiles reveal that, in most regions, highest and lowest pCO<sub>2</sub> values are

841 observed during the warmest and coldest months, respectively. This trend is particularly

842 pronounced at temperate latitudes where the seasonal pCO<sub>2</sub> amplitude can reach 60 μatm and

843 is exemplified by regions such as the western Mediterranean Sea or the eastern coast of

844 America, which become supersaturated in CO<sub>2</sub> compared to the atmosphere during the

845 summer months. However, there are a few other regions, where the lowest pCO<sub>2</sub> is found in

Deleted: T

846 the summer, such as the Baltic Sea (Thomas and Schneider, 1999). Around the equator, the

Deleted: ,

847 magnitude of the seasonal variations in pCO<sub>2</sub> is limited and does not exceed 30 μatm.

Deleted:

Deleted: however,

848 Although the general latitudinal trend of the annual mean pCO<sub>2</sub> is similar across all

Deleted: in

849 continental shelves, significant differences in the seasonality can be observed across the

Deleted: the

850 largest ocean basins. In particular, most of the East Pacific shelves, except for latitudes north

Deleted: p

Deleted: c

851 of 55°N, display limited seasonal change in pCO<sub>2</sub> (typically below 30 μatm) while the West

Deleted:

852 Pacific shelves have seasonal pCO<sub>2</sub> amplitudes that can exceed 50 μatm in temperate regions

Deleted: 40

Deleted: 60

853 and 100 μatm at high latitudes (above 55° N). Along the Atlantic shelves, the seasonal signal

869 is more pronounced in the north compared to the south, in agreement with Laruelle et al.  
 870 (2014). Overall, the North Pacific (north of 55°N) displays the most pronounced seasonal  
 871 change in pCO<sub>2</sub> with a difference of 80 μatm between summer and winter. In the Indian  
 872 Ocean, the seasonal dynamics of pCO<sub>2</sub> is partly regulated by seasonal upwelling induced by  
 873 the Monsoon (Liu et al., 2010). In this basin north the equator, April, May and June are the  
 874 months having the highest pCO<sub>2</sub> and the seasonal variations do not exceed 30 μatm. In  
 875 contrast, the seasonal cycle is quite pronounced in the Indian Ocean south of the equator (~50  
 876 μatm).

Deleted: above

Deleted: displaying

Deleted: 40

Deleted: 60

877 Latitudinal profiles of SST (Fig 8, bottom) are similar in all coastal oceans with minimal  
 878 seasonal variations around the equator and amplitudes as large as 20°C at temperate latitudes.

Deleted: 4

Deleted: and display

879 The comparison between the seasonal pCO<sub>2</sub> and SST profiles allows us to assess the  
 880 contribution of temperature-induced changes in CO<sub>2</sub> solubility to the seasonal pCO<sub>2</sub> variations,  
 881 in the continental shelf waters. However, other factors such as seasonal upwelling and  
 882 biological activity also strongly influence coastal pCO<sub>2</sub> and contribute to the complexity of  
 883 the seasonal pCO<sub>2</sub> profiles. To quantify the effect of temperature on seasonal variations of  
 884 pCO<sub>2</sub>, the latter is normalized to the mean temperature at different latitudes in each oceanic

Deleted: bility

885 basin (Fig. 8) using the formula proposed by Takahashi et al. (1993):

Deleted: 5

$$886 \quad pCO_{2(SSTmean)} = pCO_{2,obs} \times \exp(0.0423 \times (T_{mean} - T_{obs})) \quad (1)$$

Deleted: n

887 where pCO<sub>2(SSTmean)</sub> is the temperature normalized pCO<sub>2</sub>, pCO<sub>2,obs</sub> is the observed pCO<sub>2</sub> at  
 888 the observed temperature T<sub>obs</sub> and T<sub>mean</sub> is the yearly mean temperature at the considered

Deleted:  $npCO_2$

Formatted: Not Superscript/ Subscript

889 location. In sea-water, an increase in water temperature induces a decrease in gas solubility

890 which leads to a higher water pCO<sub>2</sub>. Thus, comparing pCO<sub>2(SSTmean)</sub> with observed pCO<sub>2</sub>

Deleted: n

902 monthly values provides a quantitative estimate of the influence of seasonal temperature  
903 change on the seasonality of pCO<sub>2</sub>.

904 For most latitudes and oceanic basins, pCO<sub>2</sub> is minimum in late winter or early spring, i.e., at  
905 the time when pCO<sub>2</sub>(SSTmean) has its maximum. pCO<sub>2</sub> also generally displays a maximum in  
906 summer, while pCO<sub>2</sub>(SSTmean) reaches its minimum then (Fig. 9). The amplitude of the changes  
907 in pCO<sub>2</sub>(SSTmean) is quite consistent across oceans and about 2 to 3 times larger than that of  
908 pCO<sub>2</sub>. Between 45°N and 60° N, the variations in pCO<sub>2</sub>(SSTmean) largely exceed 100 μatm (up  
909 to 220 μatm at 60° N in the West Pacific). In these regions, the magnitude of the seasonal  
910 temperature changes is also maximum and reaches 20° C between winter and summer (Fig. 5).

911 A seasonal signal in pCO<sub>2</sub> with a minimum in late winter or spring when pCO<sub>2</sub>(SSTmean) is  
912 maximal can also be identified. However, the magnitude of the seasonal variations in pCO<sub>2</sub> is  
913 significantly smaller than those of pCO<sub>2</sub>(SSTmean), suggesting that other processes such as  
914 biological uptake or transport/mixing partly offsets the temperature effect on solubility. In the  
915 subpolar western Pacific shelves (60° N), a second pronounced dip in pCO<sub>2</sub> following a  
916 weaker one in spring is observed in summer, which suggests the occurrence of a pronounced  
917 summer biological activity taking up large amounts of CO<sub>2</sub>. This would also explain the sharp  
918 increase in pCO<sub>2</sub> in the following month, as a result of the degradation of organic matter

919 synthesized during the summer bloom. Although this region is also the one subjected to the  
920 strongest seasonal temperature, the amplitude of the seasonal pCO<sub>2</sub>(SSTmean) which reaches  
921 220μatm suggests that non thermal processes drive most of the seasonal pCO<sub>2</sub> variations in  
922 the regions. At 20° N, the amplitude of the changes in both pCO<sub>2</sub> and pCO<sub>2</sub>(SSTmean) are lower  
923 than at higher latitudes. pCO<sub>2</sub> varies by ~30μatm between summer and winter in all oceanic  
924 basin while the seasonal variations in pCO<sub>2</sub>(SSTmean) are more pronounced in the Pacific

Deleted: all

Formatted: Not Highlight

Deleted: npCO<sub>2</sub>

Deleted: npCO<sub>2</sub>

Deleted: 5

Deleted: npCO<sub>2</sub>

Deleted: npCO<sub>2</sub>

Deleted: 180

Deleted: 4

Deleted: npCO<sub>2</sub>

Deleted: npCO<sub>2</sub>

Deleted: T

Deleted: gradient as evidenced by

Deleted: npCO<sub>2</sub>

Deleted: 200μatm

Formatted: Subscript

Deleted: npCO<sub>2</sub>

Deleted: npCO<sub>2</sub>

941 (~60 $\mu$ atm) than in the Atlantic or the Indian Oceans. In the Southern Hemisphere, the  
942 seasonal variations in pCO<sub>2</sub> are not as pronounced as in the Northern Hemisphere suggesting  
943 that the changes induced by the solubility pump are compensated by biological activities. At  
944 10°S and 30°S, the seasonal variations in pCO<sub>2</sub> rarely exceed 30  $\mu$ atm in either basin with a  
945 minimum observed around August.

Deleted:

946

#### 947 4. Summary

948 This study presents the first global high-resolution monthly pCO<sub>2</sub> maps for continental shelf  
949 waters at an unprecedented 0.25° spatial resolution. We show that when tailored for the  
950 specific conditions of shelf systems, the SOM-FFN method previously employed in the open  
951 ocean is capable of reproducing well-known and well-observed features of the pCO<sub>2</sub> field in  
952 the coastal ocean. Our continuous shelf product allows, for the first time, to analyze the  
953 dominant spatial patterns of pCO<sub>2</sub> across all ocean basins and their seasonality. The data  
954 product associated to this manuscript consists of a netcdf file containing the pCO<sub>2</sub> for ice-free  
955 cells at a 0.25° spatial resolution for each of the 216 month of the simulation period (from  
956 January 1998 to December 2015). 12 maps representing mean pCO<sub>2</sub> fields calculated for each  
957 month over the simulation period are also provided. This data product can be combined with  
958 wind field products such as ERA-interim (Dee, 2010; Dee et al., 2011) or CCMP (Atlas et al.,  
959 2011) to compute spatially and temporally resolved air-sea CO<sub>2</sub> fluxes across the global shelf  
960 region, including the Arctic. Maps including pCO<sub>2</sub> for ice covered cells are also available but  
961 should be treated with care because the dynamics of CO<sub>2</sub> fluxes through sea ice are still  
962 poorly understood and air-sea gas transfer velocities in partially sea ice covered areas cannot  
963 be predicted from classical wind speed relationships (Lovely et al. 2015)

Deleted: ,

Deleted: 204

Deleted: 2014

Formatted: Subscript

Deleted: Climatologically averaged pCO<sub>2</sub> maps for each month

970

971 **5. Data availability**

972 The version 4 of the SOCAT database (Bakker et al., 2016) can be downloaded from

973 www.socat.info/upload/SOCAT v4.zip. The observation-based global monthly gridded sea

974 surface pCO<sub>2</sub> product is provided by Landschützer, et al. (2015; doi:

975 10.3334/CDIAC/OTG.SPCO2\_1982\_2011\_ETH\_SOM-FFN.), was downloaded from

976 http://cdiac.ornl.gov/ftp/oceans/SPCO2\_1982\_2011\_ETH\_SOM\_FFN and is now available at:

977 https://www.nodc.noaa.gov/ocads/oceans/SPCO2\_1982\_2015\_ETH\_SOM\_FFN.html. The

978 LDEOv2015 database (Takahashi et al., 2015; doi: 10.3334/CDIAC/OTG.NDP088(V2015))

979 was downloaded from http://cdiac.ornl.gov/oceans/LDEO Underway Database/. The global

980 atmospheric reanalysis ERA-interim datasets (Dee et al., 2011,

981 http://doi.wiley.com/10.1002/qj.828) are accessible on the European Centre for

982 Medium-Range Weather Forecasts (ECMWF) website. SST and SSS were extracted from the

983 Met Office's EN4 data set (Good et al., 2009; doi:10.1002/2013JC009067). The bathymetry

984 used is the global ETOPO2 database (US Department of Commerce, 2006), which can be

985 downloaded from http://www.ngdc.noaa.gov/mgg/fliers/06mgg01.html. The sea ice

986 concentrations are derived from the global 25 km resolution monthly data product compiled

987 by the NSIDC (National Snow and Ice Cover Data; Cavalieri et al., 1996).

