



1FFNN-LSCE: A two-step neural network model for the 2reconstruction of surface ocean pCO₂ over the Global 3Ocean.

4

5Anna Denvil-Sommer¹, Marion Gehlen¹, Mathieu Vrac¹, Carlos Mejia²

6¹Laboratoire des Sciences du Climat et de l'Environnement (LSCE), Institut Pierre Simon Laplace (IPSL),

7CNRS/CEA/UVSQ/Univ. Paris-Saclay, Orme des Merisiers, Gif-Sur-Yvette, 91191, France

8²Sorbonne Université, CNRS, IRD, MNHN, Institut Pierre Simon Laplace (IPSL), Paris, 75005, France

9

10Correspondence to: Anna Denvil-Sommer (anna.sommer.lab@gmail.com)

11

12Abstract.

13A new Feed-Forward Neural Network (FFNN) model is presented to reconstruct surface ocean partial
14pressure of carbon dioxide (pCO₂) over the global ocean. The model consists of two steps: (1)
15reconstruction of pCO₂ climatology and (2) reconstruction of pCO₂ anomalies with respect to the
16climatology. For the first step, a gridded climatology was used as the target, along with sea surface salinity
17and temperature (SSS and SST), sea surface height (SSH), chlorophyll *a* (Chl), mixed layer depth (MLD),
18as well as latitude and longitude as predictors. For the second step, data from the Surface Ocean CO₂ Atlas
19(SOCAT) provided the target. The same set of predictors was used during step 2 augmented by their
20anomalies. During each step, the FFNN model reconstructs the non-linear relations between pCO₂ and the
21ocean predictors. It provides monthly surface ocean pCO₂ distributions on a 1°x1° grid for the period 2001-
222016. Global ocean pCO₂ was reconstructed with a satisfying accuracy compared to independent
23observational data from SOCAT. However, errors are larger in regions with poor data coverage (e.g. Indian
24Ocean, Southern Ocean, subpolar Pacific). The model captured the strong interannual variability of surface
25ocean pCO₂ with reasonable skills over the Equatorial Pacific associated with ENSO (El Niño Southern
26Oscillation). Our model was compared to three pCO₂ mapping methods that participated in the Surface
27Ocean pCO₂ Mapping intercomparison (SOCOM) initiative. We found a good agreement in seasonal and
28interannual variability between the models over the global ocean. However, important differences still exist
29at the regional scale, especially in the Southern hemisphere and in particular, the Southern Pacific and the
30Indian Ocean, as these regions suffer from poor data-coverage. Large regional uncertainties in
31reconstructed surface ocean pCO₂ and sea-air CO₂ fluxes have a strong influence on global estimates of
32CO₂ fluxes and trends.

33



341. Introduction.

35

36The global ocean is a major sink of excess CO₂ emitted to the atmosphere since the beginning of the
37industrial revolution. In 2011, the best estimate of the ocean inventory of anthropogenic carbon (C_{ant})
38amounted to 155 ± 30 PgC or 28% of cumulated total CO₂ emissions attributed the human activities since
391750 (Ciais et al., 2013). Between 2000 and 2009, the yearly average ocean C_{ant} uptake was 2.3 ± 0.7 PgC
40yr⁻¹ (Ciais et al., 2013). ~~These global estimates hide, however,~~ substantial regional and inter-annual
41fluctuations (Rödenbeck et al., 2015), which need to be quantified in order to track the evolution of the
42Earth's carbon budget (e.g. Le Quéré et al., 2018).

43

44 Until recently, most estimates of inter-annual air-sea CO₂ flux variability were based on atmospheric
45inversions (Peylin et al., 2005, 2013; Rödenbeck et al., 2005) or global ocean circulation models (Orr et al.,
462001; Aumont and Bopp, 2006; Le Quéré et al., 2010). However, models tend to underestimate the
47variability of air-sea CO₂ fluxes (Le Quéré et al., 2003), while atmospheric inversions suffer from a still
48sparse network of atmospheric CO₂ measurements (Peylin et al., 2013). These approaches are increasingly
49complemented by data-based techniques relying on *in situ* measurements of CO₂ fugacity (e.g.
50Landschützer et al., 2016; Rödenbeck et al., 2014, 2015; Takahashi et al., 2002, 2009, Landschützer et al.,
512013; Schuster et al., 2013; Nakaoka et al., 2013; Fay et al., 2014). These techniques rely on a variety of
52data-interpolation approaches developed to provide estimates in time and space of surface ocean pCO₂
53(Rödenbeck et al., 2015) such as statistical interpolation, linear and non-linear regressions, or model-based
54regressions or tuning (Rödenbeck et al., 2014, 2015). These methods have their advantages, ~~as well as~~
55disadvantages ~~and~~ are compared and discussed in Rödenbeck et al. (2015). This intercomparison did not
56allow identifying a single optimal technique, but rather pleaded in favour of exploiting the ensemble of
57methods.

58

59Artificial neural networks (ANN) have been widely used to reconstruct surface ocean pCO₂ (open ocean:
60Lefèvre et al., 2005; Friedrich and Oschlies, 2009b; Telszewski et al., 2009; Landschützer et al., 2013;
61Nakaoka et al., 2013; Zeng et al. 2014; coastal region: Laruelle et al., 2017). ANN fill the spatial and
62temporal gaps based on calibrated non-linear statistical relationships between pCO₂ and its oceanic and
63atmospheric drivers. The existing products usually present monthly fields with a 1°x1° spatial resolution
64and capture a large part of temporal-spatial variability. **Methods based on ANN are able to represent the**
65**large class of pCO₂-driver relationships, but they are sensitive to the number of data used in the training**
66**algorithm and can generate artificial variability in regions with sparse data coverage.**

67

68This study proposes an alternative implementation of a neural network applied to the reconstruction of
69surface ocean pCO₂ over the period 2001-2016. It belongs to the category of **Forward Feed Neural**



72 Networks (FFNN) and consists of a two-step approach: (1) the reconstruction of monthly climatologies of
73 global surface ocean $p\text{CO}_2$ based on data from Takahashi et al. (2009), and (2) the reconstruction of
74 monthly anomalies (with respect to the monthly climatologies) on a $1^\circ \times 1^\circ$ grid exploiting the Surface
75 Ocean CO_2 Atlas (SOCAT) (Bakker et al., 2016). The model is easily applied to the global ocean without
76 any boundaries between the ocean basins or regions. However, as mentioned before, it is still sensitive to
77 the observational coverage. This limitation is partly overcome by the two-step approach as the
78 reconstruction of monthly climatologies draws on a larger data set, thereby keeping FFNN output close to
79 realistic values. Furthermore, the reconstruction of monthly climatologies during the first step allows taking
80 into account a potential change in seasonal cycle in response to climate change when applied to time slices
81 or to model output providing the drivers, but no carbon cycle variables.

82 The remainder of this paper is structured as follows: section 2 introduces data sets used during this study
83 and describes the neural network; section 3 presents results for its validation and qualification, as well as a
84 comparison to three mapping methods part of the Surface Ocean $p\text{CO}_2$ Mapping intercomparison
85 (SOCOM) exercise (Rödenbeck et al., 2015). Results and perspectives are summarized in the last section.

86

87 2. Data and method.

88

89 2.1. Data.

90 The standard set of variables known to represent physical, chemical and biological drivers of surface ocean
91 $p\text{CO}_2$ – mean state and variability – (Takahashi et al., 2009; Landschützer et al., 2013) were used as input
92 variables (or predictors) for training the FFNN algorithm. These are sea surface salinity (SSS), sea surface
93 temperature (SST), mixed layer depth (MLD), chlorophyll *a* concentration (CHL), atmospheric CO_2 mole
94 fraction ($x\text{CO}_{2,\text{atm}}$). Based on Rodgers et al. (2009) who reported a strong correlation between natural
95 variations in dissolved inorganic carbon (DIC) and sea surface height (SSH), SSH was added as a new
96 driver to this list.

97 For the first step, the reconstruction of monthly climatologies, the Takahashi et al. (2009) monthly $p\text{CO}_2$
98 gridded climatology ($1^\circ \times 1^\circ$) was used as the target. The original climatology was constructed by an
99 advection-based interpolation method on a $4^\circ \times 5^\circ$ grid. It was interpolated on the $1^\circ \times 1^\circ$ SOCAT grid which
100 is also the final output for the FFNN.

101 For the second step, the observational data-base SOCAT v5 (Bakker et al., 2016) provided the target. We
102 used a gridded version of this dataset that was derived by combining all SOCAT data collected within a
103 $1^\circ \times 1^\circ$ box during a specific month. SOCAT v5 represents global observations of sea surface fugacity of CO_2
104 ($f\text{CO}_2$) over the period 1970 to 2016. It includes data from moorings, ships and drifters. These data are
105 distributed irregularly over the global ocean with 188274 gridded measurements over the Northern
106 hemisphere and 76065 over the Southern hemisphere. In order to ensure a satisfying spatial and temporal
107 data coverage, we limited the reconstruction to the period 2001–2016, which represents ~77% of the data



base (Fig. 1(a)).

The following formula is used to convert $f\text{CO}_2$ to $p\text{CO}_2$ (Körtzinger et al., 1999):

$$f\text{CO}_2 = p\text{CO}_2 \exp\left(p \frac{B + 2\delta}{RT}\right), \quad (1)$$

where $f\text{CO}_2$ and $p\text{CO}_2$ are in μatm , p is the total pressure (Pa), $R=8.314 \text{ JK}^{-1}$ is the gas constant, T is the absolute temperature (K). Parameter B ($\text{m}^3\text{mol}^{-1}$) is estimated as: $B = (-1636.75 + 12.0408 T - 3.27957 \cdot 10^{-2} T^2 + 3.16528 \cdot 10^{-5} T^3) \cdot 10^{-6}$. The parameter δ is the cross virial coefficient ($\text{m}^3\text{mol}^{-1}$): $\delta = (57.7 - 118T) \cdot 10^{-6}$. The total pressure is from the Jena data-base (6h, $5^\circ \times 5^\circ$) (<http://www.bgc-jena.mpg.de/CarboScope/?ID=s>).

Monthly global observed physics reprocessed products distributed through the Copernicus Marine

Environment Monitoring Service (CMEMS) ($0.25^\circ \times 0.25^\circ$) (http://marine.copernicus.eu/services-portfolio/access-to-products/?option=com_csw&view=details&product_id=MULTIOBS_GLO_PHY_REP_015_002) were used for SSS,

SST and SSH. The GlobColour project provided monthly CHL distributions at $1^\circ \times 1^\circ$ resolution (http://www.globcolour.info/products_description.html). For MLD, daily data from the “Estimating the Circulation and Climate of the Ocean” (ECCO2) project Phase II, at $0.25^\circ \times 0.25^\circ$ resolution (Menemenlis et al., 2008) were used. For $x\text{CO}_2$ atmospheric, the 6h data from Jena CO_2 inversion s76_v4.1 on a $5^\circ \times 5^\circ$ grid were selected (<http://www.bgc-jena.mpg.de/CarboScope/?ID=s>). Finally, an ice mask based on daily “Operational Sea Surface Temperature and Sea Ice Analysis” (OSTIA) with a gridded $0.05^\circ \times 0.05^\circ$ resolution (Donlon et al., 2011) was applied.

