

Estimating temporal and spatial variation of ocean surface $p\text{CO}_2$

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Estimating temporal and spatial variation of ocean surface $p\text{CO}_2$ in the North Pacific using a Self Organizing Map neural network technique

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This study produced maps of the partial pressure of oceanic carbon dioxide ($p\text{CO}_2^{\text{sea}}$) in the North Pacific on a 0.25° latitude \times 0.25° longitude grid from 2002 to 2008. The $p\text{CO}_2^{\text{sea}}$ values were estimated by using a self-organizing map neural network technique to explain the non-linear relationships between observed $p\text{CO}_2^{\text{sea}}$ data and four oceanic parameters: sea surface temperature (SST), mixed layer depth, chlorophyll *a* concentration, and sea surface salinity (SSS). The observed $p\text{CO}_2^{\text{sea}}$ data was obtained from an extensive dataset generated by the volunteer observation ship program operated by the National Institute for Environmental Studies. The reconstructed $p\text{CO}_2^{\text{sea}}$ values agreed rather well with the $p\text{CO}_2^{\text{sea}}$ measurements, the root mean square error being $17.6 \mu\text{atm}$. The $p\text{CO}_2^{\text{sea}}$ estimates were improved by including SSS as one of the training parameters and by taking into account secular increases of $p\text{CO}_2^{\text{sea}}$ that have tracked increases in atmospheric CO_2 . Estimated $p\text{CO}_2^{\text{sea}}$ values accurately reproduced $p\text{CO}_2^{\text{sea}}$ data at several stations in the North Pacific. The distributions of $p\text{CO}_2^{\text{sea}}$ revealed by seven-year averaged monthly $p\text{CO}_2^{\text{sea}}$ maps were similar to Lamont-Doherty Earth Observatory $p\text{CO}_2^{\text{sea}}$ climatology and more precisely reflected oceanic conditions. The distributions of $p\text{CO}_2^{\text{sea}}$ anomalies over the North Pacific during the winter clearly showed regional contrasts between El Niño and La Niña years related to changes of SST and vertical mixing.

1 Introduction

The ocean plays an important role as a major carbon reservoir for CO_2 emitted to the atmosphere from fossil fuel burning, cement production, and biomass burning. The ocean has absorbed about 48 % of the CO_2 emitted to the atmosphere by fossil-fuel combustion since the Industrial Revolution (Sabine et al., 2004). To evaluate the global budget of oceanic CO_2 uptake, measurements of the partial pressure of CO_2 ($p\text{CO}_2^{\text{sea}}$) in surface seawater have been carried out over the global ocean, with the highest

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intensity in the equatorial Pacific (Feely et al., 1987, 2006; Ishii et al., 2009), the North Atlantic (Cooper et al., 1998; Olsen et al., 2003; Schuster et al., 2009), and the North Pacific (Inoue et al., 1995; Murphy et al., 2001a; Zeng et al., 2002; Chierici et al., 2006). A compilation of worldwide efforts to measure $p\text{CO}_2^{\text{sea}}$ on a global scale can be found in Takahashi et al. (2009). The authors led by a team at the Lamont-Doherty Earth Observatory (LDEO) computed a 35-yr $p\text{CO}_2^{\text{sea}}$ climatology (for a reference year 2000) on 4° latitude \times 5° longitude resolution and estimated the annual global air-sea CO_2 exchange at $-1.6 \pm 0.9 \text{ PgC yr}^{-1}$.

Neural network (NN) techniques can be generally described as empirical statistical tools that resolve, to certain degree, the non-linear, often discontinuous relationships among proxy parameters without any a priori assumptions. In the past decade a handful of authors reported the application of an NN technique to basin-scale $p\text{CO}_2^{\text{sea}}$ analysis (e.g. Lefèvre et al., 2005; Jamet et al., 2007; Friedrich and Oschlies, 2009a,b; Telszewski et al., 2009) concentrating mainly on the North Atlantic Ocean. Most recently, Telszewski et al. (2009) successfully applied a Self Organizing Map (SOM) based NN technique to reconstruct $p\text{CO}_2^{\text{sea}}$ distribution in the North Atlantic (10.5° N to 75.5° N , 9.5° E to 75.5° W) for three years (2004–2006) by examining non-linear/discontinuous relationship between $p\text{CO}_2^{\text{sea}}$ and ocean parameters of sea surface temperature (SST), mixed layer depth (MLD) and chlorophyll *a* concentration (CHL). One of the main benefits of this approach over the more traditional techniques such as the multiple linear regression is that there are numerous empirical relationships established (e.g. 2220 in Telszewski et al., 2009) between examined parameters allowing for more accurate representation of the highly variable system of interconnected water properties.