988

989

989 **6. Competing interests**

990 The authors declare that they have no conflict of interest.

991

992

Formatted: Font: Not Bold

Formatted: Font: Not Bold, Subscript

Formatted: Font: Not Bold

Formatted: Font: Not Bold

Formatted: Font: Not Bold

Formatted: Font: Not Bold

Formatted: Hyperlink, Font: 10,5 pt, Not Bold, English (U.S.)

Field Code Changed

Formatted: Font: Not Bold

Formatted: Font: Not Bold

Formatted: Font: Not Bold

Formatted: Font: Not Bold

Formatted: Not Highlight

Deleted: : quality controlled subsurface ocean temperature and salinity profiles and objective analyses

Formatted: Not Highlight

Formatted: Not Highlight

Formatted: Not Highlight

Formatted: Not Highlight

Formatted: Font: Not Bold

Formatted: Font: Not Bold

996 | **Acknowledgements**

Deleted: 5.

997 G. G. Laruelle and B Delille are postdoctoral researcher and research associate, respectively,  
998 of F.R.S.-FNRS. The Surface Ocean CO<sub>2</sub> Atlas (SOCAT) is an international effort, supported  
999 by the International Ocean Carbon Coordination Project (IOCCP), the Surface Ocean Lower  
1000 Atmosphere Study (SOLAS), and the Integrated Marine Biogeochemistry and Ecosystem  
1001 Research program (IMBER), in order to deliver a uniformly quality-controlled surface ocean  
1002 CO<sub>2</sub> database. The many researchers and funding agencies responsible for the collection of  
1003 data and quality control are thanked for their contributions to SOCAT. The research leading to  
1004 these results has received funding from the European Union's Horizon 2020 research and  
1005 innovation program under the Marie Skłodowska-Curie grant agreement No 643052 744  
1006 (C-CASCADES project). NG acknowledges support by ETH Zürich. PL is supported by the  
1007 Max Planck Society for the Advancement of Science.

1008

**References**

- 1010  
1011 Ali, E.: The Inorganic Carbon Cycle in the Red Sea, Master's thesis, University of Bergen,  
1012 2008.
- 1013 Anderson, L. G., Jutterström, S., Hjalmarsson, S., Wählström, I., and Semiletov, I. P.:  
1014 Out-gassing of CO<sub>2</sub> from Siberian Shelf seas by terrestrial organic matter decomposition,  
1015 *Geophys. Res. Lett.*, 36, L20601, doi:10.1029/2009GL040046, 2009.
- 1016 Antonov, J. I., Seidov, D., Boyer, T. P., Locarnini, R. A., Mishonov, A. V., Garcia, H. E.,  
1017 Baranova, O. K., Zweng, M. M., and Johnson D. R.: in *World Ocean Atlas 2009, Volume*  
1018 *2: Salinity*, NOAA Atlas NESDIS, vol. 69, edited by S. Levitus, U.S. Gov. Print. Off.,  
1019 Washington, D. C., 2010.
- 1020 Atlas, R., Hoffman, R.N., Ardizzone, J., Leidner, S.M., Jusem, J.C., Smith, D.K. and Gombos,  
1021 D.: A cross-calibrated, multiplatform ocean surface wind velocity product for  
1022 meteorological and oceanographic applications. *Bulletin of the American Meteorological*  
1023 *Society*, 92(2), 157-174, 2011.
- 1024 Bakker, D. C. E., Pfeil, B., Smith, K., Hankin, S., Olsen, A., Alin, S. R., Cosca, C., Harasawa,  
1025 S., Kozyr, A., Nojiri, Y., O'Brien, K. M., Schuster, U., Telszewski, M., Tilbrook, B., Wada,  
1026 C., Akl, J., Barbero, L., Bates, N. R., Boutin, J., Bozec, Y., Cai, W.-J., Castle, R. D.,  
1027 Chavez, F. P., Chen, L., Chierici, M., Currie, K., De Baar, H. J. W., Evans, W., Feely, R. A.,  
1028 Fransson, A., Gao, Z., Hales, B., Hardman-Mountford, N. J., Hoppema, M., Huang, W.-J.,  
1029 Hunt, C. W., Huss, B., Ichikawa, T., Johannessen, T., Jones, E. M., Jones, S., Jutterstrom,  
1030 S., Kitidis, V., Körtzinger, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Manke, A. B.,  
1031 Mathis, J. T., Merlivat, L., Metzl, N., Murata, A., Newberger, T., Omar, A. M., Ono, T.,  
1032 Park, G.-H., Paterson, K., Pierrot, D., Ríos, A. F., Sabine, C. L., Saito, S., Salisbury, J.,

1034 Sarma, V. V. S. S., Schlitzer, R., Sieger, R., Skjelvan, I., Steinhoff, T., Sullivan, K. F., Sun,  
1035 H., Sutton, A. J., Suzuki, T., Sweeney, C., Takahashi, T., Tjiputra, J., Tsurushima, N., Van  
1036 Heuven, S. M. A. C., Vandemark, D., Vlahos, P., Wallace, D. W. R., Wanninkhof, R.,  
1037 Watson, A. J.: An update to the Surface Ocean CO<sub>2</sub> Atlas (SOCAT version 2). *Earth*  
1038 *System Science Data* 6: 69-90. doi:10.5194/essd-6-69-2014, 2014.

1039 Bakker, D. C. E. et al. (92 authors) : A multi-decade record of high-quality fCO<sub>2</sub> data in  
1040 version 3 of the Surface Ocean CO<sub>2</sub> Atlas (SOCAT), *Earth Syst. Sci. Data*, 8, 383-413,  
1041 doi:10.5194/essd-8-383-2016, 2016

1042 Bates, N. R., Moran, S. B., Hansell, D. A., and Mathis, J. T.: An increasing CO<sub>2</sub> sink in the  
1043 Arctic Ocean due to sea-ice loss. *Geophys. Res. Lett.*, 33(23), L23609, doi:  
1044 10.1029/2006GL027028, 2006.

1045 Bates, N. R., and Mathis, J. T.: The Arctic Ocean marine carbon cycle: Evaluation of air-sea  
1046 CO<sub>2</sub> exchanges, ocean acidification impacts and potential feedbacks, *Biogeosciences*, 6,  
1047 2433–2459, doi:10.5194/bg-6-2433-2009, 2009.

1048 Bauer, J. E., Cai, W.-J., Raymond, P. A., Bianchi, T. S., Hopkinson, C. S., and Regnier, P. A.  
1049 G.: The changing carbon cycle of the coastal ocean, *Nature*, 504, 61–70,  
1050 doi:10.1038/nature12857, 2013.

1051 Borges, A. V., Delille, B., and Frankignoulle, M.: Budgeting sinks and sources of CO<sub>2</sub> in the  
1052 coastal ocean: Diversity of ecosystems counts, *Geophys. Res. Lett.*, 32, L14601,  
1053 doi:10.1029/2005GL023053, 2005.

1054 Bourgeois, T., Orr, J. C., Resplandy, L., Terhaar, J., Ethé, C., Gehlen, M., and Bopp, L.:  
1055 Coastal-ocean uptake of anthropogenic carbon, *Biogeosciences*, 13, 4167-4185,  
1056 doi:10.5194/bg-13-4167-2016, 2016.

Deleted:

1058 Cai, W. J.: Estuarine and coastal ocean carbon paradox: CO<sub>2</sub> sinks or sites of terrestrial  
1059 carbon incineration?, *Annu. Rev. Mar. Sci.*, 3, 123–145, 2011.

1060 Cavalieri, D. J., Parkinson, C. L., Gloersen, P., and Zwally, H.: Sea Ice Concentrations from  
1061 Nimbus-7 SMMR and DMSP SSM/I-SSMIS Passive Microwave Data, years 1990–2011,  
1062 NASA DAAC at the Natl. Snow and Ice Data Cent., Boulder, Colo. (Updated yearly.),  
1063 1996.

1064 Chen, C.T.A., and Borges, A.V.: Reconciling opposing views on carbon cycling in the coastal  
1065 ocean: continental shelves as sinks and near-shore ecosystems as sources of atmospheric  
1066 CO<sub>2</sub>, *Deep-Sea Research II*, 56 (8-10), 578-590, 2009.

1067 Chen, C. T. A., Huang, T. H., Chen, Y. C., Bai, Y., He, X., and Kang, Y.: Air-sea exchanges of  
1068 CO<sub>2</sub> in the world's coastal seas, *Biogeosciences*, 10, 6509–6544,  
1069 doi:10.5194/bg-10-6509-2013, 2013.

1070 Chen, S., Hu, C., Byrne, R. H., Robbins, L. L., and Yang, B.: Remote estimation of surface  
1071 pCO<sub>2</sub> on the West Florida Shelf, *Continental Shelf Research*, 128, 10–25, 2016.