MLD and CHL were log-transformed before their use in the FFNN algorithm because of their skewed distribution. In regions with no CHL data (high latitudes in winter) $\log(\text{CHL}) = 0$ was applied. It does not introduce discontinuities since $\log(\text{CHL})$ is close to zero in the adjacent region.

All data were averaged or interpolated on a $1^\circ \times 1^\circ$ grid and, depending on the resolution of the data set,

averaged over the month. It is worth noting that all data sets have to be normalized (i.e. centered to zero-mean and reduced to unit standard deviation) before their use in the FFNN algorithm, for example:

$$\text{SSS}_n = \frac{\text{SSS} - \bar{\text{SSS}}}{\text{std}(\text{SSS})}.$$

Normalization ensures that all predictors fall within a comparable range and therefore avoids giving more weight to predictors with large variability ranges (Kallache et al., 2011).

As surface ocean $p\text{CO}_2$ also varies spatially, geographical positions (lat, lon) were included as predictors. In order to normalize (lat, lon) the following transformation is proposed:

$$\text{lat}_n = \sin(\text{lat})$$



$$lon_n1 = \sin(lon)$$

$$lon_n2 = \cos(lon)$$

Two functions *sin* and *cos* for longitudes are used to preserve its periodical 0 to 360 degrees behavior and thus to consider the difference of positions before and after the 0° longitude. For step 2, data required for training were co-located at the SOCAT data positions that are used as target for the FFNN model. Details are provided in the next section.

147

1482.2. Method.

149

150a) Network configuration and evaluation protocol

151

In this work we use Keras, a high-level neural network Python library (“Keras: The Python Deep Learning library”, Chollet, 2015; <https://keras.io>) to build and train the FFNN models. The identification of an optimal configuration is the first step in the FFNN model building. This includes: the choice of number and size of hidden layers (i.e., intermediate layers between input and output layers), connection type, activation functions, loss function and optimization algorithm, as well as the learning rate and other low-level parameters. Based on a series of tests and their statistical results (RMS, correlation, bias) a hyperbolic tangent was chosen as an activation function for neurons in hidden layers, and a linear function for the output layer. As optimization algorithm the mini-batch gradient descent or RMSprop was used (adaptive learning rates for each weight, Chollet, 2015; Hinton et al., 2012). The number of layers and neurons depends on the problem. For totally connected layers (i.e., a neuron in a hidden layer is connected to all neurons in the precedent layer and connects all neurons in the next one), the case here, it is enough to have only one single hidden layer but two or more can help the approximation of complex functions (or complex relations between the input and the output of the problem).

165

The number of the FFNN layers and number of neurons depends on one side on the complexity of the problem: the more layers and neurons, the better the accuracy of output. However, the size also depends on the number of patterns (data) used for training. There is a well-known empirical rule advising to have a factor of 10 between number of patterns (data) and number of connections, or weights to adjust. This limits the size, the number of parameters and incidentally the number of neurons, of the FFNN. This empirical rule was followed in this study.

172

173(1) Step 1: reconstruction of monthly climatologies

FFNN reconstructs a monthly surface ocean pCO₂ climatology as a nonlinear function of SSS, SST, SSH, Chl, MLD and geographical position (longitude, latitude):



$$pCO_{2,n} = (SSS_n, SST_n, SSH_n, Chl_n, MLD_n, lon_n, lat_n) \quad (2)$$

Surface ocean pCO_2 from Takahashi et al. (2009) provided the target. The data set was divided into 50% for FFNN training and 25% for its evaluation. This 25% did not participate in the training. This set is used to monitor process performance and drive convergence. The remaining 25% (each 4th point) of the data set were used after training for the FFNN model validation. More details about the FFNN training process can be found in Rumelhart et al. (1986) and Bishop (1995). Validation and evaluation data sets were chosen quasi-regularly in space and time to take into account all regions and seasonal variability. In order to improve the accuracy of the reconstruction, the model was applied separately for each month. Tests with one model for 12 months showed a slight decrease in accuracy (not presented here). We have developed a FFNN model with 5 layers (3 hidden layers). About 17500 data were available for each month to train the model, resulting in monthly FFNN models with about 1856 parameters.

187

(2) Step 2: reconstruction of anomalies

During the second step, pCO_2 anomalies were reconstructed as a nonlinear function of SSS, SST, SSH, Chl, MLD, xCO_2 and their anomalies, as well as geographic position:

$$pCO_{2,n,anom} = (SSS_n, SST_n, SSH_n, Chl_n, MLD_n, xCO_{2,n}, SSS_{anom,n}, SST_{anom,n}, SSH_{anom,n}, Chl_{anom,n}, MLD_{anom,n}, xCO_{2,anom,n}, lon_n, lat_n) \quad (3)$$

Surface ocean pCO_2 anomalies computed as the differences between collocated pCO_2 values based on SOCAT observations and monthly pCO_2 climatologies reconstructed during the first step provided the targets:

$$pCO_{2,anom} = pCO_{2,SOCAT} - pCO_{2,clim,FFNN} \quad (4)$$

The set of target data was again divided into 50% for the training algorithm, 25% for evaluation and 25% for model validation. As in step (1) the model was trained separately for each month. There were thus 12 models sharing a common architecture but trained on different data. At this step, in order to increase the amount of data during training and to introduce information on the seasonal cycle, the model was trained using as a target pCO_2 data from the month in question as well as those from the previous and following month during the entire period 2001–2016. Figures 1 (b) and 1 (c) show an example of data distribution for the sole months of January over the period 2001–2016 (Fig. 1 (b)) and for the three months time-window December–January–February 2001–2016 used in the training algorithm of the January FFNN model (Fig. 1 (c)). In this particular example, the choice of three months provided a better cover of the region and doubled the number of data at high latitudes.

206

7K-fold cross-validation was used for evaluation and validation of the FFNN architecture. Cross-validation relied on K=4 different subsampling of the data set to draw 25% of independent data for validation (Fig. 209S1). Each sampling was tested on 5 runs of the FFNN for each month. Each of these 5 runs is characterized



209by different initial values that are chosen automatically. From these 5 results, the best was chosen based on
210root-mean-square-error (RMSE), r^2 and bias.

211
212The final model architecture had 3 layers (1 hidden layer). About 10000 samples were available for training
213for each month, thus, a model with 541 parameters was developed. Note that a higher number of
214parameters did not show a significant improvement of accuracy (not shown).

215
216b) Reconstruction of surface ocean pCO_2
217The previous section presented the development of a FFNN model for the reconstruction of global surface
218ocean pCO_2 , and the estimation of its accuracy. It allowed to identify the “optimal” FFNN architecture for
219the reconstruction of surface pCO_2 and its validation. This FFNN model was used to provide the final
220product for scientific analysis and comparison with other mapping approaches. In order to provide the final
221output, the selected FFNN architecture is trained on all available data: 100% of data for training, 100% for
222evaluation and 100% for validation. The network was executed 5 times (different initial values) and the best
223model was selected based on validation results considering root-mean-square-error (RMSE), correlation
224and bias computed between network output and SOCAT derived surface ocean pCO_2 data. The final model
225output is referred to as the FFNN-LSCE product.

226
2272.3. Computation of sea-air CO_2 fluxes.

228Sea-air CO_2 flux f was calculated following Rödenbeck et al. (2015) as:

$$229 \quad f = k p L \left(pCO_2 - pCO_2^{atm} \right) \quad (5)$$

230

231where k is the piston velocity estimated according to Wanninkhof (1992):

$$232 \quad k = \Gamma u^2 \left(Sc^{CO_2} / Sc^{Ref} \right)^{-0.5} \quad (6)$$

233The global scaling factor Γ was chosen as in Rödenbeck et al. (2014) with the global mean CO_2 piston
234velocity equaling to 16.5 cm/h. Sc corresponds to the Schmidt number estimated according to Wanninkhof
235(1992). The wind speed was computed from 6-hourly NCEP wind speed (Kalnay et al., 1996). ρ stands
236for seawater density in (4) and L for temperature-dependent solubility (Weiss, 1974). pCO_2 corresponds to
237the surface ocean pCO_2 output of the mapping method. pCO_2^{atm} was derived from the atmospheric CO_2
238mixing ratio fields provided by the Jena inversion (<http://www.bgc-jena.mpg.de/CarboScope/>).

239

2403. Results.

241

2423.1. Validation.

243The subset of data used for network validation, that is 25% of the total, represents independent observations



as they did not participate in training. The skill of the FFNN to reconstruct monthly climatologies of surface ocean $p\text{CO}_2$, was assessed by comparing collocated reconstructed $p\text{CO}_2$ and corresponding values from Takahashi et al. (2009). The global climatology was reconstructed with a satisfying accuracy during step 1 with a RMSE of $0.17 \mu\text{atm}$ and r^2 of 0.93. Model output of step 2 was assessed by K-fold cross validation as presented before: K=4 different subsamplings of independent data were drawn from the data set and the network was run 5 times on each subsampling. From these 20 results the best one was chosen based on RMSE, r^2 and bias. The combination of the four best model output was used for the statistical analysis summarized in Table 1. Metrics were computed over the full period (2001-2016) and with reference to SOCAT observations (independent data only). At the global scale, the analysis yielded a RMSE of $\sim 17.97 \mu\text{atm}$, while the absolute bias was $11.52 \mu\text{atm}$ and r^2 0.76. These results are comparable to those obtained by Landschützer et al. (2013) for the assessment of a surface ocean $p\text{CO}_2$ reconstruction based on an alternative neural network-based approach. The RMSE between SOCAT data and the climatology of $p\text{CO}_2$ from Takahashi et al. (2009) equals $41.87 \mu\text{atm}$, larger than errors computed for the regional comparison between FFNN and SOCAT (Table 1).