The North Pacific is dominated by two major current systems: the subarctic and subtropical gyres (Fig. 1). The cold Oyashio Current and the warm Kuroshio Current are the western boundary currents of the North Pacific subarctic and subtropical gyres, respectively. The two currents meet at mid-latitudes in the western North Pacific and turn toward the east as the North Pacific Current. The North Pacific has been typically characterized as a high-nutrient, low-chlorophyll region of the ocean at high latitudes

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because of the low influx of iron to the ocean surface (Dugdale and Wilkerson, 1991) and as a low-nutrient, low-chlorophyll region at low latitudes (Karl and Letelier, 2008). The subarctic North Pacific is an upwelling area, within which the transport of nutrient- and CO_2 -rich subsurface water to the surface assures high biological productivity in spring and summer. In the North Pacific there are thus quite large temporal and spatial variations of $p\text{CO}_2^{\text{sea}}$, the regional characteristics of which are generally understood from the LDEO climatology (Takahashi et al., 2009).

For analysis of temporal variability of $p\text{CO}_2^{\text{sea}}$ in the North Pacific, Takamura et al. (2010) used multiple linear regression (MLR) analysis to reconstruct $p\text{CO}_2^{\text{sea}}$ distributions as a function of SST and sea surface salinity (SSS) from 1999 to 2006 in mid-latitudes (25°N to 40°N , 120°W to 150°W , 140°E to 170°E). They resolved regional differences in secular increasing trends of $p\text{CO}_2^{\text{sea}}$, however their MLR technique could not be applied to spatial mapping. Sarma et al. (2006) used MLR relationships to estimate $p\text{CO}_2^{\text{sea}}$ from SST and satellite-based CHL observations in highlatitude regions of the eastern and western North Pacific, but the applicability of the MLR equations was limited to spring and summer.

The precise timeseries analyses of pelagic ocean $p\text{CO}_2^{\text{sea}}$ variability are limited to timeseries stations (Bates, 2007; Dore et al., 2009) where monthly $p\text{CO}_2^{\text{sea}}$ observations are available over extended time periods. Two areas of frequent shipboard observations of $p\text{CO}_2^{\text{sea}}$ other than timeseries stations are the eastern and western equatorial Pacific (Feely et al., 2006; Ishii et al., 2009), where apparent interannual $p\text{CO}_2^{\text{sea}}$ variations are known to occur as a result of the El Niño-Southern Oscillation (ENSO). Another place where there have been frequent shipboard $p\text{CO}_2^{\text{sea}}$ observations in the North Pacific is the 137°E repeat line (Midorikawa et al., 2006), where a weak but significant relationship between $p\text{CO}_2^{\text{sea}}$ and ENSO has been observed. A basin-wide analysis of observed $p\text{CO}_2^{\text{sea}}$ variability (including the analysis of the interannual signal) has not yet been successfully performed. An atmospheric CO_2 inverse model (Patra et al., 2005) and an ocean biogeochemical model (Valsala et al., 2012), however, suggest the possible correlation of the $p\text{CO}_2^{\text{sea}}$ variability with Pacific Decadal Oscillation (PDO).

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Our goal in this study was to reconstruct temporal and spatial variability of the $p\text{CO}_2^{\text{sea}}$ distribution in the North Pacific for seven years from 2002 to 2008 using the SOM technique applied to observational $p\text{CO}_2^{\text{sea}}$ dataset obtained by the NIES VOS program. We then compared the estimated $p\text{CO}_2^{\text{sea}}$ values with measured $p\text{CO}_2^{\text{sea}}$ values obtained from the NIES VOS program and other datasets in various areas of the North Pacific (Fig. 1). We also presented the change of the $p\text{CO}_2^{\text{sea}}$ distribution in response to the ENSO events.

2 Method and datasets

2.1 Method of $p\text{CO}_2^{\text{sea}}$ estimation

The study area includes the North Pacific from 10°N to 60°N and from 120°E to 90°W and is hereafter called the North Pacific, although we excluded coastal (bathymetric depth $< 500\text{m}$) and ice-covered ($\text{SST} < -1.8^\circ\text{C}$) areas from the analysis. In this study, we hypothesized that $p\text{CO}_2^{\text{sea}}$ could be estimated by a linear function of time and an SOM function (f_{SOM}) of four independent variables: SST, MLD, CHL, and SSS. The equation for $p\text{CO}_2^{\text{sea}}$ then takes the following form:

$$p\text{CO}_2^{\text{sea}} = a^*(t - t_{\text{ref}}) + f_{\text{SOM}}(\text{SST}, \text{MLD}, \text{CHL}, \text{SSS}) \quad (1)$$