1072 [Cooley, S. R., V. J. Coles, A. Subramaniam, and P. L. Yager \(2007\), Seasonal variations in the](#)  
1073 [Amazon plume-related atmospheric carbon sink, \*Global Biogeochem. Cycles\*, 21,](#)  
1074 [GB3014, doi:10.1029/2006GB002831.](#)

1075 Crossland, C. J., Kremer, H. H., Lindeboom, H. J., Marshall Crossland, J. I., and LeTissier, M.  
1076 D. A. (Eds.): *Coastal Fluxes in the Anthropocene*, *Global Change – The IGBP Series*: 232  
1077 pp, Berlin, Heidelberg, Springer-Verlag, Germany, 2005.

1078 Dee, D.P.: The ERA-Interim reanalysis: Configuration and performance of the data  
1079 assimilation system. *Q. J. R. Meteorol. Soc.*, 137, pp.553–597, 2010.

1080 [Dee, D. P., Uppala, S. M., Simmons, A. J., Berrisford, P., Poli, P., Kobayashi, S., Andrae, U.,](#)

1081 [Balmaseda, M. A., Balsamo, G., Bauer, P., Bechtold, P., Beljaars, A. C. M., van de Berg,](#)  
1082 [L., Bidlot, J., Bormann, N., Delsol, C., Dragani, R., Fuentes, M., Geer, A. J., Haimberger,](#)  
1083 [L., Healy, S. B., Hersbach, H., Hòlm, E. V., Isaksen, L., Kallberg, P., Köhler, M.,](#)  
1084 [Matricardi, M., McNally, A. P., Monge-Sanz, B. M., Morcrette, J. J., Park, B. K., Peubey,](#)  
1085 [C., de Rosnay, P., Tavolato, C., Thépaut, J. N. and Vitart, F.: The ERA-Interim reanalysis:](#)  
1086 [Configuration and performance of the data assimilation system, Q. J. R. Meteorol. Soc.,](#)  
1087 [137\(656\), 553–597, doi:10.1002/qj.828, 2011.](#)

1088 Doney, S. C.: The Growing Human Footprint on Coastal and Open-Ocean Biogeochemistry,  
1089 Science 328(5985), 1210-1216, doi:10.1126/science.1185198, 2010.

1090 [Good, S. A., M. J. Martin and N. A. Rayner, 2013. EN4: quality controlled ocean temperature](#)  
1091 [and salinity profiles and monthly objective analyses with uncertainty estimates, Journal of](#)  
1092 [Geophysical Research: Oceans, 118, 6704-6716, doi:10.1002/2013JC009067](#)

1093 Gruber, N.: Ocean biogeochemistry: Carbon at the coastal interface, Nature, 517, 148–149,  
1094 doi:10.1038/nature14082, 2015.

1095 Grimm, R., Notz, D., Glud, R.N., Rysgaard, S. and Six, K.D.: Assessment of the sea-ice  
1096 carbon pump: Insight from a three-dimensional ocean-sea-ice-biogeochemical model  
1097 (MPIOM/HAMOCC). Elementa: Science of the Anthropocene, 4:000136, doi:  
1098 10.12952/journal.elementa.000136, 2016.

1099 [Ibáñez, J. S. P., D. Diverres, M. Araujo, and N. Lefèvre \(2015\), Seasonal and interannual](#)  
1100 [variability of sea-air CO2 fluxes in the tropical Atlantic affected by the Amazon River](#)  
1101 [plume, Global Biogeochem. Cycles, 29, 1640–1655, doi:10.1002/2015GB005110.](#)

1102 Landschützer, P., Gruber, N., Bakker, D. C. E., Schuster, U., Nakaoka, S., Payne, M. R., Sasse,  
1103 T., and Zeng, J.: A neural network-based estimate of the seasonal to inter-annual

1104 variability of the Atlantic Ocean carbon sink, *Biogeosciences*, 10, 7793-7815,  
1105 doi:10.5194/bg-10-7793-2013, 2013.

1106 Landschützer, P., Gruber, N., Bakker, D. C. E., and Schuster, U.: Recent variability of the  
1107 global ocean carbon sink, *Global Biogeochemical Cycles*, 28, 927–949,  
1108 doi:10.1002/2014GB004853, 2014.

1109 Landschützer, P., Gruber, N., Haumann, F. A. Rödenbeck, C. Bakker, D.C.E. , van Heuven, S.  
1110 Hoppema, M., Metzl, N., Sweeney, C., Takahashi, T., Tilbrook, B. and Wanninkhof, R.:  
1111 The reinvigoration of the Southern Ocean carbon sink, *Science*, 349, 1221-1224. doi:  
1112 10.1126/science.aab2620, 2015.

1113 Landschützer, P., Gruber, N. Bakker, D.C.E.: Decadal variations and trends of the global  
1114 ocean carbon sink, *Global Biogeochemical Cycles*, 30, doi:10.1002/2015GB005359, 2016

1115 Laruelle, G. G., Dürr, H. H., Slomp, C. P., and Borges, A. V.: Evaluation of sinks and sources  
1116 of CO<sub>2</sub> in the global coastal ocean using a spatially-explicit typology of estuaries and  
1117 continental shelves, *Geophys. Res. Lett.*, 37, L15607, doi: 10.1029/2010gl043691, 2010.

1118 Laruelle, G. G., Dürr, H. H., Lauerwald, R., Hartmann, J., Slomp, C. P., Goossens, N., and  
1119 Regnier, P. A. G.: Global multi-scale segmentation of continental and coastal waters from  
1120 the watersheds to the continental margins, *Hydrol. Earth Syst. Sci.*, 17, 2029–2051,  
1121 doi:10.5194/hess-17-2029-2013, 2013.

1122 Laruelle, G. G., Lauerwald, R., Pfeil, B., and Regnier, P.: Regionalized global budget of the  
1123 CO<sub>2</sub> exchange at the air-water interface in continental shelf seas, *Global Biogeochemical*  
1124 *Cycles*, 28, 1199–1214, doi:10.1002/2014GB004832, 2014.

1125 Laruelle, G. G., Lauerwald, R., Rotschi, J., Raymond, P. A., Hartmann, J., and Regnier, P.:  
1126 Seasonal response of air–water CO<sub>2</sub> exchange along the land–ocean aquatic continuum of

1127 the northeast North American coast., *Biogeosciences*, 12, 1447-1458,  
1128 doi:10.5194/bg-12-1447-2015, 2015.

1129 Liu, K.-K., Atkinson, L., Quinones, R., and Talaue-McManus, L. (Eds.): Carbon and Nutrient  
1130 Fluxes in Continental Margins, *Global Change – The IGBP Series*, 3, Springer-Verlag  
1131 Berlin Heidelberg, 2010.

1132 Lohrenz, S. E., and Cai, W.-J.: Satellite ocean color assessment of air-sea fluxes of CO<sub>2</sub> in a  
1133 river-dominated coastal margin, *Geophys. Res. Lett.*, 33, L01601,  
1134 doi:10.1029/2005GL023942, 2006.

1135 Lovely, A., Loose, B., Schlosser, P., McGillis, W., Zappa C., Perovich, D., Brown, S., Morell,  
1136 T., Hsueh, D., and Friedrich, R.: The Gas Transfer through Polar Sea ice experiment:  
1137 Insights into the rates and pathways that determine geochemical fluxes. *J. Geophys. Res.*  
1138 *Ocean*. 120:8177–8194, 2015.

1139 Locarnini, R. A., Mishonov, A. V., Antonov, J. I., Boyer, T. P., Garcia, H. E., Baranova, O. K.,  
1140 Zweng, M. M., and Johnson D. R.: *World Ocean Atlas 2009, Volume 1: Temperature*,  
1141 *NOAA Atlas NESDIS*, vol. 69, edited by S. Levitus, U.S. Gov. Print. Off., Washington, D.  
1142 C., 2010.

1143 Moreau, S., Vancoppenolle, M., Bopp, L., Aumont, O., Madec, G., Delille, B., Tison, J.-L.,  
1144 Barriat, P.-Y. and Goosse, H.: Assessment of the sea-ice carbon pump: Insights from a  
1145 three-dimensional ocean-sea-ice-biogeochemical model (NEMO-LIM-PISCES). *Elementa:*  
1146 *Science of the Anthropocene*, 4:000122, doi: 10.12952/journal.elementa.000122, 2016.

1147 Nakaoka, S., Telszewski, M., Nojiri, Y., Yasunaka, S., Miyazaki, C., Mukai, H., and Usui, N.:  
1148 Estimating temporal and spatial variation of ocean surface pCO<sub>2</sub> in the North Pacific  
1149 using a self-organizing map neural network technique, *Biogeosciences*, 10, 6093-6106,

1150 doi:10.5194/bg-10-6093-2013, 2013.

1151 NASA Goddard Space Flight Center, Ocean Ecology Laboratory, Ocean Biology Processing  
1152 Group; (Dataset Release 2016): MODIS-Aqua chlorophyll Data; NASA Goddard Space  
1153 Flight Center, Ocean Ecology Laboratory, Ocean Biology Processing Group, 2016.

1154 Omer, W. M. M.: Ocean acidification in the Arabian Sea and the Red Sea. Master's thesis,  
1155 University of Bergen, 2011.

1156 Parmentier, F.-J. W., Christensen, T. R., Sørensen, L. L., Rysgaard, S., McGuire, A. D., Miller,  
1157 P. A., and Walker, D. A.: The impact of lower sea-ice extent on Arctic greenhouse-gas  
1158 exchange, *Nature Climate Change*, 3, 195–202, doi:10.1038/nclimate1784, 2013.