258

Figure 2 (a) shows the time mean difference between the estimated $p\text{CO}_2$ and $p\text{CO}_2$ from SOCAT v5 data used for validation $\text{mean}_t(p\text{CO}_{2,i,j,\text{FFNN}} - p\text{CO}_{2,i,j,\text{SOCAT}})$. Large differences occurred at high latitudes, in equatorial regions, along the Gulf Stream and Kuroshio currents – the regions with strong horizontal gradient of $p\text{CO}_2$. Moreover the standard deviation of residuals (Figure 2 (b)) in these regions was larger indicating that the model fails to accurately reproduce the temporal variability. The reduced skill of the model in these regions reflects the poor data coverage along with a strong seasonal variability (e.g. Southern Ocean) and/or high kinetic energy (e.g. Southern Ocean, Kuroshio and Gulf Stream currents) (Fig. 1 (a)). At the scale of ocean regions, (Table 1) the largest RMSE and bias were computed for the Pacific Subpolar ocean (RMSE = $34.77 \mu\text{atm}$, bias = $23.12 \mu\text{atm}$), while the lowest correlation coefficient was obtained for the equatorial Atlantic ocean ($r^2 = 0.57$). These low scores directly reflect low data density and are to be contrasted with those obtained over regions with better data coverage (e.g. Subtropical Pacific: RMSE = $15.86 \mu\text{atm}$, bias = $9.9 \mu\text{atm}$, $r^2 = 0.77$ or Subpolar Atlantic: RMSE = $22.99 \mu\text{atm}$, bias = $15.04 \mu\text{atm}$, $r^2 = 0.76$). Despite large time mean differences computed over the eastern Equatorial Pacific, scores are satisfying at the regional scale indicating error compensation by improved scores over the western basin. Scores are low in the Southern hemisphere (Table 1) and time mean differences are large (Fig. 2 (a)) reflecting sparse data coverage (Fig. 1 (a)).

275

276 3.2. Qualification.

This section presents the assessment of the final time series of reconstructed surface ocean $p\text{CO}_2$. The time series was computed using the best monthly models as described in section 2.2, as well as 100% of data for



learning, evaluation and validation.

Results of the FFNN-LSCE mapping model were compared to three published mapping methods which participated in the “Surface Ocean pCO₂ Mapping Intercomparison” (SOCOM) exercise presented in Rödenbeck et al. (2015) (<http://www.bgc-jena.mpg.de/SOCOM/>). These methods are: (1) Jena-MLS (Rödenbeck et al., 2014), a statistical interpolation scheme (data-driven mixed-layer scheme; principal drivers: ocean-internal carbon sources/sinks, SST, wind speed, mixed-layer depth climatology, alkalinity climatology); (2) JMA-MLR (Iida et al., 2015), based on multi-linear regressions with SST, SSS and Chl *a* as independent variables, and (3) ETH-SOMFFN (Landschützer et al., 2014), a combined two-step neural network model with SST, SSS, MLD, Chl *a*, xCO₂ as drivers. Qualification followed methods and analyses proposed by Rödenbeck et al. (2015). The time series of pCO₂ and sea-air flux CO₂ (*f*) were assessed over 17 biomes defined by Fay and McKinley (2014) (Fig. 3, Table 2). These biomes were derived based on coherence in SST, Chl *a*, ice fraction, maximum MLD and represent regions of coherent biogeochemical dynamics.

291

We followed the protocol and diagnostics proposed in Rödenbeck et al. (2015) for the comparison of the mapping methods between each other, respectively to observations. The following diagnostics were computed: (1) the relative interannual variability (IAV) mismatch R^{iav} (in %) and (2) the amplitude of interannual variations. The relative interannual variability (IAV) mismatch R^{iav} (in %) is the ratio of the mismatch amplitude M^{iav} of the difference between the model output and observations (its temporal standard deviation) and the mismatch amplitude $M^{iav}_{benchmark}$ of the “benchmark”. The $M^{iav}_{benchmark}$ was derived from the mean seasonal cycle of the corresponding model output where the trend of increasing yearly atmospheric pCO₂ was added (see details in Rödenbeck et al., 2015). It corresponds to a climatology corrected for increasing atmospheric CO₂, but without interannual variability.

$$R^{iav} = \frac{M^{iav}}{M^{iav}_{benchmark}} * 100\% \quad (6)$$

where

$$M^{iav} = std \left(mean \left(pCO_{2,Model} - pCO_{2,SOCAT} \right) \right),$$

$$M^{iav}_{benchmark} = std \left(mean \left(D_{season} \right) \right),$$

where “mean” is a mean over the region and year and

$$D_{season} = \left(pCO_{2,SS} + trend \left(CO_{2,atm} \right) \right) - pCO_{2,SOCAT},$$

pCO_{2,SS} is the seasonal cycle of pCO₂ from the corresponding mapping method. CO_{2,atm} estimates from xCO₂ Jena CO₂ inversion s76_v4.1 were used.

R^{iav} provides information on the capability of each method to reproduce the IAV compared to observations: a smaller R^{iav} stands for better fit compared to the reference. The amplitude of the interannual variations,



311 A^{lav} , of sea-air flux of CO_2 (its 2-month running mean). A^{lav} is estimated as the temporal standard deviation
312 over the period.

313

314 3.2.1. Interannual variability.

315

316 The time series of [global](#) averaged surface ocean pCO_2 over the period 2001-2016 are presented in Figure 4
317 for FFNN-LSCE and the three other models. Surface ocean pCO_2 (μatm) varied between 4 mapping
318 methods in the range of $\pm 7 \mu atm$ (Fig. 4 (a)). Modeled pCO_2 values were at the lower end for ETH-
319 SOMFFN and JMA-MLR, while FFNN-LSCE and Jena-MLS13 computed higher values. The same
320 behavior was found for 12-month running mean time series (Fig. 4 (b)). Figure 4 (c) shows the 12-month
321 running mean of difference between computed pCO_2 and SOCAT data (model – SOCAT) over the globe.
322 JMA-MLR mostly underestimated observed pCO_2 with a strong interannual variability of the misfit,
323 especially at the end of the period with up to $-5 \mu atm$. The difference between ETH-SOMFFN output and
324 SOCAT data fluctuates in the range of $\pm 1 \mu atm$, with an increase in amplitude up to $-2 \mu atm$ from 2010
325 onward. Jena-MLS13 overestimated observations with the difference in the range of 0-1 μatm . The
326 difference between FFNN-LSCE and SOCAT varies around zero between -0.7 and 1 μatm .

327

328 The model was assessed next at biome scale. Results for all biomes are presented in the supplementary
329 material (Fig. S2, S3, S4). Two biomes with contrasting dynamics are discussed hereafter in greater detail:
330 (1) the Equatorial East Pacific (biome 6) characterized by a strong IAV of surface ocean pCO_2 and sea-air
331 CO_2 fluxes in response to ENSO, the El Niño Southern Oscillation (Feely et al., 1999; Rödenbeck et al.,
332 2015), and (2) North Atlantic Permanently Stratified biome (biome 11) with a well-marked seasonal cycle,
333 but little IAV (Schuster et al., 2013). Results for these biomes are presented in Figure 5.

334

335 Biome 6 is relatively well-covered by observations and represents a key region for testing the skill of the
336 model to reproduce the observed strong IAV linked to ENSO. El Niño events are characterized by positive
337 SST anomalies, reduced upwelling and decreased surface ocean pCO_2 values. These episodes could be
338 identified in all model time series (Fig. 5 (a)) with reduced pCO_2 levels in 2004/2005 and 2006/2007 (weak
339 El Niño), 2002/2003 and 2009/2010 (moderate El Niño), and 2015/2016 (strong El Niño). JMA-MLR (blue
340 curve) tended to underestimate pCO_2 during weak El Niño events. It was underestimated during the La
341 Niña 2011-2012 event by Jena-MLS13. FFNN-LSCE and ETH-SOMFFN, both based on a neural network
342 approach yielded similar results despite differences in network architecture and predictor data sets.

343

344 Data coverage is particularly high over Biome 11 (Fig. 5 (b), (d), (f)). The seasonal cycle in this biome is
345 dominantly driven by temperature. Modeled seasonal variability showed a good agreement across the
346 ensemble of methods (Fig. 5(b)) with an increase in spring-summer and a decrease in autumn-winter.



347 However, the amplitude can be different by up to 10 μatm between different models. The seasonal
348 amplitude of pCO_2 computed by JMA-MLR increased from smaller values at the beginning of the time
349 series to higher ones in the middle of the period 2005-2012. The variability of seasonal amplitude was the
350 highest for Jena-MLS13 in line with the 12-month running mean time series (Fig. 5 (d)). Again, similar
351 seasonal amplitude and year-to-year variability of surface ocean pCO_2 were obtained with FFNN-LSCE
352 and ETH-SOMFFN (Fig. 5 (b), (d)). The yearly pCO_2 mismatch (Fig. 5 (f)) shows that observed surface
353 ocean pCO_2 was underestimated by JMA-MLR at the beginning and at the end of the period by up to -6
354 μatm , and overestimated during 2007-2011 by up to 8 μatm . Jena-MLS13 shows mostly positive
355 differences in the range 0-2 μatm over the full period. FFNN-LSCE and ETH-SOMFFN vary around zero
356 and between -2 – 2 μatm , being close to each other.

357

358 3.2.2. Sea-air CO_2 flux variability.

359

360 Sea-air exchange of CO_2 was estimated using the same gas exchange formulation (4) and wind data speed
361 (6-hourly NCEP wind speed) for each mapping data (Rödenbeck et al., 2005). It is worth noting that the
362 sea-air flux is sensitive to the choice of wind speed data set (Roobaert et al., 2018).

363

364 Figure 6 (a) presents the global 12-month running mean of the air-sea CO_2 flux for four mapping methods.
365 All models showed an increase in CO_2 uptake in response to increasing atmospheric CO_2 levels, albeit with
366 a strong between-model variability in multi-annual trends. There is less agreement between the methods
367 compared to reconstructions of surface ocean pCO_2 variability (Fig. 4 (b)). This results from the
368 contribution of uncertainties in air-sea CO_2 flux estimations over regions with poor data-coverage (mostly
369 in the South Hemisphere: South Pacific, South Atlantic, Indian Ocean, South Ocean; see Fig. S5).
370 Nevertheless, the relative IAV mismatch was less than 30% for all methods (Fig. 6 (b)), suggesting a
371 reasonable fit to observational data. The relative IAV mismatch is, however, a global score and it is biased
372 towards regions with good data coverage (Rödenbeck et al., 2015). The time series reconstructed in this
373 study is too short to capture decadal variations and in particular the strengthening of the sink from 2000
374 onward (Landschützer et al., 2016). FFNN-LSCE computed a slowdown of ocean CO_2 uptake between
375 2010 and 2013 with a flux of $\sim -1.8 \text{ GtC yr}^{-1}$ compared to $\sim -2.2 \text{ GtC yr}^{-1}$ for ETH-SOMFFN. A leveling-off
376 was also found for JMA-MLR, albeit shifted in time. In general, the amplitudes of reconstructed CO_2 fluxes
377 across all four methods agreed within 0.2-0.36 PgC/yr . The weighted mean of IAV (horizontal line in Fig. 6
378 (b)) computed from the four methods included here was 0.253 PgC/yr . This value is close to the one of
379 Rödenbeck et al. (2015) for the complete ensemble of SOC models (0.31 PgC/yr) estimated for the
380 period 1992-2009. The largest amplitude was obtained for ETH-SOMFFN, $\sim 0.348 \text{ PgC/yr}$. On the other
381 hand, FFNN-LSCE has the smallest amplitude with 0.206 PgC/yr . Jena-MLS13 and JMA-MLR lie very
382 close to the weighted mean value with 0.257 PgC/yr and 0.221 PgC/yr , respectively. The weighted mean



and the dispersion of individual models around it, reflect the period of analysis (2001-2015, ETH-SOMFFN output provided up to 2015) and the total number of models contributing to it (see for comparison Rödenbeck et al., 2015). As such it does not provide information on the skill of any particular model.