In Eq. (1) “ a ” is the secular rate of change of atmospheric CO_2 in $\mu\text{atm day}^{-1}$, “ t ” denotes the date, and the reference date “ t_{ref} ” is set to 30 June 2005. The use of SSS in this study is consistent with the suggestion by Telszewski et al. (2009). In addition, we assumed $p\text{CO}_2^{\text{sea}}$ to be a linear function of time to take into account the influence of anthropogenic CO_2 emissions on $p\text{CO}_2^{\text{sea}}$, an effect that could not be accounted for by SST, MLD, CHL, or SSS. The anthropogenic influence on $p\text{CO}_2^{\text{sea}}$ is considered negligible for relatively short analyses e.g. three years (cf., Lefèvre et al., 2005; Telszewski et al., 2009), but it builds up to around $10\mu\text{atm}$ after seven years. Midorikawa et al. (2006) reported that the secular trend of $p\text{CO}_2^{\text{sea}}$ varied from 1.3 to $1.8\mu\text{atm yr}^{-1}$

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(close to the rate of increase of atmospheric CO_2) in the western subtropical North Pacific based on their measurements over 20 yr along 137°E . Wong et al. (2010) also reported that their 30-yr time series of measurements along line P showed that the long-term trend of $p\text{CO}_2^{\text{sea}}$ tracked the increase of atmospheric CO_2 in the eastern subarctic region. Takahashi et al. (2006) concluded that for the most part the increase of oceanic CO_2 in the North Pacific followed the increase of atmospheric CO_2 for the last 35 yr. We assumed in this study that the secular trend of $p\text{CO}_2^{\text{sea}}$ was approximately a constant fraction of the rate of change of atmospheric CO_2 over the North Pacific. Specifically, we assumed the value of the coefficient a in Eq. (1) to be 4.82×10^{-3} ($= 1.76/365.285$) $\mu\text{atm day}^{-1}$, which is the rate of increase of atmospheric CO_2 concentration converted from the CO_2 mole fractions ($x\text{CO}_2^{\text{air}}$) in the GlobalVIEW- CO_2 dataset (GLOBALVIEW-CO2, 2011) for the North Pacific region during the period of analysis.

The method for reconstructing $p\text{CO}_2^{\text{sea}}$ is based on the methodology of Telszewski et al. (2009), but we allocated about three times as many neurons on a flat sheet map (53×115) to improve the estimate. A neuron in this study is a vector that has four components: SST, MLD, CHL, and SSS. The values of these components, the training dataset, are prospectively normalized linearly (SST, SSS) or logarithmically (MLD, CHL) to create an even distribution among the input variables (cf., Fig. 3 of Telszewski et al., 2009). As indicated schematically in Fig. 2, three processes are executed in order to estimate basin-wide $p\text{CO}_2^{\text{sea}}$ fields in the SOM analysis procedure.

First, a neuron's weight vectors (x_j), which are linearly initialized, are repeatedly trained by input vectors (y_j), by being presented with the normalized SST, MLD, CHL, and SSS values, until the statistical composition of the training dataset is extracted and the neural network sufficiently represents the non-linear inter-dependence of proxy parameters used in training (Training Process in Fig. 2a). At each step, Euclidean distances (D) are calculated between the weight vectors of neurons and the input vector:

$$D(x_i, y_j) = [(x_{i_SST} - y_{j_SST})^2 + (x_{i_MLD} - y_{j_MLD})^2 + (x_{i_CHL} - y_{j_CHL})^2 + (x_{i_SSS} - y_{j_SSS})^2]^{0.5} \quad (2)$$

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The neuron closest to the training data point in Euclidean distance terms, here called the winner, is adjusted towards its value by a fraction of this distance dictated by the linearly time-decreasing learning function. At the same time, the neurons in the vicinity of the winner are also adjusted towards the value of the training data point, by a fraction of winner's adjustment in accordance with time-decreasing Gaussian function, as explained by Kohonen (2001). This process results in clustering of similar neurons and self-organization of the map. The observed $p\text{CO}_2^{\text{sea}}$ dataset is not required at this stage of the analysis.