1159 Pfeil, B., Olsen, A., Bakker, D. C. E., Hankin, S., Koyuk, H., Kozyr, A., Malczyk, J., Manke,  
1160 A., Metzl, N., Sabine, C. L., Akl, J., Alin, S. R., Bates, N., Bellerby, R. G. J., Borges, A.,  
1161 Boutin, J., Brown, P. J., Cai, W.-J., Chavez, F. P., Chen, A., Cosca, C., Fassbender, A. J.,  
1162 Feely, R. A., González-Dávila, M., Goyet, C., Hales, B., Hardman-Mountford, N., Heinze,  
1163 C., Hood, M., Hoppema, M., Hunt, C. W., Hydes, D., Ishii, M., Johannessen, T., Jones, S.  
1164 D., Key, R. M., Körtzinger, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lenton, A.,  
1165 Lourantou, A., Merlivat, L., Midorikawa, T., Mintrop, L., Miyazaki, C., Murata, A.,  
1166 Nakadate, A., Nakano, Y., Nakaoka, S., Nojiri, Y., Omar, A. M., Padin, X. A., Park, G.-H.,  
1167 Paterson, K., Perez, F. F., Pierrot, D., Poisson, A., Ríos, A. F., Santana-Casiano, J. M.,  
1168 Salisbury, J., Sarma, V. V. S. S., Schlitzer, R., Schneider, B., Schuster, U., Sieger, R.,  
1169 Skjelvan, I., Steinhoff, T., Suzuki, T., Takahashi, T., Tedesco, K., Telszewski, M., Thomas,  
1170 H., Tilbrook, B., Tjiputra, J., Vandemark, D., Veness, T., Wanninkhof, R., Watson, A. J.,  
1171 Weiss, R., Wong, C. S., and Yoshikawa-Inoue, H.: A uniform, quality controlled Surface  
1172 Ocean CO<sub>2</sub> Atlas (SOCAT), *Earth System Science Data* 5: 125-143.

1173 doi:10.5194/essd-5-125-2013, 2013.

1174 Regnier, P., Friedlingstein, P., Ciais, P., Mackenzie, F. T., Gruber, N., Janssens, I. A., Laruelle,  
1175 G. G., Lauerwald, R., Luyssaert, S., Andersson, A. J., Arndt, S., Arnosti, C., Borges, A. V.,  
1176 Dale, A. W., Gallego-Sala, A., Godd ris, Y., Goossens, N., Hartmann, J., Heinze, C., Ilyina,  
1177 T., Joos, F., LaRowe, D. E., Leifeld, J., Meysman, F. J. R., Munhoven, G., Raymond, P. A.,  
1178 Spahni, R., Suntharalingam, P. and Thullner, M.: Anthropogenic perturbation of the  
1179 carbon fluxes from land to ocean. *Nature Geoscience*, 6, doi:10.1038/ngeo1830, 2013.

1180 R denbeck, C., Bakker, D. C. E., Gruber, N., Iida, Y., Jacobson, A. R., Jones, S., Landsch tzer,  
1181 P., Metzl, N., Nakaoka, S., Olsen, A., Park, G.-H., Peylin, P., Rodgers, K. B., Sasse, T. P.,  
1182 Schuster, U., Shutler, J. D., Valsala, V., Wanninkhof, R., and Zeng, J.: Data-based  
1183 estimates of the ocean carbon sink variability – first results of the Surface Ocean pCO<sub>2</sub>  
1184 Mapping intercomparison (SOCOM), *Biogeosciences*, 12, 7251-7278,  
1185 doi:10.5194/bg-12-7251-2015, 2015.

1186 Sabine, C. L., et al. (76 authors): Surface Ocean CO<sub>2</sub> Atlas (SOCAT) gridded data products,  
1187 *Earth System Science Data*, 5, 145–153, doi:10.5194/essd-5-145-2013, 2013  
1188

1189 Sasse, T. P., McNeil, B. I., and Abramowitz, G.: A new constraint on global air-sea CO<sub>2</sub> fluxes  
1190 using bottle carbon data, *Geophys. Res. Lett.*, 40, 1594–1599, doi:10.1002/grl.50342,  
1191 2013.

1192 [Sarma, V. V. S. S., Monthly variability in surface pCO<sub>2</sub> and net air-sea CO<sub>2</sub> flux in the](#)  
1193 [Arabian Sea, \*J. Geophys. Res.\*, 108 \(C8\), 3255, doi:10.1029/2001JC001062, 2003.](#)

1194 Shadwick, E. H., Thomas, H., Comeau, A., Craig, S. E., Hunt, C. W., and Salisbury, J. E.:  
1195 Air-Sea CO<sub>2</sub> fluxes on the Scotian Shelf: seasonal to multi-annual variability,  
1196 *Biogeosciences*, 7, 3851–3867, doi:10.5194/bg-7-3851-2010, 2010.

1197 Signorini, S. R., Mannino, A., Najjar Jr., R. G., Friedrichs, M. A. M., Cai, W.-J., Salisbury, J.,  
1198 Wang, Z. A., Thomas, H., and Shadwick, E.: Surface ocean pCO<sub>2</sub> seasonality and sea-air  
1199 CO<sub>2</sub> flux estimates for the North American east coast, *J. Geophys. Res.-Oceans*, 118,  
1200 5439–5460, doi:10.1002/jgrc.20369, 2013.

1201 Takahashi, T., Olafsson, J., Goddard, J. G., Chipman, D. W., and Sutherland, S. C.: Seasonal  
1202 variation of CO<sub>2</sub> and nutrients in the high-latitude surface oceans: A comparative study.  
1203 *Global Biogeochemical Cycles*, 7(4), 843–878, 1993.

1204 Takahashi, T., Sutherland, S., and Kozyr A.: Global ocean surface water partial pressure of  
1205 CO<sub>2</sub> database: Measurements performed during 1957–2011 (Version 2011).  
1206 ORNL/CDIAC-160, NDP-088(V2011), Carbon Dioxide Information Analysis Center,  
1207 Oak Ridge Natl. Lab., U.S. Dep. of Energy, Oak Ridge, Tenn., 2012.

1208 Takahashi, T., Sutherland, S. C., and Kozyr, A.: Global Ocean Surface Water Partial Pressure  
1209 of CO<sub>2</sub> Database: Measurements Performed During 1957-2015 (Version 2015).  
1210 ORNL/CDIAC-160, NDP-088(V2015). Carbon Dioxide Information Analysis Center,  
1211 Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, doi:  
1212 10.3334/CDIAC/OTG.NDP088(V2015), 2016.

1213 Thomas, H., and Schneider, B.: The seasonal cycle of carbon dioxide in Baltic Sea surface  
1214 waters, *J. Mar. Syst.*, 22, 53-67, 1999.

1215 Turi, G., Lachkar, Z., and Gruber, N.: Spatiotemporal variability and drivers of pCO<sub>2</sub> and air–  
1216 sea CO<sub>2</sub> fluxes in the California Current System: an eddy-resolving modeling study,  
1217 *Biogeosciences*, 11, 671-690, doi:10.5194/bg-11-671-2014, 2014.

1218 U.S. Department of Commerce, National Oceanic and Atmospheric Administration, National  
1219 Geophysical Data Center. 2006. 2-minute Gridded Global Relief Data (ETOPO2v2).

1220 <http://www.ngdc.noaa.gov/mgg/fliers/06mgg01.html>. Accessed 26 Dec 2008.

1221 Vancoppenolle M., Meiners, K. M., Michel, C., Bopp, L., Brabant, F., Carnat, G., Delille, B.,  
1222 Lannuzel, D., Madec, G., Moreau, S., Tison, J.-L., and van der Merwe, P.: Role of sea ice  
1223 in global biogeochemical cycles: Emerging views and challenges, *Quaternary Science*  
1224 *Reviews*, 79, 207-230, doi:10.1016/j.quascirev.2013.04.011, 2013.

1225 Wanninkhof, R., Park, G.-H., Takahashi, T., Sweeney, C., Feely, R., Nojiri, Y., Gruber, N.,  
1226 Doney, S. C., McKinley, G. A., Lenton, A., Le Quéré, C., Heinze, C., Schwinger, J.,  
1227 Graven, H., and Khatiwala, S.: Global ocean carbon uptake: magnitude, variability and  
1228 trends, *Biogeosciences*, 10, 1983-2000, doi: 10.5194/bg-10-1983-2013, 2013.

1229 Walsh, J. J.: *On the nature of continental shelves*, Academic Press, San Diego, New York,  
1230 Berkeley, Boston, London, Sydney, Tokyo, Toronto, 1988.

1231 Wijesekera, H. W., J. S. Allen, and P. A. Newberger, Modeling study of turbulent mixing over  
1232 the continental shelf: Comparison of turbulent closure schemes, *J. Geophys. Res.*, 108(C3),  
1233 3103, doi:10.1029/2001JC001234, 2003

1234 Yasunaka, S., Murata, A., Watanabe, E., Chierici, M., Fransson, A., van Heuven, S., Hoppema,  
1235 M., Ishii, M., Johannessen, T., Kosugi, N., Lauvset, S. K., Mathis, J. T., Nishino, S., Omar,  
1236 A. M., Olsen, A., Sasano, D., Takahashi, T., and Wanninkhof, R.: Mapping of the air-sea  
1237 CO<sub>2</sub> flux in the Arctic Ocean and its adjacent seas: Basin-wide distribution and seasonal  
1238 to interannual variability. *Polar Science*, 10(3):323-334, doi:10.1016/j.polar.2016.03.006,  
1239 2016.

1240 Zeng, J., Nojiri, Y., Landschützer, P., Telszewski, M., and Nakaoka, S.: A global surface ocean  
1241 fCO<sub>2</sub> climatology based on a feed-forward neural network, *J. Atmos. Ocean Technol.*, 31,  
1242 1838-1849, 2014.



1244 Table 1: Datasets used to create the environmental forcing files. The original spatial and  
 1245 temporal resolution and the main manipulations applied for their use in the SOM\_FFN are  
 1246 also reported.