The interannual variability of reconstructed sea-air CO₂ fluxes (12-month running mean) showed a good agreement for biome 6 (East Pacific Equatorial, Fig. 7 (a)). A small discrepancy was found at the beginning of the period. A strong increase was computed by Jena-MLS13 for 2010-2014 that was also identified on pCO₂ variability (Fig. 5 (a)). Despite this Jena-MLS13 has a low relative IAV (26.24%). This confirms a tendency mentioned in Rödenbeck et al. (2015) that mapping products with a small IAV show larger amplitude. FFNN-LSCE and ETH-SOMFFN yielded comparable results (Fig. 7 (a), (c)) with relative IAV mismatches of 46.13% and 53.26%, respectively, and with amplitudes ~ 0.03 PgC/yr. Interannual variability reproduced by JMA-MLR falls within the range of the other models (Fig. 7 (c)), but with a R^{IAV} of ~68.46%.

Reconstructed sea-air CO₂ fluxes over the North Atlantic Subtropical Permanently Stratified region (biome 11) show large between model differences in amplitudes and variability. The two models based on a neural network show again a good agreement with R^{IAV} of 17% for FFNN-LSCE and 20% for ETH-SOMFFN. Jena-MLS13 produced a strong seasonal variability (Fig. 7 (b)) up to 0.06 PgC/yr, and small R^{IAV} of ~11%. JMA-MLR did not reproduce a decrease of sea-air CO₂ at the middle of period by up to 0.02 PgC/yr (Fig. 7 (b)). The model is characterized by a R^{IAV} of 46.48% and an amplitude of 0.013 PgC/yr.

3.3. Sea-air CO₂ flux trend.

The long-term trend of sea-air CO₂ fluxes is dominantly driven by the increase in atmospheric CO₂ (see Fig. S7). On shorter time scales, such as for the period 2001-2016, the interannual variability at regional scale reflects natural mode of climate variability and local oceanographic dynamics (Heinze et al., 2015).

Figure 8 shows the linear trends of sea-air CO₂ fluxes for FFNN-LSCE (a), Jena-MLS13 (b), ETH-SOMFFN (c) and JMA-MLR (d). A total negative trend was computed for all models, albeit with large regional contrasts, and FFNN-LSCE falls within the range: Jena-MLS13, -0.0028 PgC/yr; FFNN-LSCE, -0.0032 PgC/yr; JMA-MLR, -0.0037 PgC/yr; ETH-SOMFFN, -0.0059 PgC/yr. FFNN-LSCE computed negative trends over most of the Atlantic basin, Indian Ocean and South of 40°S, which contrasts with decreasing fluxes over the Pacific and locally in the Antarctic Circumpolar current. At first order this broad regional pattern is found in all models. Regional maxima and minima are, however, more pronounced in Jena-MLS13 (Fig. 8 (b)) and ETH-SOMFFN (Fig. 8 (c)), while a patchy distribution at sub-basin scale is



419 diagnosed for JMA-MLR.

420

421 The agreement in sign of computed linear trends from four models is presented in Fig. 9. Over most of the
422 ocean, all four models show very close sea-air CO₂ tendency. In the Indian Ocean (biome 14), on the other
423 hand a positive trend was computed for JMA-MLR (0.0004 PgC/yr) while the three other models present a
424 negative trend. These differences between models were also found in the Pacific Ocean, especially the
425 Southern Pacific. In the Eastern Equatorial Pacific region (biome 6) a total negative trend equal to
426 -4.03×10^{-5} PgC/yr was computed for ETH-SOMFFN, which contrasts with positive trends suggested by
427 FFNN-LSCE (6.68×10^{-5} PgC/yr) and Jena-MLS13 (3×10^{-4} PgC/yr). All models reproduced a maximum in
428 the southern part of biome 6 but they disagree about its amplitude and spatial distribution. Almost
429 everywhere over the Atlantic Ocean the mapping methods produced the same sign of linear trend (Fig. 9).
430 Only in the eastern part of the subtropical North Atlantic Jena-MLS13 gave a positive linear trend of fCO₂
431 (Fig. 8 (b)).

432

433 According to FFNN-LSCE, the global ocean took up in average 1.55 PgC/yr between 2001-2015. This
434 estimate is consistent with results from the other three models (Table 3) (see Table S1 for estimations per
435 biomes). The spread between individual models falls in the range of the error reported in Landschützer et
436 al. (2016), ± 0.4 -0.6 PgC/yr. Per biome, estimates of CO₂ sea-air fluxes provided by FFNN-LSCE are
437 similarly in good agreement with those derived from the other models.

438

439 4. Summary and conclusion.

440

441 We proposed a new model for the reconstruction of monthly surface ocean pCO₂. The model is applied
442 globally and allows a seamless reconstruction without introducing boundaries between the ocean basins or
443 biomes. Our model relies on a two-step approach based on Feed-Forward Neural Networks (FFNN-LSCE).
444 The first step corresponds to the reconstruction of a monthly pCO₂ climatology. It allows us to keep the
445 output of the FFNN close to the observed values in the region with the poor data cover. Moreover, it allows
446 to include a potential change in seasonal cycle in response to climate change from drivers to carbon cycle
447 variables. At the second step pCO₂ anomalies are reconstructed according to climatology from the first step.
448 The model was applied over the period 2001-2016. Validation with independent data at global scale
449 indicated an accuracy of 17.57 μ atm, r^2 of ~ 0.76 and an absolute bias of 11.52 μ atm. In order to assess the
450 model further, it was compared to three different mapping models: ETH-SOMFFN (self-organizing maps +
451 neural network), Jena-MLS13 (statistical interpolation), JMA-MLR (linear regression) (Rödenbeck et al.,
452 2015). Network qualification followed the protocol and diagnostics proposed in Rödenbeck et al. (2015).
453 Reconstructed surface ocean pCO₂ distributions were in good agreement with other models and
454 observations. The seasonal variability was reproduced satisfyingly by FFNN-LSCE, the yearly pCO₂



455 mismatch varied around zero, and relative IAV mismatch was 7.55%. FFNN-LSCE proved skillful in
456 reproducing the interannual variability of surface ocean pCO₂ over the Eastern Equatorial Pacific in
457 response to ENSO. Reductions in surface ocean pCO₂ during El Niño events were well reproduced. The
458 comparison between reconstructed and observed pCO₂ values yielded a RMSE of 15.73 μatm, r² of 0.79
459 and an absolute bias of 10.33 μatm over the Equatorial Pacific. The relative IAV misfit in this region was
460 ~17%. Despite an overall good agreement between models, important differences still exist at the regional
461 scale, especially in the Southern hemisphere and in particular, the Southern Pacific and the Indian Ocean.
462 These regions suffer from poor data-coverage. Large regional uncertainties in reconstructed surface ocean
463 pCO₂ and sea-air CO₂ fluxes have a strong influence on global estimates of CO₂ fluxes and trends.

464

465

466 **Code and data availability.**

467

468 Python code for pCO₂ climatology reconstruction, 1st step of FFNN-LSCE model:

469 <https://files.lsce.ipsl.fr/public.php?service=files&t=016351132f69db55f1e6eda948665237>

470

471 Python code for reconstruction of pCO₂ anomalies, 2nd step of FFNN-LSCE model:

472 <https://files.lsce.ipsl.fr/public.php?service=files&t=9304199cf79efd688837e891383287c3>

473

474 Data of FFNN-LSCE pCO₂ are available on request: anna.sommer.lab@gmail.com

475

476 **Author contribution.**

477 ADS, MG, MV and CM contributed to the development of the methodology and designed the experiments,
478 ADS carried them out. ADS developed the model code and performed the simulations. ADS prepared the
479 manuscript with contributions from all co-authors.

480

481

482 **Acknowledgments.**

483 Authors would like to thank Frederic Chevallier and Gilles Reverdin for their suggestions. Authors would
484 like to gratefully acknowledge funding by the AtlantOS project (EU Horizon 2020 research and innovation
485 program, grant agreement no. 2014-633211). MV also acknowledges funding by the CoCliServ project
486 (ERA4CS program).

487

488 **References**

489

490 Aumont, O., and Bopp, L.: Globalizing results from ocean in situ iron fertilization studies, Global
491 Biogeochem. Cycles, 20, GB2017, doi:10.1029/2005GB002591, 2006.



492
493Bakker, D. C. E., Pfeil, B., Landa, C. S., Metzl, N., O'Brien, K. M., Olsen, A., Smith, K., Cosca, C.,
494Harasawa, S., Jones, S. D., Nakaoka, S.-I. et al.: A multi-decade record of high-quality fCO₂ data in version
4953 of the Surface Ocean CO₂ Atlas (SOCAT), *Earth Syst. Sci. Data*, 8, 383–413,
496<https://doi.org/10.5194/essd-8-383-2016>, 2016.
497
498Bishop, C.M.: *Neural Networks for Pattern Recognition*, Oxford Univ. Press, Cambridge, U. K., 1995.
499
500Bricaud, A., Meija, C., Blondeau-Patissier, D., Claustre, H., Crepon, M., and Thiria, S.: Retrieval of
501pigment concentrations and size structure of algal populations from the absorption spectra using
502multilayered perceptrons, *Appl. Opt.*, 46, 8, 1251–1260, 2006.
503
504Chollet, F., et al.: Keras. <https://keras.io>, 2015.
505
506Ciais P., Sabine C., Bala G. et al.: Carbon and other biogeochemical cycles. In: *Climate Change 2013: The*
507*Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the*
508Intergovernmental Panel on Climate Change[Stocker, T. F., D. Qin, G.-K. Plattner, M. Tignor, S. K. Allen,
509J. Boschung, A. Nauels, Y. Xia, V. Bex and P. M. Midgley (eds.)]. Cambridge University Press, Cambridge,
510United Kingdom and New York, NY, USA, 2013.
511
512Donlon, C.J., Martin, M., Stark, J.D., Roberts-Jones, J., Fiedler, E., and Wimmer, W.: The Operational Sea
513Surface Temperature and Sea Ice analysis (OSTIA), *Remote Sensing of the Environment*, doi:
51410.1016/j.rse.2010.10.017, 2011.
515
516Fay, A. R. and McKinley, G. A.: Global open-ocean biomes: mean and temporal variability, *Earth Syst. Sci.*
517*Data*, 6, 273–284, doi:10.5194/essd-6-273-2014, 2014.
518
519Fay, A.R., McKinley, G.A., and Lovenduski, N.S.: Southern Ocean carbon trends: Sensitivity to methods,
520*Geophys. Res. Lett.*, 41, 6833–6840, doi:10.1002/2014GL061324, 2014.
521
522Feely, R. A., Wanninkhof, R., Takahashi, T., and Tans, P.: Influence of El Niño on the equatorial Pacific
523contribution to atmospheric CO₂ accumulation, *Nature*, 398, 597–601, 1999.
524
525Friedrich, T., and Oschlies, A.: Basin-scale pCO₂ maps estimated from ARGO float data: A model study, *J.*
526*Geophys. Res.*, 114, C10012, doi:10.1029/2009JC005322, 2009a.
527
528Friedrich, T., and Oschlies, A.: Neural network-based estimates of North Atlantic surface pCO₂ from
529satellite data: A methodological study, *J. Geophys. Res.*, 114, C03020, doi: 10.1029/2007JC004646, 2009b.
530
531Gross, L., Thiria, S., Frouin, R., and Mitchell, B.G.: Artificial neural networks for modeling transfer
532function between marine reflectance and phytoplankton pigment concentration, *J. Geophys. Res.*, 105, C2,
5333483–3949, doi: 10.1029/1999jc900278, 2000.
534
535Hinton, G., Srivastava, N., and Swersky, K.: Lecture 6a: Overview of mini-batch gradient descent. *Neural*
536*Networks for Machine Learning. Slides:*
537http://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf, 2012.
538
539Iida, Y., Kojima, A., Takatani, Y., Nakano, T., Midorikawa, T., and Ishii, M.: Trends in pCO₂ and sea-air
540CO₂ flux over the global open oceans for the last two decades, *J. Oceanogr.*, 71, 637–661,
541doi:10.1007/s10872-015-0306-4, 2015.
542
543Kalnay, E., Kanamitsu, M., Kistler, R., Collins, W., Deaven, D., Gandin, L., Iredell, M., Saha, S., White,
544G., Woollen, J., Zhu, Y., Chelliah, M., Ebisuzaki, W., Higgins, W., Janowiak, J., Mo, K. C., Ropelewski, C.,