Second, each neuron is labeled with an observed $p\text{CO}_2^{\text{sea}}$ value. Technically, the labeling process follows the same principles as the training process. The labeling data, which in this study consists of the observed $p\text{CO}_2^{\text{sea}}$ value assigned to a reference year by adding/subtracting the assumed temporal change of $p\text{CO}_2^{\text{sea}}$ and coincided with normalized SST, MLD, CHL, and SSS values, is presented to the neural network and a winner neuron is found (Labeling Process in Fig. 2b). Instead of adjusting the winner's value, it is labeled with the $p\text{CO}_2^{\text{sea}}$ value of the labeling data. This process is carried out for each of the observed $p\text{CO}_2^{\text{sea}}$ values. After the labeling process, most neurons are labeled with a $p\text{CO}_2^{\text{sea}}$ value. Neurons are consequently represented by five-dimensional vectors.

Third, the labeled SOM neurons are used to assign $p\text{CO}_2^{\text{sea}}$ values to the geographical grid points of the North Pacific (Mapping Process in Fig. 2c). The initial training data set is being presented to the trained and labeled SOM map. Upon computing the winner neuron, no adjustments are being made. Instead, the training data is assigned a $p\text{CO}_2^{\text{sea}}$ value of the winner neuron. This value becomes a $p\text{CO}_2^{\text{sea}}$ estimate for time and location determined by the spatio/temporal coordinates of each training data.

The reconstructed $p\text{CO}_2^{\text{sea}}$ distributions obtained as a result of this work will be available for scientific purposes at the website <http://soop.jp>.

2.2 Training data set (SST, MLD, CHL, SSS)

We used four high-resolution datasets, one for SST, MLD, CHL, and SSS to train the SOM. We obtained observed SST datasets from the Merged satellite and in situ data Global Daily Sea Surface Temperatures (MGDSST) Project (<http://goos.kishou.go.jp/rtrtdb/database.html>) at a daily frequency and 0.25° latitude \times 0.25° longitude resolution (Kurihara et al., 2006). We obtained daily assimilated MLD estimates from the GLObal Ocean ReanalYses and Simulations (GLORYS) model by Mercator Ocean (Le Centre National de la Recherche Scientifique, France) with a horizontal resolution of 0.25° latitude \times 0.25° longitude (Bernard et al., 2006; Ferry et al., 2010). Satellite CHL data were obtained from MODIS-Aqua and SeaWiFS Level 3 Standard products provided by NASA/GFSC/DAAC at a frequency of eight per day and resolution of 9 km (<http://oceancolor.gsfc.nasa.gov>). We obtained assimilated SSS estimates from the MOVE/MRI.COM-NP model of the Meteorological Research Institute, Japan at a frequency of 10 per day and horizontal resolution of 0.5° latitude and 0.5° longitude (Usui et al., 2006). For the analysis all parameters were re-gridded onto a frequency of one per day and horizontal resolution of 0.25° latitude \times 0.25° longitude.

2.3 $p\text{CO}_2^{\text{sea}}$ datasets for labeling

To estimate $p\text{CO}_2^{\text{sea}}$ fields in the North Pacific, it was necessary to label the trained SOM neurons with $p\text{CO}_2^{\text{sea}}$ values. In the labeling process, observed $p\text{CO}_2^{\text{sea}}$ data together with corresponding SST, MLD, CHL and SSS values were needed. We used a subset of the North Pacific dataset collected by the NIES VOS program. The $p\text{CO}_2^{\text{sea}}$ data is available for public use on the web page <http://soop.jp>. Information related to the four VOS lines is summarized in Table 1, and their composite cruise routes are depicted in Fig. 3. The commercial ships collaborating in the NIES-VOS program have taken part in trans-Pacific cruises between Japan and North America (10° N to 55° N, 140° E to 230° E) since March 1995 and between Japan and Oceania (45° S to 35° N, 140° E to 180° E) since July 2006. The ships have sailed regularly at intervals of about

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5–8 weeks between Japan and North America or Oceania. The volunteer ship that has sailed to North America sailed to the northern part of North America in the early part of the NIES-VOS program but since 2003 the route has occasionally shifted to the southeast to pass through the Panama Canal (Supplement Fig. 1). In contrast, the ship that has sailed between Japan and Oceania has sailed regularly as a member of a bi-weekly service fleet and the shipping route has been mostly fixed.

Although we reconstructed $p\text{CO}_2^{\text{sea}}$ in the North Pacific after 2002, in the analysis we used some in situ data for years 1998–2001 due to the insufficient data coverage especially in the subarctic region for years 2002–2008. The addition of $p\text{CO}_2^{\text{sea}}$ data from 1998 to 2001 to the labeling dataset improved the coverage of monthly measurements (Supplement Fig. 2). The improved coverage facilitated reproduction of the rapid drawdown of $p\text{CO}_2^{\text{sea}}$ due to phytoplankton photosynthesis during the spring bloom in the highly productive western mid-high latitude region.