<u>Predictor</u>	<u>dataset</u>	<u>resolution</u>	<u>reference</u>	<u>Manipulation</u>
<u>SST</u>	<u>EN4</u>	<u>0.25°, daily</u>	<u>Good et al., 2013</u>	<u>Monthly average</u>
<u>SSS</u>	<u>EN4</u>	<u>0.25°, daily</u>	<u>Good et al., 2013</u>	<u>Monthly average</u>
<u>Bathymetry</u>	<u>ETOPO2</u>	<u>2 minutes</u>	<u>US Department of Commerce, 2006</u>	<u>Aggregation to 0.25°</u>
<u>Sea ice</u>	<u>NSIDC</u>	<u>0.25°, monthly</u>	<u>Cavalieri et al., 1996</u>	<u>Monthly rate of change in sea ice coverage</u>
<u>Chlorophyll a</u>	<u>SeaWifs, MODIS</u>	<u>9km, monthly</u>	<u>NASA, 2016</u>	<u>Aggregation to 0.25°</u>
<u>Wind speed</u>	<u>ERA</u>	<u>0.25°, 6hours</u>	<u>Dee et al., 2011</u>	<u>Monthly average</u>

1247  
 1248

Formatted: Justified

1249 Table 2: List of the biogeochemical provinces, their geographic distribution and the  
 1250 environmental predictors used to calculate surface ocean pCO<sub>2</sub>. SSS stands for sea surface  
 1251 salinity, SST for sea surface temperature, Bathy for bathymetry, Ice for sea-ice cover, Chl for  
 1252 chlorophyll concentration and Wind for wind speed.

Province	SSS	SST	Bathy	Ice	Chl	Wind
P1	X	X	X		X	X
P2	X	X	X		X	X
P3	X	X	X		X	X
P4	X	X	X		X	X
P5	X	X	X	X	X	X
P6	X	X	X	X	X	X
P7	X	X	X	X	X	X
P8	X	X	X	X		X
P9	X	X	X	X		X
P10	X	X	X	X		X

Deleted: 1

Formatted: Justified

Deleted: and

Deleted: X

Deleted: X

Deleted: X

1253

1259 Table 3: Root mean squared error between observed and calculated pCO<sub>2</sub> in the different biogeochemical provinces. The SOM-FFN results are compared to  
 1260 data extracted from the LDEO database (Takahashi et al, 2014) and the overlapping cells from the Landschützer et al. (2016) pCO<sub>2</sub> climatology.

Province	Surface	Ice Cover	SOCAT*	Landschützer		2016	LDEO	
	Area (km <sup>2</sup> )	(%)	Bias (µatm)	RMSE (µatm)	Bias (µatm)	RMSE (µatm)	Bias (µatm)	RMSE (µatm)
P1	8.2 10 <sup>6</sup>	0	0.0	19.1	2.0	27.2	2.0	20.5
P2	10.9 10 <sup>6</sup>	0	0.2	24.7	9.3	24.2	1.3	27.2
P3	4.4 10 <sup>6</sup>	0	-0.3	16.1	2.2	37.9	2.3	22.7
P4	16.6 10 <sup>6</sup>	0	-0.2	31.2	8.0	21.1	-1.6	33.0
P5	7.5 10 <sup>6</sup>	57.1	0.0	34.2	11.5	30.9	-1.4	38.0
P6	4.8 10 <sup>6</sup>	0	0.0	24.3	6.8	18.1	1.3	27.9
P7	9.3 10 <sup>6</sup>	0.0	0.1	37.2	0.7	23.5	-0.2	52.5
P8	3.3 10 <sup>6</sup>	38.5	0.2	46.8	13.9	70.1	3.9	51.4
P9	2.9 10 <sup>6</sup>	54.3	-0.1	23.0	-5.2	42.5	-2.5	33.4
P10	9.0 10 <sup>6</sup>	45.8	0.0	35.7	-9.7	50.9	1.6	53.1
	76.9 10 <sup>6</sup>		0.0	32.9	3.9	34.7	0.0	39.2

- Deleted: 2
- Deleted: v3.0
- Deleted: 15.5
- Deleted: -5.4
- Deleted: 27.8
- Deleted: 8.6
- Deleted: 26...7.2.5
- Deleted: -0.4
- Deleted: 29.3
- Deleted: 6
- Deleted: 1.6
- Deleted: 17.9
- Deleted: 5.4
- Deleted: 5
- Deleted: -0.2
- Deleted: 4.1
- Deleted: 7
- Deleted: 1.8
- Deleted: 25.7
- Deleted: 3.1
- Deleted: 23.6
- Deleted: -
- Deleted: 43.7
- Deleted: 8...6.1
- Deleted: 8
- Deleted: 15.4
- Deleted: 0.2
- Deleted: 28.5

1261

Table 4: Biases and root mean squared error (RMSE) between observed and calculated pCO<sub>2</sub> using only SST, SSS and bathymetry (STB) or SST, SSS, bathymetry and chlorophyll (STBC) as predictors.

Province	SOCAT*				LDEO*			
	Bias (µatm)		RMSE (µatm)		Bias (µatm)		RMSE (µatm)	
	STB	STBC	STB	STBC	STB	STBC	STB	STBC
<b>P1</b>	<u>0.0</u>	<u>-0.2</u>	<u>20.8</u>	<u>21.0</u>	<u>2.4</u>	<u>2.0</u>	<u>21.7</u>	<u>21.5</u>
<b>P2</b>	<u>-0.1</u>	<u>0.1</u>	<u>26.9</u>	<u>27.8</u>	<u>0.5</u>	<u>0.8</u>	<u>29.0</u>	<u>29.6</u>
<b>P3</b>	<u>0.0</u>	<u>-0.5</u>	<u>22.7</u>	<u>21.3</u>	<u>3.0</u>	<u>2.3</u>	<u>27.1</u>	<u>26.8</u>
<b>P4</b>	<u>0.0</u>	<u>-0.2</u>	<u>33.0</u>	<u>33.0</u>	<u>-1.7</u>	<u>-2.3</u>	<u>33.8</u>	<u>33.8</u>
<b>P5</b>	<u>0.2</u>	<u>0.1</u>	<u>52.7</u>	<u>42.2</u>	<u>-1.7</u>	<u>-0.9</u>	<u>56.9</u>	<u>44.5</u>
<b>P6</b>	<u>0.0</u>	<u>0.1</u>	<u>26.8</u>	<u>26.5</u>	<u>-0.5</u>	<u>0.6</u>	<u>28.9</u>	<u>28.0</u>
<b>P7</b>	<u>0.4</u>	<u>0.3</u>	<u>44.3</u>	<u>44.1</u>	<u>1.2</u>	<u>0.3</u>	<u>59.3</u>	<u>58.8</u>
<b>P8</b>	<u>0.1</u>	<u>0.4</u>	<u>82.6</u>	<u>80.0</u>	<u>9.1</u>	<u>9.0</u>	<u>56.3</u>	<u>58.5</u>
<b>P9</b>	<u>0.1</u>	<u>0.9</u>	<u>34.7</u>	<u>36.5</u>	<u>-2.6</u>	<u>-2.8</u>	<u>39.8</u>	<u>41.8</u>
<b>P10</b>	<u>-0.3</u>	<u>0.7</u>	<u>49.8</u>	<u>49.5</u>	<u>-3.9</u>	<u>-3.0</u>	<u>76.5</u>	<u>75.4</u>
<b>Global</b>	<u>0.1</u>	<u>0.2</u>	<u>43.9</u>	<u>42.4</u>	<u>0.0</u>	<u>0.0</u>	<u>48.0</u>	<u>45.0</u>

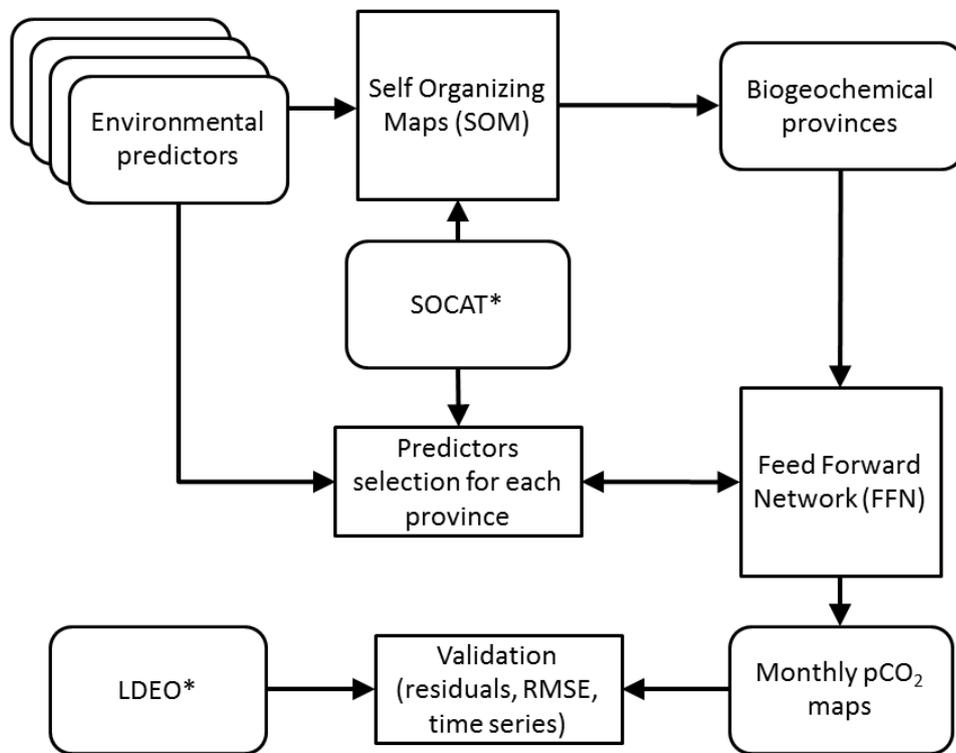


Figure 1: Schematic scheme of the different steps involved in the SOM-FFN artificial neural network calculations leading to continuous monthly pCO<sub>2</sub> maps over the 1998-2015 period.