- 545Wang, J., Leetmaa, A., Reynolds, R., Jenne, R., and Joseph, D.: The NCEP/NCAR 40-year reanalysis
546project, B. Am. Meteorol. Soc., 77, 437–471, 1996.
- 547
- 548Kallache, M., Vrac, M., Naveau, P., Michelangeli, P.-A.: Non-stationary probabilistic downscaling of
549extreme precipitation, J. Geophys. Res. - Atmospheres, 116, D05113, doi:10.1029/2010JD014892, 2011.
- 550
- 551Körtzinger, A.: Methods of Seawater Analysis, chap. Determination of carbon dioxide partial pressure
552(pCO₂), 149–158, Verlag Chemie, 1999.
- 553
- 554Landschützer, P., Gruber, N., Bakker, D. C. E., Schuster, U., Nakaoka, S., Payne, M. R., Sasse, T. P., and
555Zeng, J.: A neural network-based estimate of the seasonal to inter-annual variability of the Atlantic Ocean
556carbon sink, Biogeosciences, 10, 7793–7815, <https://doi.org/10.5194/bg-10-7793-2013>, 2013.
- 557
- 558Landschützer, P., Gruber, N., Bakker, D. C. E., and Schuster, U.: Recent variability of the global ocean
559carbon sink, Global Biogeochem. Cy., 28, 927–949, <https://doi.org/10.1002/2014GB004853>, 2014.
- 560
- 561Landschützer, P., Gruber, N. & Bakker, D. C. E.: Decadal variations and trends of the global ocean carbon
562sink, Glob. Biogeochem. Cycles, 30, 1396–1417, <https://doi.org/10.1002/2015GB005359>, 2016.
- 563
- 564Laruelle, G. G., Landschützer, P., Gruber, N., Tison, J.-L., Delille, B., and Regnier, P.: Global high-
565resolution monthly pCO₂ climatology for the coastal ocean derived from neural network interpolation,
566Biogeosciences, 14, 4545–4561, <https://doi.org/10.5194/bg-14-4545-2017>, 2017.
- 567
- 568Lefèvre, N., Watson, A. J., and Watson, A. R.: A comparison of multiple regression and neural network
569techniques for mapping *in situ* pCO₂ data, Tellus, 57B, 375–384,
570<https://doi.org/10.3402/tellusb.v57i5.16565>, 2005.
- 571
- 572Le Quéré, C., and Coauthors: Two decades of ocean CO₂ sink and variability, Tellus, 55B, 649–656,
573<https://doi.org/10.1034/j.1600-0889.2003.00043.x>, 2003.
- 574
- 575Le Quéré, C., Takahashi, T., Buitenhuis, E. T., Rödenbeck, C., and Sutherland, S. C.: Impact of climate
576change and variability on the global oceanic sink of CO₂, Glob. Biogeochem. Cy., 24, GB4007,
577doi:10.1029/2009GB003599, 2010.
- 578
- 579Le Quéré, C., Andrew, R. M., Friedlingstein, P., Sitch, S., Pongratz, J., Manning, A. C., et al.: Global
580carbon budget 2017, Earth System Science Data, 10 (1), 405–448. <https://doi.org/10.5194/essd-10-405-5812018>, 2018.
- 582
- 583Majkut, J. D., Carter, B.R., Frölicher, T.L., Dufour, C.O., Rodgers, K.B., and Sarmiento, J.L.: An observing
584system simulation for Southern Ocean carbon dioxide uptake, Philos. Trans. Roy. Soc. London, A372,
58520130046, doi:<https://doi.org/10.1098/rsta.2013.0046>, 2014.
- 586
- 587Mejia, C., Thiria, S., Tran, N., and Crepon, M.: Determination of the Geophysical Model Function of ERS1
588Scatterometer by the use of Neural Networks, J. Geophys. Res., Vol. 103, No. C6, PP 12853–12868,
589<https://doi.org/10.1029/97JC02178>, 1998.
- 590
- 591Menemenlis, D., Campin, J., Heimbach, P., Hill, C., Lee, T., Nguyen, A., Schodlok, M., and Zhang, H.:
592ECCO2: High resolution global ocean and sea ice data synthesis, Mercator Ocean, Quarterly Newsletter,
59331, 13–21, 2008.
- 594
- 595Nakaoka, S., Telszewski, M., Nojiri, Y., Yasunaka, S., Miyazaki, C., Mukai, H., and Usui, N.: Estimating
596temporal and spatial variation of ocean surface pCO₂ in the North Pacific using a self-organizing map
597neural network technique, Biogeosciences, 10, 6093–6106, doi:10.5194/bg-10-6093-2013, 2013.



598
599Organelli, E., Barbieux, M., Claustre, H., Schmechtig, C., Poteau, A., Bricaud, A., Boss, E., Briggs, N.,
600Dall'Olmo, G., D'Ortenzio, F., Leymarie, E., Mangin, A., Obolensky, G., Penkerch, C., Prieur, L., Roesler,
601C., Serra, R., Uitz, J., and Xing, X.: Two databases derived from BGC-Argo float measurements for marine
602biogeochemical and bio-optical applications, *Earth Syst. Sci. Data*, 9, 861-880,
603<https://doi.org/10.5194/essd-9-861-2017>, 2017.

604
605Orr, J. C., Monfray, P., Maier-Reimer, E., Mikolajewicz, U., Palmer, J., Taylor, N. K., Toggweiler, J. R.,
606Sarmiento, J. L., Quere, C. L., Gruber, N., Sabine, C. L., Key, R. M. and Boutin, J.: Estimates of
607anthropogenic carbon uptake from four three-dimensional global ocean models, *Global Biogeochem. Cycl.*,
60815, 43–60, <https://doi.org/10.1029/2000GB001273>, 2001.

609
610Peylin, P., Bousquet, P., Le Quéré, C., Sitch, S., Friedlingstein, P., McKinley, G., Gruber, N., Rayner, P.,
611and Ciais, P.: Multiple constraints on regional CO₂ flux variations over land and oceans, *Glob.*
612*Biogeochem. Cycles*, 19, GB1011, <https://doi.org/10.1029/2003GB002214>, 2005.

613
614Peylin, P., Law, R. M., Gurney, K. R., Chevallier, F., Jacobson, A. R., Maki, T., Niwa, Y., Patra, P. K.,
615Peters, W., Rayner, P. J., Rödenbeck, C., van der Laan-Luijkx, I. T., and Zhang, X.: Global atmospheric
616carbon budget: results from an ensemble of atmospheric CO₂ inversions, *Biogeosciences*, 10, 6699-6720,
617<https://doi.org/10.5194/bg-10-6699-2013>, 2013.

618
619Rödenbeck, C.: Estimating CO₂ sources and sinks from atmospheric mixing ratio measurements using a
620global inversion of atmospheric transport, Technical Report 6, Max Planck Institute for Biogeochemistry,
621Jena, available at: http://www.bgc-jena.mpg.de/uploads/Publications/TechnicalReports/tech_report6.pdf,
6222005.

623
624Rödenbeck, C., Bakker, D. C. E., Metzl, N., Olsen, A., Sabine, C., Cassar, N., Reum, F., Keeling, R. F., and
625Heimann, M.: Interannual sea-air CO₂ flux variability from an observation-driven ocean mixed-layer
626scheme, *Biogeosciences*, 11, 4599–4613, doi:10.5194/bg-11-4599-2014, 2014.

627
628Rödenbeck, C., Bakker, D. C. E., Gruber, N., Iida, Y., Jacobson, A. R., Jones, S., Landschützer, P. et al.:
629Data-based estimates of the ocean carbon sink variability—first results of the Surface Ocean pCO₂
630Mapping intercomparison (SOCOM), *Biogeosciences*, 12, 7251–7278, [https://doi.org/10.5194/bg-12-7251-](https://doi.org/10.5194/bg-12-7251-2015)
6312015, 2015.

632
633Rodgers, K. B., Key, R. M., Gnanadesikan, A., Sarmiento, J. L., Aumont, O., Bopp, L. et al.: Using
634altimetry to help explain patchy changes in hydrographic carbon measurements, *J. Geophys. Res.*, 114,
635C09013, doi:10.1029/2008JC005183, 2009.

636
637Roobaert, A., Laruelle, G. G., Landschützer, P., and Regnier, P.: Uncertainty in the global oceanic CO₂
638uptake induced by wind forcing: quantification and spatial analysis, *Biogeosciences*, 15, 1701-1720,
639<https://doi.org/10.5194/bg-15-1701-2018>, 2018.

640
641Rumelhart, D.E., Hinton, G.E., & Williams, R.J.: Learning internal representations by backpropagating
642errors, *Nature*, 323, 533–536, 1986.

643
644Sauzède, R., Claustre, H., Uitz, J., Jamet, C., Dall'Olmo, G., D'Ortenzio, F., Gentili, B., Poteau, A., and
645Schmechtig, C.: A neural network-based method for merging ocean color and Argo data to extend surface
646bio-optical properties to depth: Retrieval of the particulate backscattering coefficient, *J. Geophys. Res.*
647*Oceans*, 121, 2552–2571, doi:10.1002/2015JC011408, 2016.