Murphy et al. (2001b) and Fransson et al. (2006) have described the ocean surface CO_2 measurement system used by the NIES VOS program. The non-dispersive infrared analyzer used for those measurements was changed from a Licor 6262 to a Licor 7000 for the M/S *Pyxis* cruises in 2006 (Table 1). The CO_2 standard gases were calibrated by the NIES and are traceable to the World Meteorological Organization scale. The flow-through tandem equilibrator provides a continuous $p\text{CO}_2^{\text{sea}}$ output with high temporal resolution (Murphy et al., 2001b). The $p\text{CO}_2^{\text{sea}}$ measurements were made every 10 s and the $p\text{CO}_2^{\text{sea}}$ data were 10 min averages of those measurements accompanied by supplementary values of observed atmospheric and oceanic parameters. The $p\text{CO}_2^{\text{sea}}$ data were then averaged on a daily basis within 0.25° latitude \times 0.25° longitude grid boxes. Consequently, the number of $p\text{CO}_2^{\text{sea}}$ data by the NIES VOS program amounted to 317 332 and a total of 73 284 $p\text{CO}_2^{\text{sea}}$ data were binned as the labeling dataset.

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2.4 Other oceanic CO_2 datasets used for the validation of estimated $p\text{CO}_2^{\text{sea}}$

To validate $p\text{CO}_2^{\text{sea}}$ values reconstructed by the SOM analysis, we used the fugacity of oceanic CO_2 ($f\text{CO}_2^{\text{sea}}$) dataset from the Surface Ocean CO_2 Atlas (SOCAT; <http://www.socat.info>) database. That dataset has been in the public domain since September 2011 and has been subject to quality control as a part of an international collaboration of more than 10 institutes (including the NIES) which work on ocean surface CO_2 observations (Pfeil et al., 2012). In the North Pacific, the SOCAT database contains the $f\text{CO}_2^{\text{sea}}$ values measured mainly by NIES, the Japan Meteorological Agency (JMA), the Japan Agency for Marine-Earth Science and Technology (JAMSTEC), and the United States National Oceanic and Atmospheric Administration (NOAA). The average bias between the observed $p\text{CO}_2^{\text{sea}}$ and $f\text{CO}_2^{\text{sea}}$ values was calculated to be $0.3 \pm 0.1\%$. No corrections were made when comparing the two datasets because the uncertainty of the estimated $p\text{CO}_2^{\text{sea}}$ values was much larger than the difference (see Sect. 2.7.1 for details).

Underway $p\text{CO}_2^{\text{sea}}$ data and mooring $p\text{CO}_2^{\text{sea}}$ data collected by Wong and Johannessen (2010) and Sabine et al. (2010), respectively, were obtained from the Carbon Dioxide Information Analysis Center (CDIAC; <http://cdiac.ornl.gov/oceans/>). We used those data for the comparisons near Ocean Station P (50°N , 145°W). In addition, we used $p\text{CO}_2^{\text{sea}}$ values calculated from measurements of dissolved inorganic carbon (DIC) and total alkalinity (TA) at two stations: Station KNOT (44°N , 155°E ; Wakita et al., 2010) and Station ALOHA (23°N , 158°W ; Dore et al., 2009).

2.5 Ranges of the training/labeling dataset

As explained by Telszewski et al. (2009), one of the biggest advantages of SOM analysis over the more traditional methods is the fact that the temporal and spatial distribution of proxy parameters in the training and labeling datasets does not influence the analysis. Instead ranges covered by these parameters in each dataset, and more precisely their relative overlap determines whether the SOM will be able to reconstruct the

distribution of the predicted parameter. Ranges of the training/labeling datasets and the trained neurons are summarized in Table 2. The training dataset SSTs varied between -1.8°C and 32.7°C ; the MLD ranged from 1 m to more than 500 m; CHL varied from 0 to more than 10 mg m^{-3} ; and the range of SSS was 30.15–35.69. The values in the labeling datasets and neurons covered most of the range of values in the training dataset. However, the maximum MLDs in the labeling dataset (416 m) and in the neurons (194 m) were substantially lower than the maximum MLD in the training dataset ($> 500\text{ m}$; Table 2). Our results indicate that the correlation between $p\text{CO}_2^{\text{sea}}$ and MLD was not apparent when the MLD was deeper than 200 m (not shown), a result also reported for the North Atlantic by Telszewski et al. (2009).