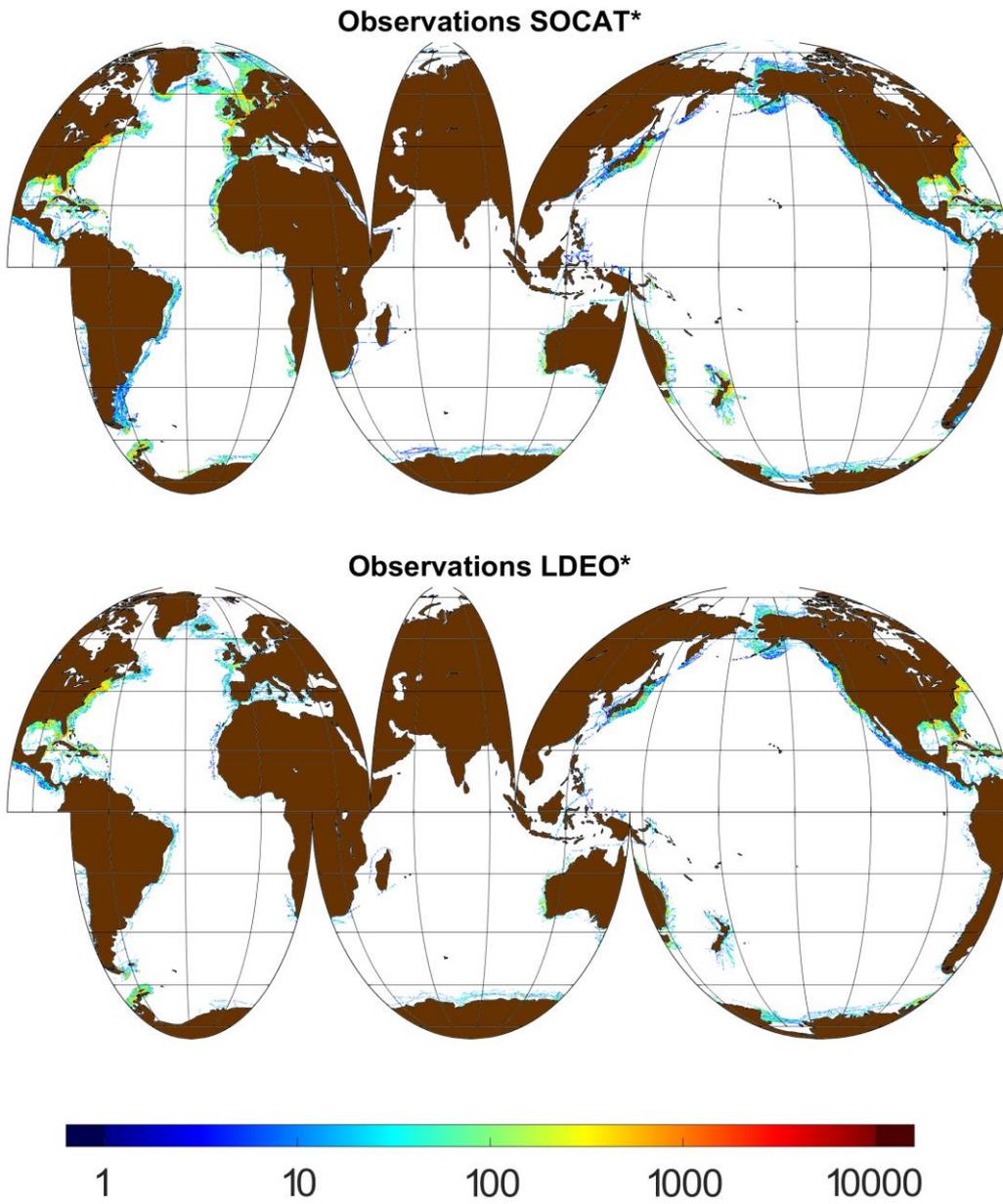


Figure 2: Number of observations contained in each 0.25° grid cell of the SOCAT\* (top) and LDEO\* (bottom) databases.

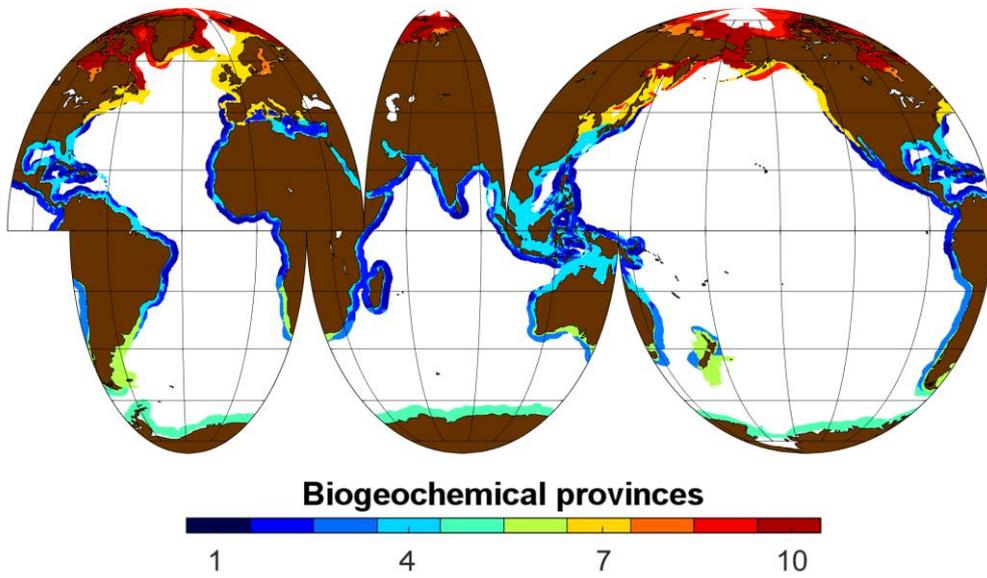
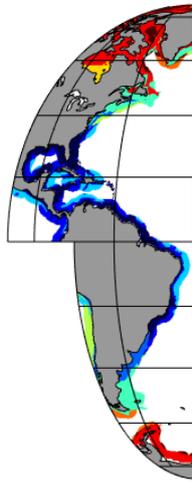


Figure 3: Map of the 10 different biogeochemical provinces generated by the artificial neural network method SOM-FFN.



1

Deleted:

Formatted: Font: 12 pt

Deleted: 1

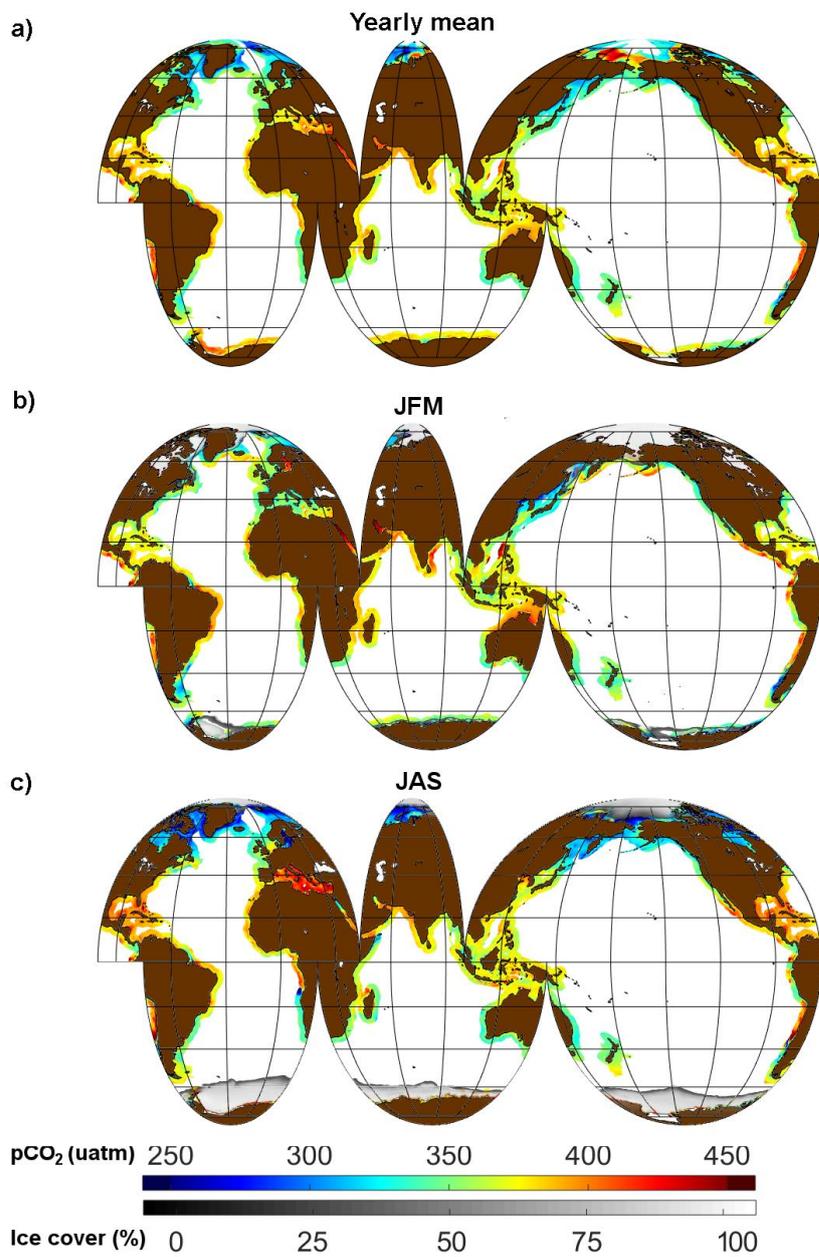


Figure 4: Climatological mean  $p\text{CO}_2$  for (a) the long-term averaged  $p\text{CO}_2$  (rainbow color scale) and sea-ice coverage (black-white color scale). The long-term average  $p\text{CO}_2$  corresponds to roughly the nominal year 2006, as the average was formed over the full analysis period from 1998 through 2015; (b) the months of January, February and March; and (c) the months of July, August and September.

Partial view of Figure 4 on the right side of the page, showing the right edge of the maps and color scales.