648
649Schuster, U., McKinley, G. A., Bates, N., Chevallier, F., Doney, S. C., Fay, A. R., González-Dávila, M.,
650Gruber, N., Jones, S., Krijnen, J., Landschützer, P., Lefèvre, N., Manizza, M., Mathis, J., Metzl, N., Olsen,



651A., Rios, A. F., Rödenbeck, C., Santana-Casiano, J. M., Takahashi, T., Wanninkhof, R., and Watson, A. J.:
652An assessment of the Atlantic and Arctic sea–air CO₂ fluxes, 1990–2009, *Biogeosciences*, 10, 607–627,
653<https://doi.org/10.5194/bg-10-607-2013>, 2013.

654
655Takahashi, T., Sutherland, S.C., Wanninkhof, R., Sweeney, C., Feely, R.A., Chipman, D.W., Hales, B.,
656Friederich, G., Chavez, F., Sabine, C., et al.: Climatological mean and decadal change in surface ocean
657pCO₂, and net sea–air CO₂ flux over the global oceans, *Deep.-Sea Res. II*, 56(8–10), 554–577,
658<https://doi.org/10.1016/j.dsr2.2008.12.009>, 2009.

659
660Takahashi, T., Sutherland, S. C., Sweeney, C., Poisson, A., Metzl, N. et al.: Global sea–air CO₂ flux based
661on climatological surface ocean pCO₂, and seasonal biological and temperature effects, *Deep.-Sea Res. II*,
66249, 1601–1622, [https://doi.org/10.1016/S0967-0645\(02\)00003-6](https://doi.org/10.1016/S0967-0645(02)00003-6), 2002.

663
664Telszewski, M., Chazottes, A., Schuster, U., Watson, A. J., Moulin, C., Bakker, D. C. E., González-Dávila,
665M., Johannessen, T., Körtzinger, A., Lüger, H., Olsen, A., Omar, A., Padin, X. A., Ríos, A. F., Steinhoff, T.,
666Santana-Casiano, M., Wallace, D.W.R., and Wanninkhof, R.: Estimating the monthly pCO₂ distribution in
667the North Atlantic using a self-organizing neural network, *Biogeosciences*, 6, 1405–1421, doi:10.5194/bg-
6686-1405-2009, 2009.

669
670Wanninkhof, R.: Relationship between wind speed and gas exchange over the ocean, *J. Geophys. Res.-*
671*Oceans*, 97, 7373–7382, <https://doi.org/10.1029/92JC00188>, 1992.

672
673Weiss, R.: Carbon dioxide in water and seawater: the solubility of a non-ideal gas, *Mar. Chem.*, 2, 203–205,
674[https://doi.org/10.1016/0304-4203\(74\)90015-2](https://doi.org/10.1016/0304-4203(74)90015-2), 1974.

675
676Williams, N.L., Juraneck, L.W., Feely, R.A., Johnson, K.S., Sarmiento, J.L., Talley, L.D., Dickson, A.G.,
677Gray, A.R., Wanninkhof, R., Russell, J.L., Riser, S.C., Takeshita, Y.: Calculating surface ocean pCO₂ from
678biogeochemical Argo floats equipped with pH: An uncertainty analysis, *Global Biogeochemical Cycles*,
67931:591–604, <https://doi.org/10.1002/2016GB005541>, 2017.

680
681Zeng, J., Nojiri, Y., Landschützer, P., Telszewski, M., and Nakaoka, S.: A global surface ocean fCO₂
682climatology based on a feed-forward neural network, *J. Atmos. Ocean Technol.*, 31, 1838–1849,
683<https://doi.org/10.1175/JTECH-D-13-00137.1>, 2014.

684

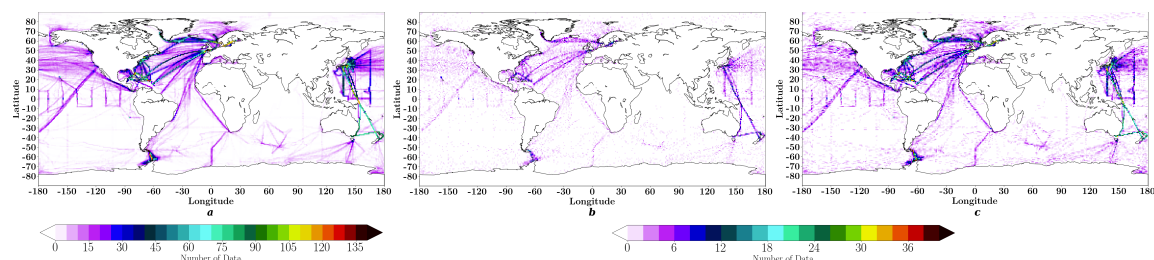


Figure 1: Spatial distribution of SOCAT data (number of measurements per grid point): (a) - period 2001-2016; (b) - all months January for period 2001-2016; (c) - all months December-January-February for period 2001-2016.

687
688



689

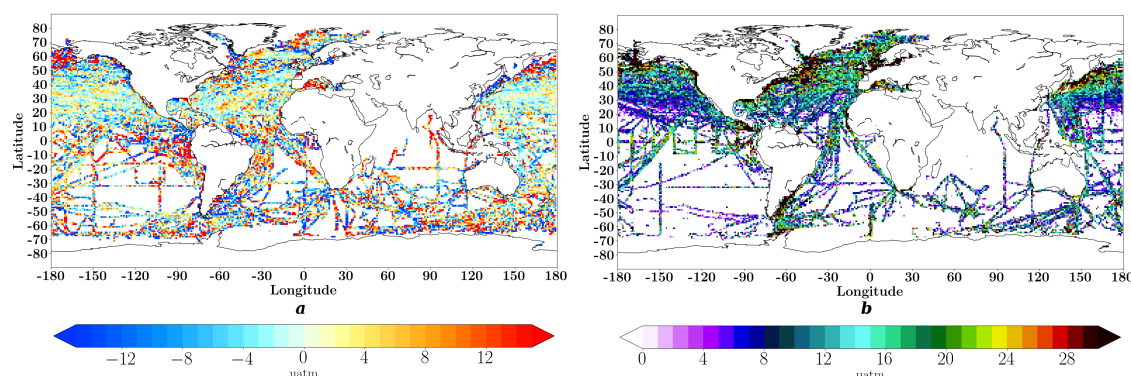


Figure 2: Time mean differences (uatm) (a) between monthly FFNN-LSCE pCO₂ and SOCAT pCO₂ data used for evaluation of the model over the period 2001-2016 and its std (b).

691

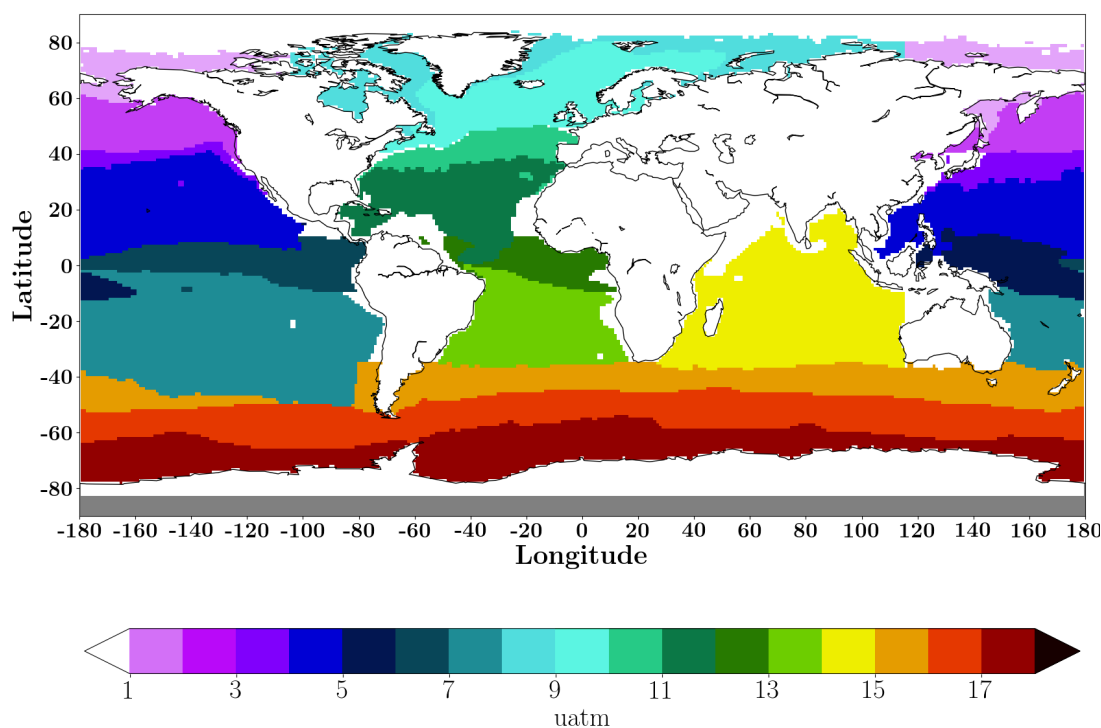


Figure 3: Map of biomes (after Rodenbeck et al. (2015); and Fay and McKinley (2014)) used for comparison. See table 2 for biome names.