2.6 Reconstructing $p\text{CO}_2^{\text{sea}}$ distributions in winter at high latitudes

The three products, SST, MLD, and SSS, provided full basin-wide coverage from 2002 to 2008. However, the CHL data were affected by the lack of satellite coverage from November to January at high latitudes of the North Pacific (north of 45°N) due to the low-angle of the sun during that time and enormous atmospheric correction required to retrieve the signal. To reconstruct $p\text{CO}_2^{\text{sea}}$ for this area during those months, we assumed that $p\text{CO}_2^{\text{sea}}$ could be adequately characterized by only three parameters: SST, MLD and SSS. The rationale for this assumption is that biological activity is relatively low during the winter at high latitudes (e.g. Imai et al., 2002). Therefore, we prepared another SOM trained by three parameters SST, MLD and SSS. We generated complete $p\text{CO}_2^{\text{sea}}$ maps in the study area by combining the $p\text{CO}_2^{\text{sea}}$ values obtained with the fourparameter SOM including CHL with the values obtained with the three-parameter SOM excluding CHL in the area north of 45°N during the period from November to January. We checked the difference between the $p\text{CO}_2^{\text{sea}}$ values estimated with the four-parameter SOM and the three-parameter SOM in the region between 40°N and 45°N and found the difference to be negligibly small from November to January because of the relatively low biological activity during that time. The implication is that combining the results from the two SOMs does not produce any bias.

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2.7 Uncertainty and improvement of the $p\text{CO}_2^{\text{sea}}$ estimate

2.7.1 Uncertainty

For each in situ $p\text{CO}_2^{\text{sea}}$ measurement, the corresponding SOM $p\text{CO}_2^{\text{sea}}$ estimate was determined on the basis of the spatial (0.25° longitude \times 0.25° latitude grid) and temporal (daily intervals between 1 January 2002 and 31 December 2008) coordinates associated with the measurement. We calculated the root mean square error (RMSE) between observed $p\text{CO}_2^{\text{sea}}$ and estimated $p\text{CO}_2^{\text{sea}}$ values as follows:

$$\text{RMSE} = \sqrt{\frac{\sum (p\text{CO}_2^{\text{sea}}(\text{estimated})^2 - p\text{CO}_2^{\text{sea}}(\text{observed})^2)}{n}} \quad (3)$$

where n is the number of points in the labeling dataset. The RMSE provided an estimate of the uncertainty of the method in reproducing the in situ measurements and equaled $17.6 \mu\text{atm}$, or 5.0% of the average $p\text{CO}_2^{\text{sea}}$ of the in situ dataset. A scatter plot of the estimated $p\text{CO}_2^{\text{sea}}$ against the observed $p\text{CO}_2^{\text{sea}}$ (Fig. 4) shows that the values are clustered around the 1 : 1 line with slightly more scatter at high $p\text{CO}_2^{\text{sea}}$ over $400 \mu\text{atm}$.

Zeng et al. (2002) estimated the distribution of monthly average $p\text{CO}_2^{\text{sea}}$ in the North Pacific based on data from the NIES VOS program from 1995 to 1999 and reported that the estimated $p\text{CO}_2^{\text{sea}}$ agreed with the in situ $p\text{CO}_2^{\text{sea}}$ to within a RMSE of $24.9 \mu\text{atm}$. Sarma et al. (2006) used a MLR method to estimate the distribution of monthly average $p\text{CO}_2^{\text{sea}}$ in the North Pacific during the spring-summer period in 1998 and reported that the derived $p\text{CO}_2^{\text{sea}}$ agreed with the shipboard $p\text{CO}_2^{\text{sea}}$ observations to within a RMSE of 17–23 μatm . Although the present study represents a much longer period of time than the previous reports, the RMSE achieved in this study is comparable to or better than the RMSEs achieved in the shorter studies.