Deleted:

Formatted: Font: 12 pt

Deleted: 2

Deleted: 2014

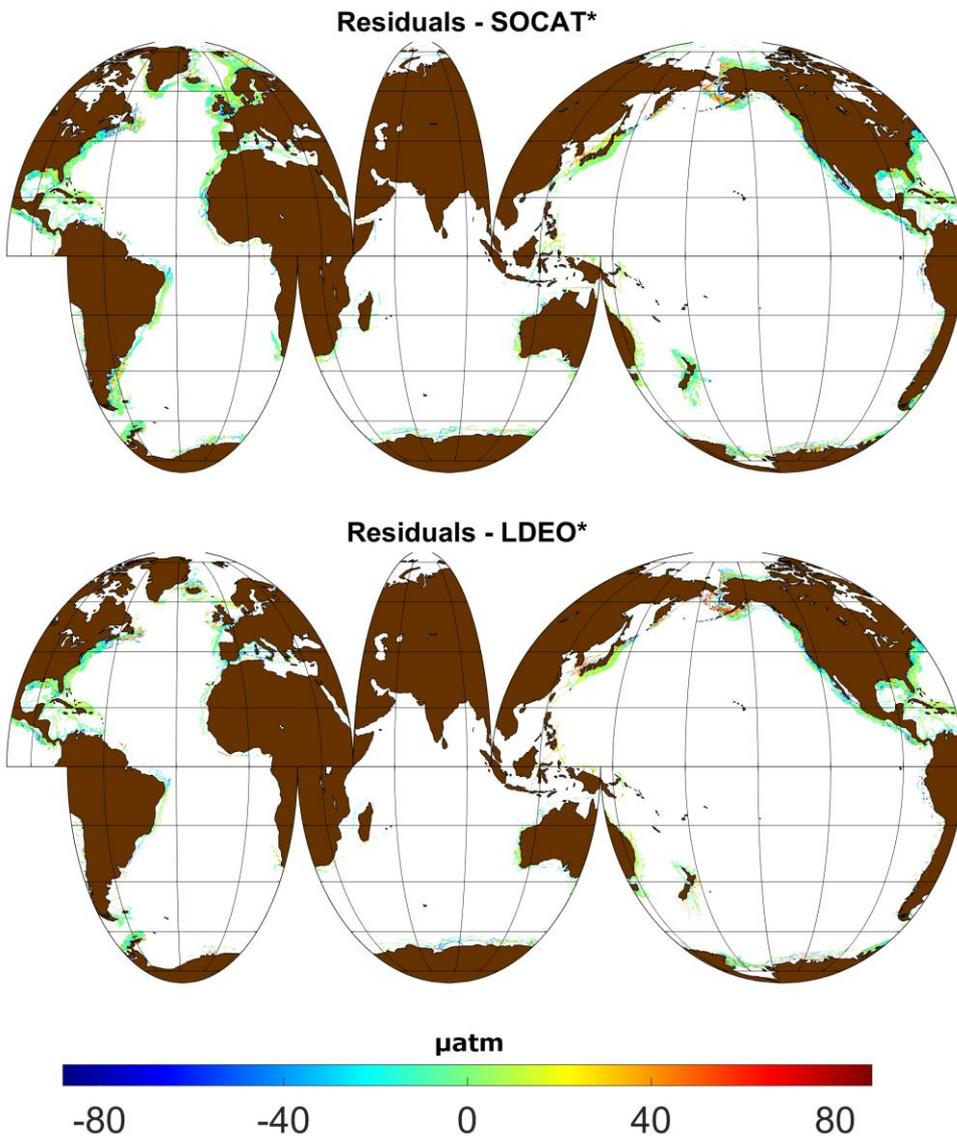


Figure 5: Mean residuals calculated as the difference between the SOM FFM  $pCO_2$  outputs and  $pCO_2$  observations from SOCAT\* (top) and LDEO\* (bottom).

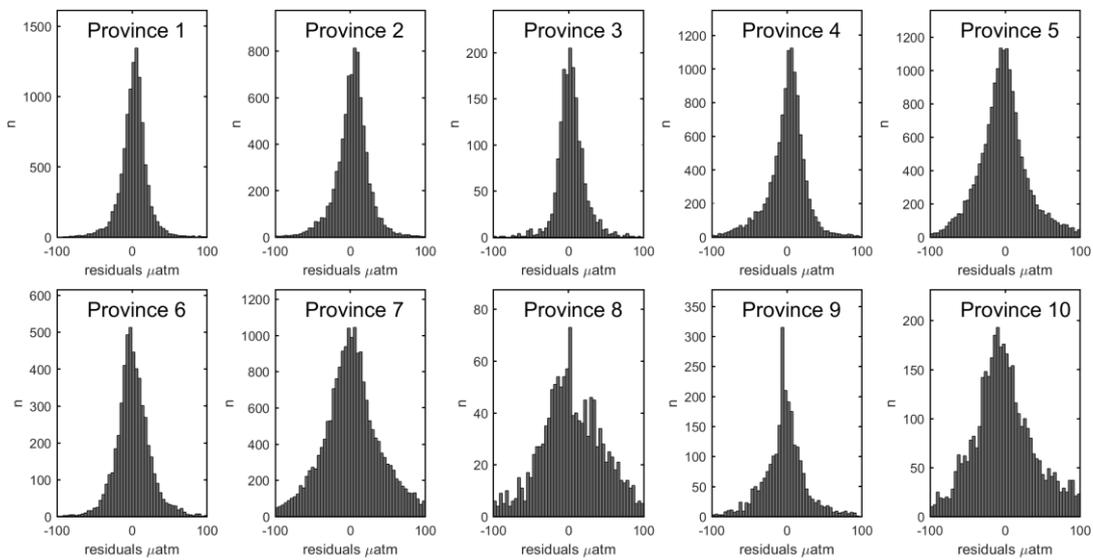
Formatted: Font: 12 pt

Formatted: Justified

Formatted: Subscript

Formatted: Subscript

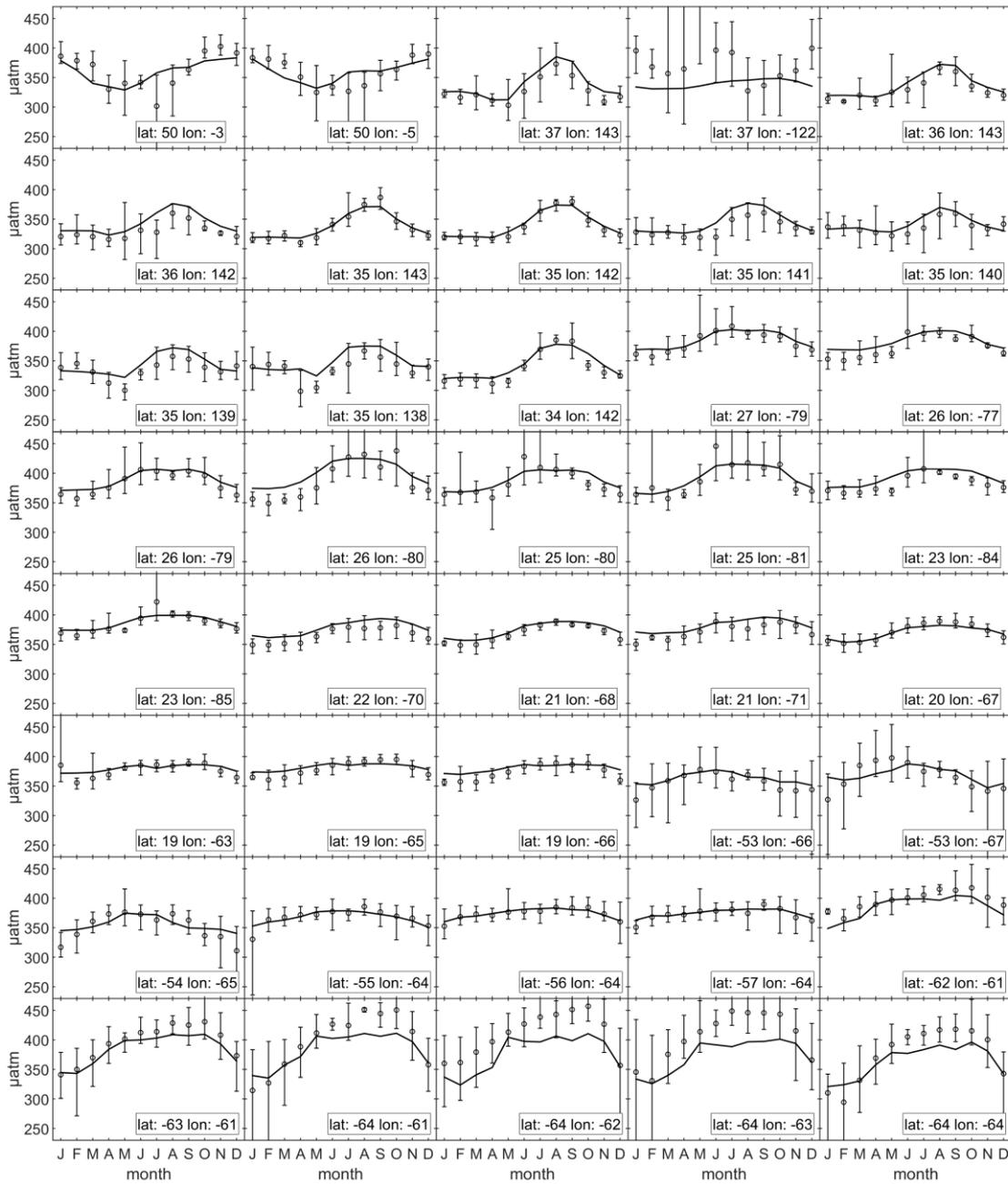
Formatted: Justified, Line spacing: 1,5 lines, Widow/Orphan control



Formatted: Font: 12 pt

Figure 6: Histograms reporting the distribution of residuals between observed (LDEO\*) and computed (SOM\_FFN) pCO<sub>2</sub> in each biogeochemical province.