693

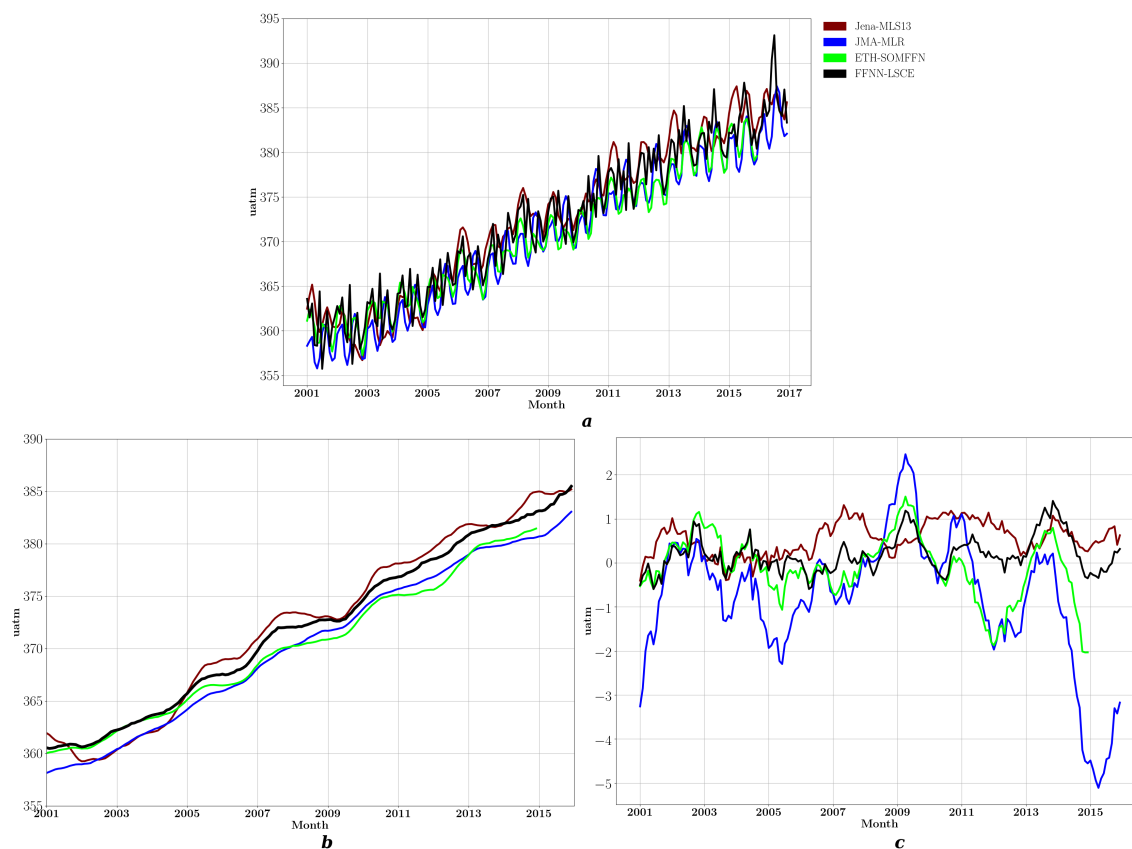


Figure 4: Global oceanic pCO₂: black - FFNN-LSCE, blue - JMA, brown - Jena, green - ETH-SOMFFN; (a) - monthly time series averaged over the glob, (b) - 12-month running mean averaged over the glob, (c) - yearly pCO₂ mismatch (difference of mapping methods and SOCAT data).



695

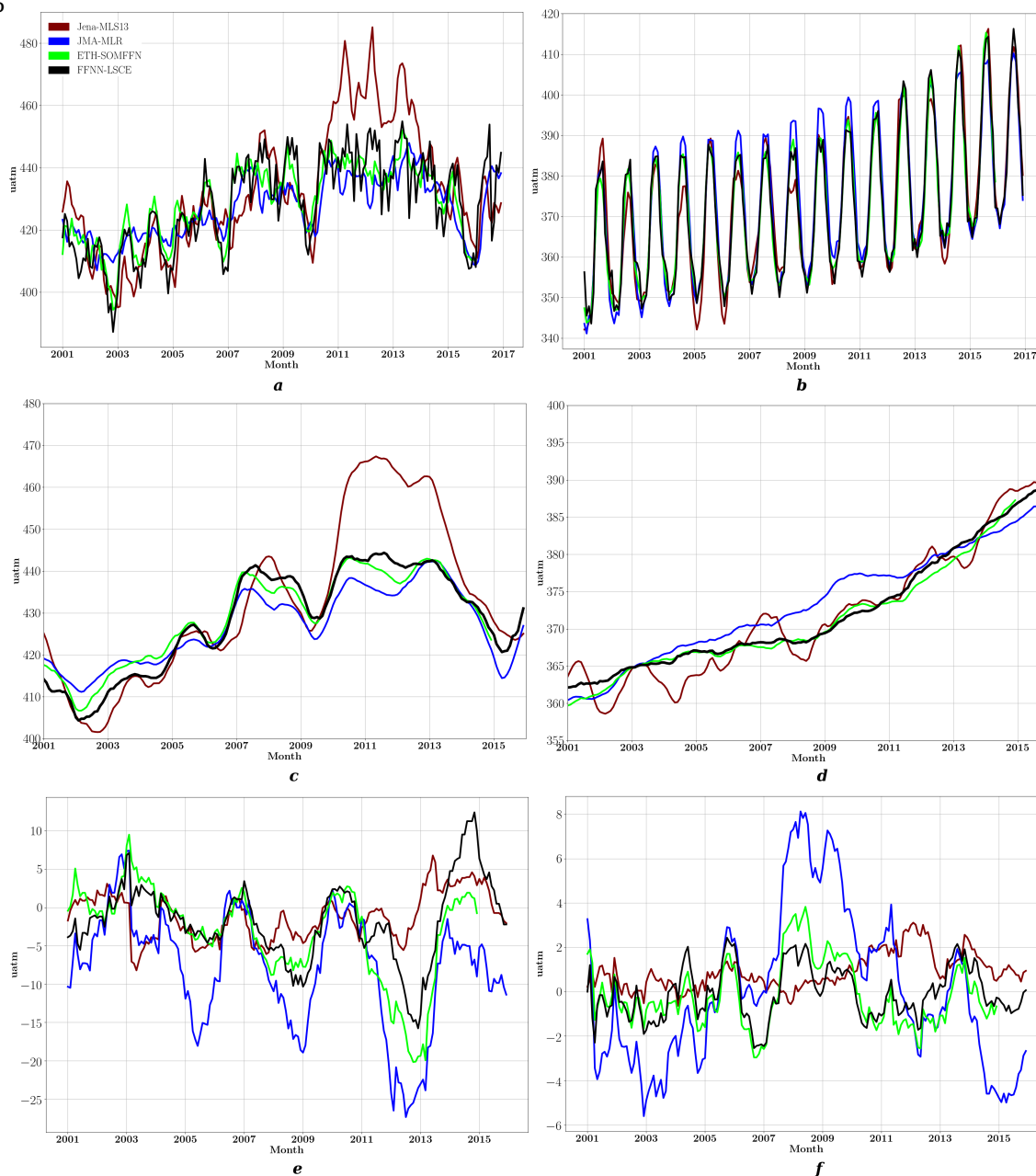


Figure 5: East Pacific Equatorial (biome 6) (left) and North Atlantic Subtropical Permanently Stratified (biome 11) (right) oceanic pCO_2 : black – FFNN, blue – JMA, brown – Jena, green – ETH-SOMFFN; (a), (b) – monthly time series averaged over biome; (c), (d) – 12-month running mean averaged over biome; (e), (f) – yearly pCO_2 mismatch (difference of mapping methods and SOCAT data).

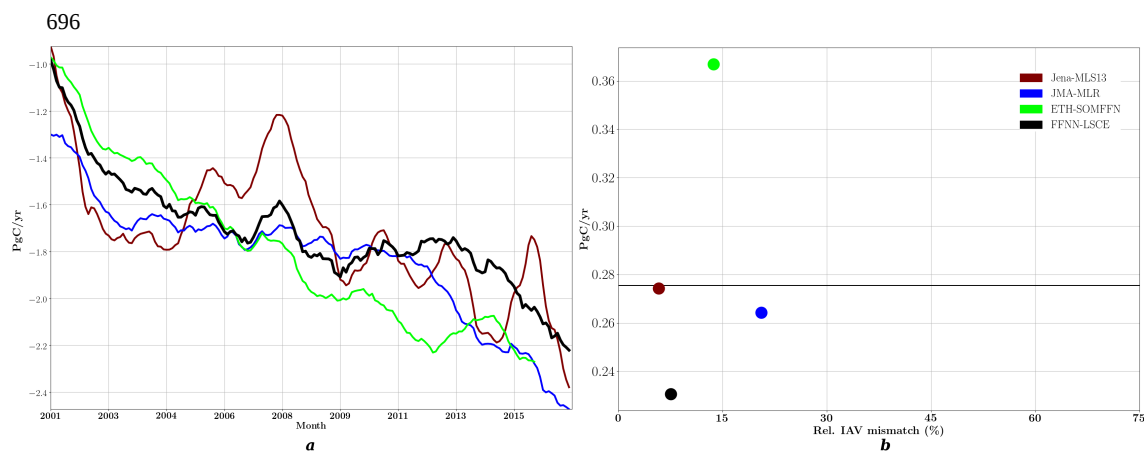


Figure 6: (a) – Interannual sea-air CO₂ flux (12-month running mean) in the global ocean; (b) – amplitude of interannual CO₂ flux plotted against the relative IAV mismatch amplitude. The weighted mean is given as a horizontal line.

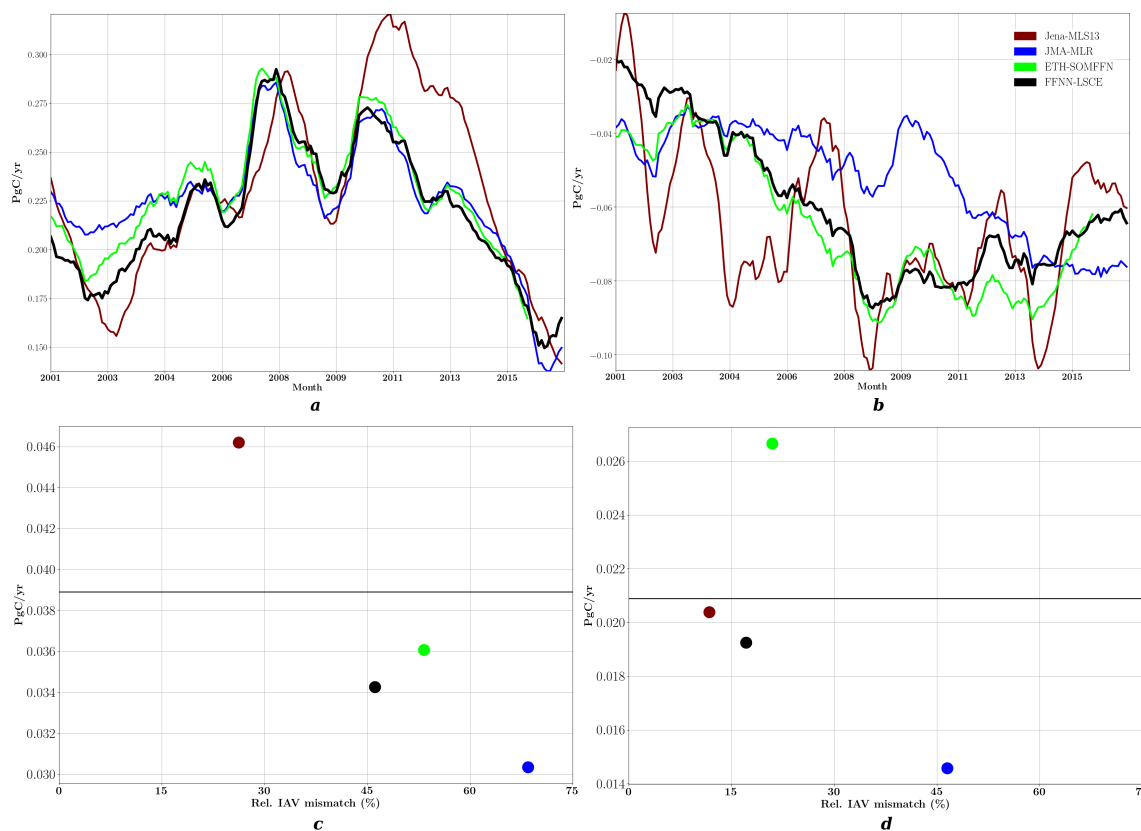


Figure 7: East Pacific Equatorial (biome 6) (left) and North Atlantic Subtropical Permanently Stratified (biome 11) (right): (a), (b) – Interannual sea-air CO₂ flux (12-month running mean) in the global ocean; (c), (d) – amplitude of interannual CO₂ flux plotted against the relative IAV mismatch amplitude. The weighted mean is given as a horizontal line.