2.7.2 Improvement in the NN scheme

We have implemented two major improvements over the previous attempt to utilize SOM neural network to compute the $p\text{CO}_2^{\text{sea}}$ distribution. In the first one we followed the suggestion of Telszewski et al. (2009) to use the SSS dataset as one of the training datasets to improve $p\text{CO}_2^{\text{sea}}$ estimates. To quantify the improvement achieved by using the SSS dataset, we generated another $p\text{CO}_2^{\text{sea}}$ map derived with a three-parameter SOM that excluded SSS and compared the result with the four-parameter SOM result. The RMSE of the three-parameter SOM estimate was $20.0 \mu\text{atm}$. Use of SSS in the training dataset therefore reduced the RMSE by 12 %. The $p\text{CO}_2^{\text{sea}}$ distributions were also improved by the use of the SSS data. To visualize the differences, we mapped seven-year averaged monthly $p\text{CO}_2^{\text{sea}}$ distributions in February and August derived with and without inclusion of SSS in the training dataset (Fig. 5). The estimated $p\text{CO}_2^{\text{sea}}$ derived from the three-parameter SOM in February is characterized by a smaller longitudinal difference in mid latitudes than the $p\text{CO}_2^{\text{sea}}$ derived from the four-parameter SOM. Furthermore, use of the four-parameter SOM enabled reconstruction of quite high $p\text{CO}_2^{\text{sea}}$ values in August in the eastern low/mid-latitude region, where the North Pacific current flows, whereas use of the three-parameter SOM failed to reproduce this feature. Figure 6 shows the temporal variation of $p\text{CO}_2^{\text{sea}}$ derived with the two SOMs in the region (37°N , 140°W). It clearly shows that the agreement between observed and estimated $p\text{CO}_2^{\text{sea}}$ values was better for the four-parameter SOM than the three-parameter SOM. The RMSE in the region was improved from $15.9 \mu\text{atm}$ to $10.6 \mu\text{atm}$ by inclusion of SSS. The improvement was especially apparent during the summer when high $p\text{CO}_2^{\text{sea}}$ values (about $400 \mu\text{atm}$) were observed. The reason why inclusion of SSS improved the $p\text{CO}_2^{\text{sea}}$ estimate is unclear. Inclusion of SSS in the SOM analysis may facilitate differentiation between temporal and spatial oceanic variability that could not be elucidated with only SST, MLD, and CHL.

Taking into account the influence of anthropogenic CO_2 emissions on the trend of $p\text{CO}_2^{\text{sea}}$ was the second improvement introduced by this work. As described above it

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was done by adding or subtracting $1.76 \mu\text{atm yr}^{-1}$ ($4.82 \times 10^{-3} \mu\text{atm day}^{-1}$) to project observed $p\text{CO}_2^{\text{sea}}$ values to the $p\text{CO}_2^{\text{sea}}$ values in the reference year of 2005 (Eq. 1). The improvement of the $p\text{CO}_2^{\text{sea}}$ estimate by making this correction was not spatially uniform. For example, the RMSEs were reduced by adding the term from $10.2 \mu\text{atm}$ to $9.1 \mu\text{atm}$ in the Station P area, from $8.8 \mu\text{atm}$ to $7.4 \mu\text{atm}$ in the WST area, and from $10.8 \mu\text{atm}$ to $7.9 \mu\text{atm}$ in the Station ALOHA area. In contrast, the improvements at Station KNOT area and the KE area were unclear (see in Fig. 1). Overall, inclusion of the secular trend effect slightly, but statistically significantly ($p < 0.05$), reduced the RMSE for the whole of the North Pacific.

3 Temporal and spatial variation of $p\text{CO}_2^{\text{sea}}$

3.1 Mapping of seven-year averaged monthly $p\text{CO}_2^{\text{sea}}$ distributions

Figure 7 presents a comparison of seven-year (2002 to 2008) averaged monthly $p\text{CO}_2^{\text{sea}}$ distributions derived from SOM results for February, May, August, and November with LDEO $p\text{CO}_2^{\text{sea}}$ climatology (Takahashi et al., 2009). The comparison reveals that the reconstructed $p\text{CO}_2^{\text{sea}}$ maps are generally similar to the LDEO climatology however the resolution of the SOM estimated $p\text{CO}_2^{\text{sea}}$ distributions is much higher, and the results more precisely resolve some oceanic features. Both studies show high $p\text{CO}_2^{\text{sea}}$ values (over $400 \mu\text{atm}$) at high latitudes in the North Pacific in February, however the SOM reconstructed $p\text{CO}_2^{\text{sea}}$ distribution shows $p\text{CO}_2^{\text{sea}}$ rich water between the Bering Sea and the coast of northern Japan along the axis of the cold, southward-flowing Eastern Kamchatka Current. As described in Sect. 2.7.2, high $p\text{CO}_2^{\text{sea}}$ values are apparent from June to October in the eastern low/mid-latitude region, where the North Pacific Current and the California Current flow, and the high $p\text{CO}_2^{\text{sea}}$ field dominates. With respect to the coastal region, low estimates of $p\text{CO}_2^{\text{sea}}$ stretch along the coastline from the Aleutian Islands to the California Peninsula from May to October, when the concentration of phytoplankton is high.