Formatted: Subscript



Deleted:

Formatted: Font: 12 pt

Deleted: 3

Deleted: √2014

Figure 7: Climatological monthly mean pCO<sub>2</sub> extracted from the LDEO\* database (points) and generated by the artificial neural network (lines) for grid cells having more than 40 months of data. The error bars associated with the data represent the inter-annual variability, reported as the highest and lowest recorded values for a given month at a given location.

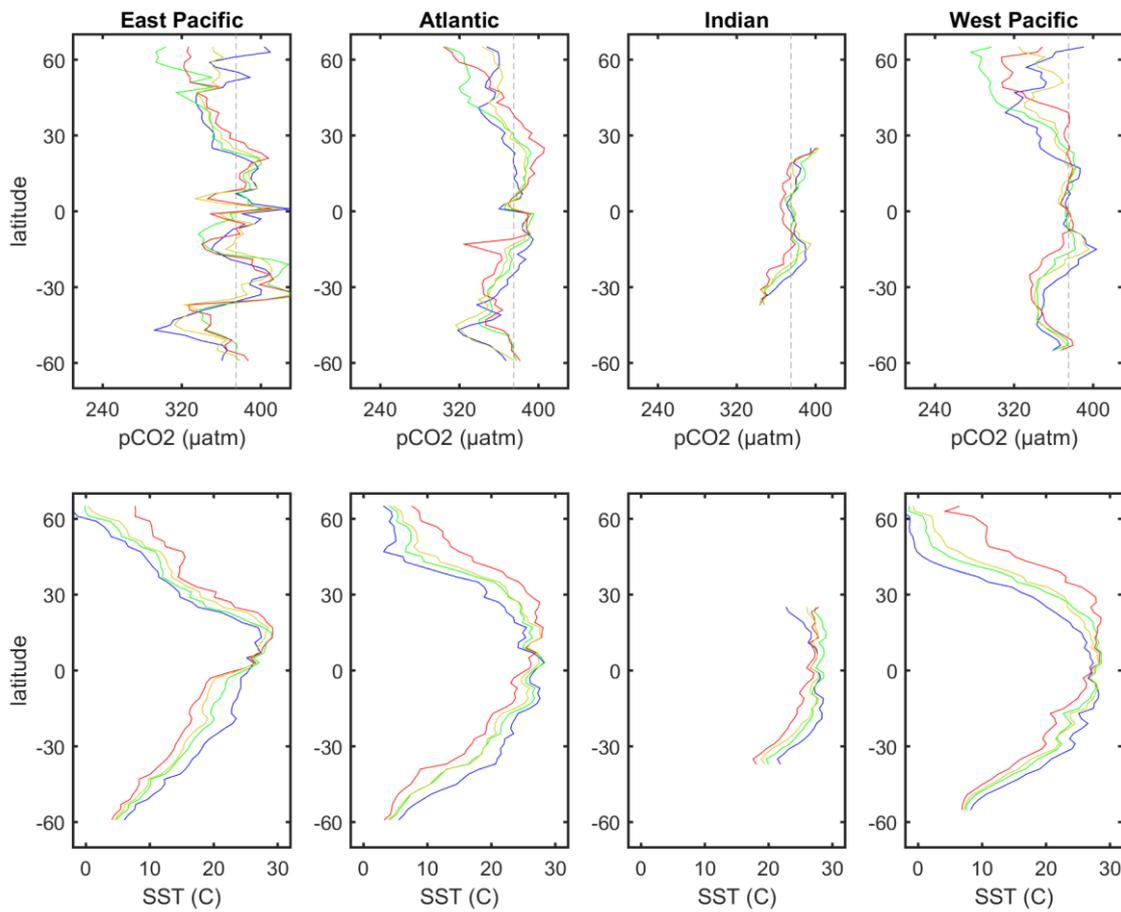
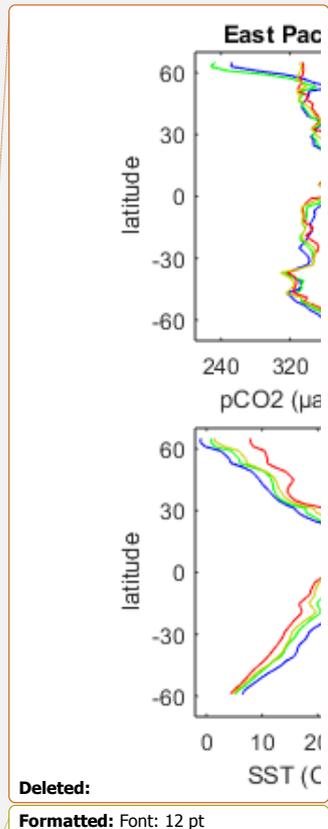


Figure 8: Seasonal-mean latitudinal profiles of  $p\text{CO}_2$  (top) and SST (bottom) for the continental shelves surrounding 4 oceanic basins. Blue lines: averages over the months of January, February and March; green lines: averages over the months of April, May and June; red lines: averages over the months of July, August and September; yellow lines: averages over the months of October, November and December. The dashed line in the top panels represents the average atmospheric  $p\text{CO}_2$  for year 2006.



Deleted:  
Formatted: Font: 12 pt

Deleted: 4

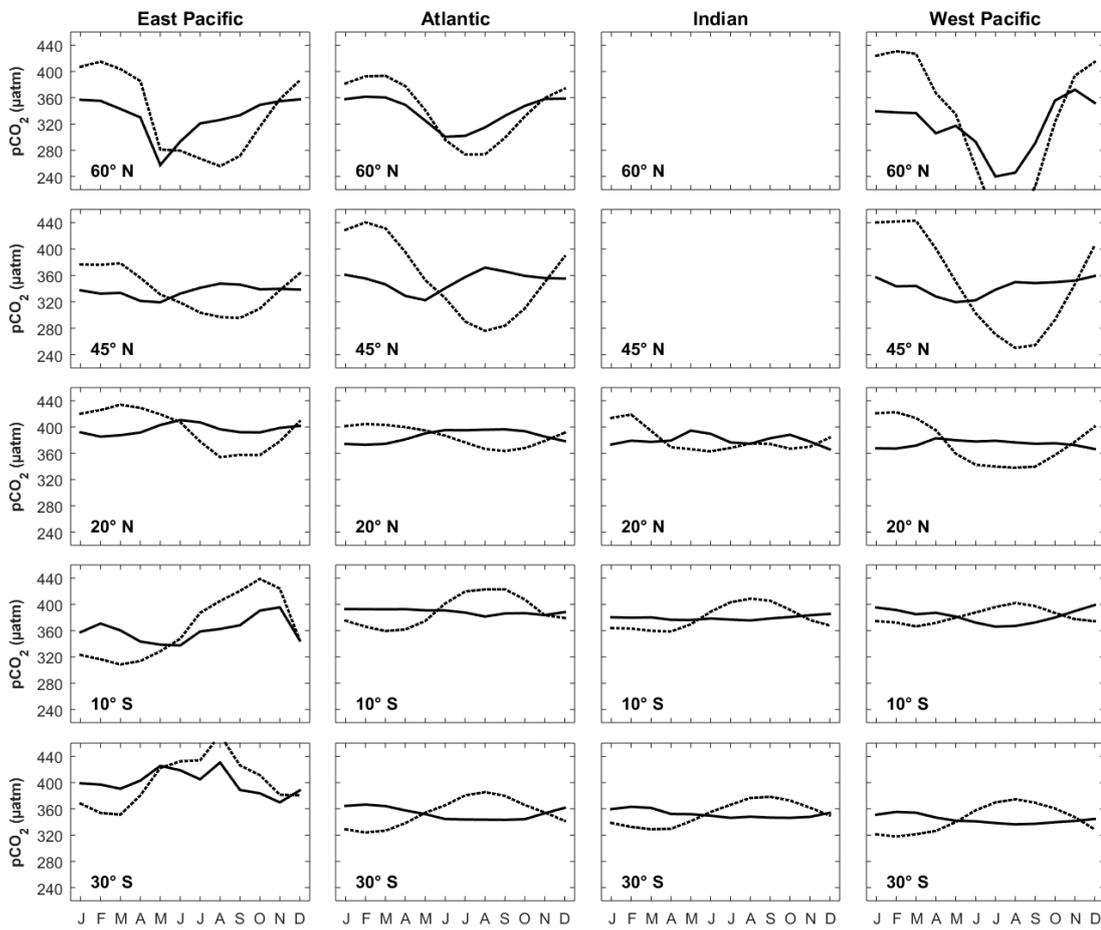
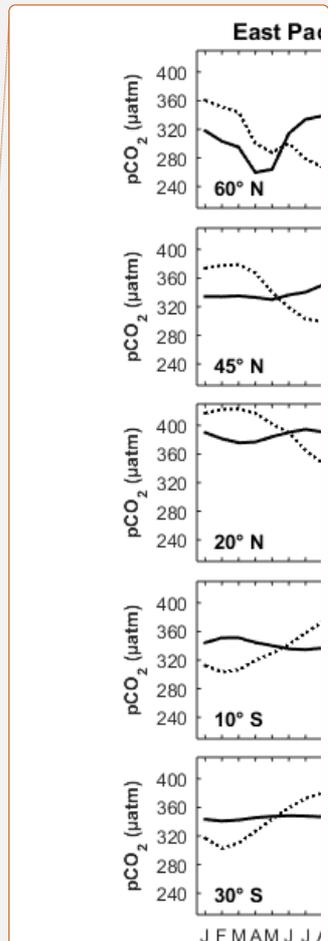


Figure 9: Seasonal cycle of observed (continuous lines) and temperature normalized pCO<sub>2</sub> (pCO<sub>2</sub>(SST<sub>mean</sub>) dashed lines) at 5 different latitudes in 4 oceanic basins.



Deleted:

Formatted: Font: 12 pt

Deleted: 5

Formatted: Subscript