700

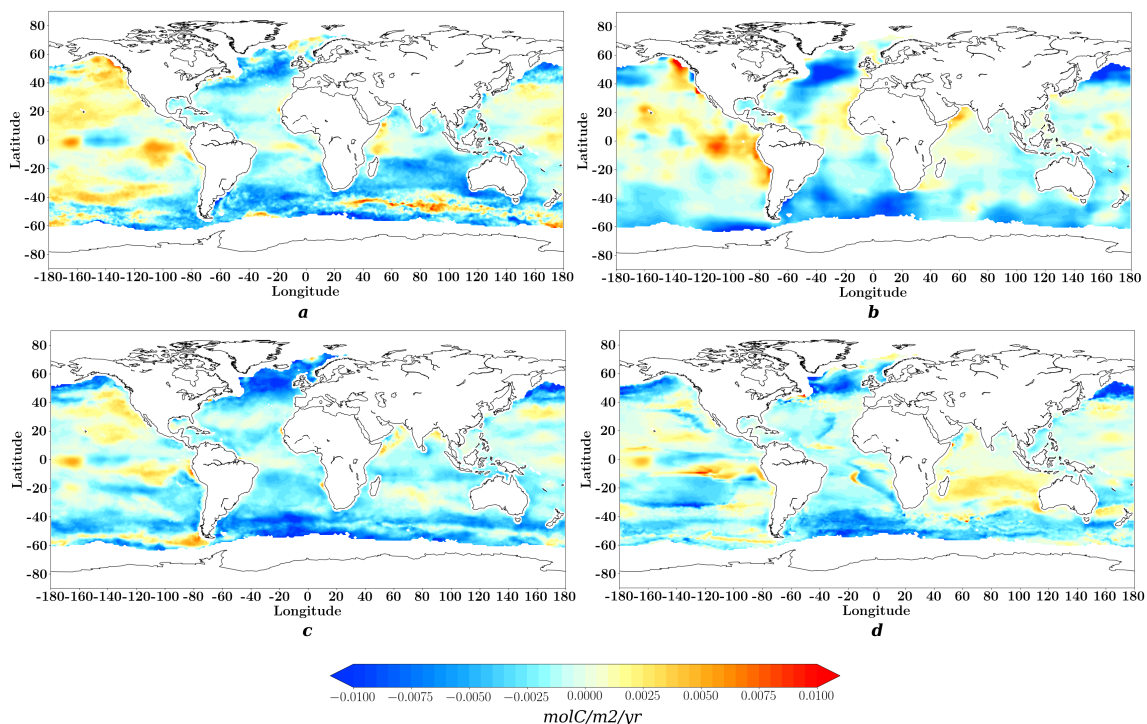


Figure 8: Linear trend of $f\text{CO}_2$ for common period 2001-2015: (a) – FFNN-LSCE; (b) – Jena-MLS13; (c) – ETH-SOMFFN; (d) – JMA-MLR.

702

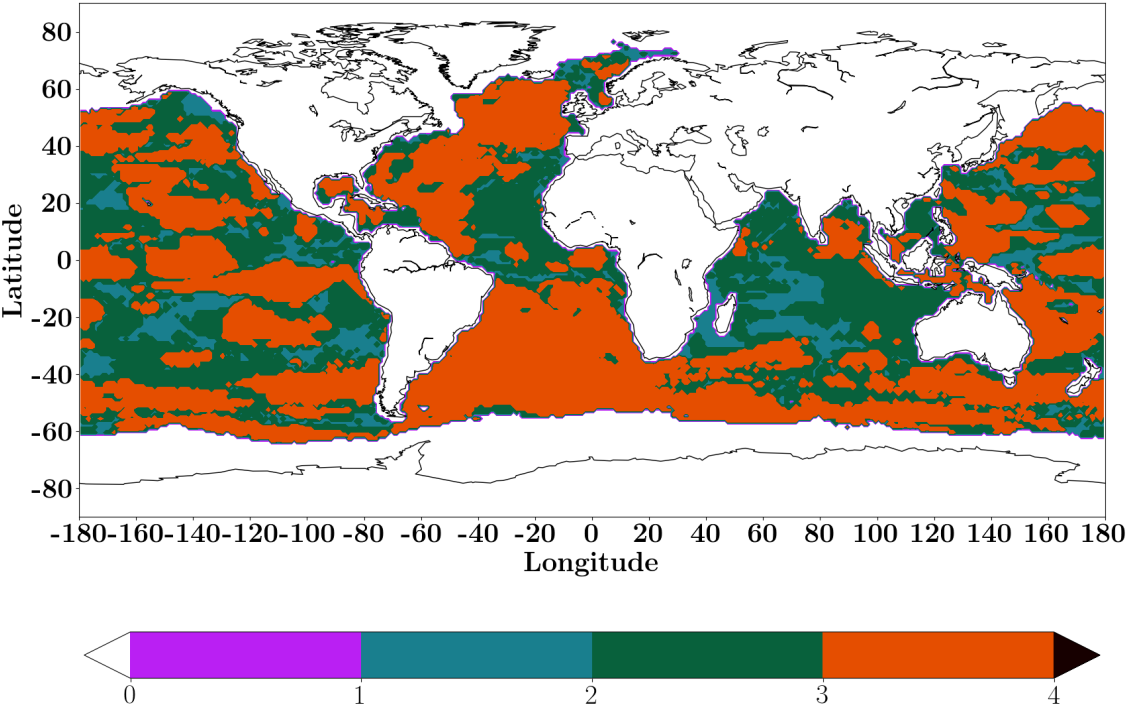


Figure 9: Agreement between four mapping methods in their linear trend of sea-air CO₂ flux. Color-bar represents the number of products that have the same sign of linear trend.

704
705
706
707
708
709
710
711
712
713
714
715
716
717
718
719
720
721
722
723
724Table 1: Statistical validation of FFNN-LSCE. Comparison between reconstructed surface ocean pCO₂ and
725pCO₂ values from SOCAT v5 data base not used in the training algorithm for the period 2001-2016 over the
726global ocean (except for regions with ice-cover) and for large oceanographic regions. In round brackets:



727 number of measurements per region

Model	Latitude boundaries	RMS (μatm)	r^2	Bias (μatm)
FFNN Global		17.97	0.76	11.52
Arctic (150)	76°N to 90°N	22.05	0.54	17.1
Atlantic Subpolar (21903)	49°N to 76°N	22.99	0.76	15.04
Pacific Subpolar (4529)	49°N to 76°N	34.77	0.65	23.12
Atlantic Subtropical (41331)	18°N to 49°N	17.28	0.69	11.27
Pacific Subtropical (41867)	18°N to 49°N	15.86	0.77	9.9
Atlantic Equatorial (7300)	18°S to 18°N	17.27	0.57	11.44
Pacific Equatorial (27092)	18°S to 18°N	15.73	0.79	10.33
South Atlantic (3002)	44°S to 18°S	17.81	0.63	12.28
South Pacific (12934)	44°S to 18°S	13.52	0.63	9.36
Indian Ocean (2871)	44°S to 30°N	17.25	0.62	11.6
Southern Ocean (16334)	90°S to 44°S	17.4	0.58	11.92

728

729 Table 2: Biomes from Fay and McKinley (2014) used for time series comparison (Fig. 3)

Number	Name
1	(Omitted) North Pacific Ice
2	North Pacific Subpolar Seasonally Stratified
3	North Pacific Subtropical Seasonally Stratified
4	North Pacific Subtropical Permanently Stratified
5	West Pacific Equatorial
6	East Pacific Equatorial
7	South Pacific Subtropical Permanently Stratified
8	(Omitted) North Atlantic Ice
9	North Atlantic Subpolar Seasonally Stratified
10	North Atlantic Subtropical Seasonally Stratified
11	North Atlantic Subtropical Permanently Stratified
12	Atlantic Equatorial
13	South Atlantic Subtropical Permanently Stratified
14	Indian Ocean Subtropical Permanently Stratified



15	Southern Ocean Subtropical Seasonally Stratified
16	Southern Ocean Subpolar Seasonally Stratified
17	Southern Ocean Ice

730

731 Table 3: Mean of sea-air CO₂ flux (PgC/yr) over the Global Ocean and per regions for period in common

732 (2001-2015). Averages over the period 2001-2009 are presented between brackets. The last column

733 presents a comparison to best estimates from Schuster et al. (2013) for the Atlantic Ocean (1990 – 2009).

Region	Latitude boundaries	FFNN-LSCE	ETH-SOMFFN	Jena-MLS13	JMA-MLR	Schuster et al. (2013), 1990-2009
Global		-1.55 (-1.44)	-1.67 (-1.47)	-1.55 (-1.41)	-1.74 (-1.62)	---
Arctic	76°N to 90°N	-0.001	-0.001	-0.001	-0.001	-0.12±0.06
Atlantic Subpolar	49°N to 76°N	-0.15 (-0.15)	-0.14 (-0.12)	-0.15 (-0.15)	-0.16 (-0.15)	-0.21±0.06
Pacific Subpolar	49°N to 76°N	-0.003 (-0.005)	-0.009 (-0.004)	-0.006 (-0.004)	-0.027 (-0.021)	---
Atlantic Subtropical	18°N to 49°N	-0.21 (-0.19)	-0.21 (-0.19)	-0.2 (-0.18)	-0.21 (-0.2)	-0.26±0.06
Pacific Subtropical	18°N to 49°N	-0.45 (-0.46)	-0.49 (-0.48)	-0.47 (-0.46)	-0.49 (-0.47)	---
Atlantic Equatorial	18°S to 18°N	0.085 (0.09)	0.085 (0.095)	0.08 (0.082)	0.1 (0.11)	0.12±0.04
Pacific Equatorial	18°S to 18°N	0.42 (0.41)	0.4 (0.4)	0.44 (0.42)	0.38 (0.37)	---
South Atlantic	44°S to 18°S	-0.17 (-0.16)	-0.18 (-0.16)	-0.18 (-0.17)	-0.23 (-0.22)	-0.14±0.04
South Pacific	44°S to 18°S	-0.33 (-0.34)	-0.4 (-0.39)	-0.35 (-0.34)	-0.49 (-0.47)	---
Indian Ocean	44°S to 30°N	-0.25 (-0.2)	-0.32 (-0.29)	-0.27 (-0.26)	-0.27 (-0.29)	---
South Ocean	90°S to 44°S	-0.38	-0.29	-0.36	-0.26	---

734

735

736

737

738

739

740