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The reconstructed $p\text{CO}_2^{\text{sea}}$ distributions in this study clearly show a tongue of very low $p\text{CO}_2^{\text{sea}}$ (about $320 \mu\text{atm}$) water distributed (except in August) uniformly between the western and central mid-latitude regions of the North Pacific (Fig. 7). Such low $p\text{CO}_2^{\text{sea}}$ values are attributed to high rates of photosynthesis (Kameda, 2003) and cooling of the seawater that occurred mainly in the subtropics. In addition, a band of relatively high $p\text{CO}_2^{\text{sea}}$ caused mainly by a seasonal rise in temperature was also apparent during the period from May to September in the western North Pacific between 15°N and 30°N . The temperature rise began in April and amounted to about $2\text{--}5^\circ \text{C}$. Following the temperature dependence of $p\text{CO}_2^{\text{sea}}$ given by Takahashi et al. (1993), $\delta \ln p\text{CO}_2^{\text{sea}} / \delta T = 0.0423^\circ \text{C}^{-1}$, the expected $p\text{CO}_2^{\text{sea}}$ rise due to the temperature effect is about $30\text{--}70 \mu\text{atm}$. The observed increase in expected $p\text{CO}_2^{\text{sea}}$ is only about half of the expected $p\text{CO}_2^{\text{sea}}$ rise due to temperature effects. The increase may have been attenuated by other factors such as photosynthetic uptake of CO_2 .

3.2 Reproducibility of temporal $p\text{CO}_2^{\text{sea}}$ variations in each of six regions

To facilitate a discussion about the temporal variations of $p\text{CO}_2^{\text{sea}}$ in the North Pacific, Fig. 8 shows the time series of area-averaged $p\text{CO}_2^{\text{sea}}$ estimated in this study along with the estimates of Takamura et al. (2010). The grid size of all the averaged areas except in the Station KNOT area is set to 4° latitude \times 5° longitude, whereas the Station KNOT area is set to 43.5°N to 45.5°N , 153°E to 157°E to exclude the transition zone between the Kuroshio and the Oyashio. The panels in Fig. 8 also include comparisons between the observed $p\text{CO}_2^{\text{sea}}$ data from various observation programs and the data from the NIES VOS program in the same area. The estimated $p\text{CO}_2^{\text{sea}}$ values at each location generally agree well with observed values and other estimates, most of the data lying within the spatial variability (twice the spatial standard deviation; $2\text{-}\sigma$) calculated for each area. However disagreements greater than $20 \mu\text{atm}$ between estimated $p\text{CO}_2^{\text{sea}}$ and observed $p\text{CO}_2^{\text{sea}}$, as exemplified in the area surrounding Station KNOT (Fig. 8a), occur occasionally. The calculated $p\text{CO}_2^{\text{sea}}$ in Station P area generally agree well with

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the data from the NIES VOS program as well as with $p\text{CO}_2^{\text{sea}}$ values measured by an underway system from 2002 to 2003 and by a moored buoy system from 2007 to 2008 (Fig. 8b). The largest seasonal amplitudes tend to coincide with the largest disagreements between the estimates (Zeng et al., 2002). The calculated $p\text{CO}_2^{\text{sea}}$ values in the KE area of the eastern mid-latitude region (Fig. 8c) agree well with the NIES dataset as well as with the $f\text{CO}_2^{\text{sea}}$ values from the SOCAT dataset, all $p\text{CO}_2^{\text{sea}}$ values lying within the spatial variability. The results of Takamura et al. (2010) also agree with the $p\text{CO}_2^{\text{sea}}$ measurements to within 15–20 μatm , and the temporal pattern of those data is generally consistent with the $p\text{CO}_2^{\text{sea}}$ estimates within the spatial variability from this study. The temporal variations of $p\text{CO}_2^{\text{sea}}$ in the WST area (Fig. 8d) and Station ALOHA area (Fig. 8e) agree well with the $p\text{CO}_2^{\text{sea}}$ values in the SOCAT dataset, even though the observed $p\text{CO}_2^{\text{sea}}$ data used for the labeling process in the SOM analysis rarely existed in these areas. The calculated $p\text{CO}_2^{\text{sea}}$ values in the EST area (Fig. 8f) also agree well with the data from the NIES VOS program. As shown in the Fig. 8d–f, the patterns of variation were similar in the WST area, the Station ALOHA area, and the EST area. Keeping in mind that only data obtained by the NIES VOS program were used in the SOM labeling process, these results suggest that the labeling process allows labeled SOM neurons to effectively learn $p\text{CO}_2^{\text{sea}}$ variations from $p\text{CO}_2^{\text{sea}}$ values observed in other subtropical areas. This confirms the notion that the SOM technique overcomes problems associated with temporal and spatial data scarcity.

3.3 Difference of $p\text{CO}_2^{\text{sea}}$ distributions during ENSO events

The ENSO has a large influence on the climate of the North Pacific (IPCC, 2007), and large fluctuations of $p\text{CO}_2^{\text{sea}}$ coincided with the ENSO cycle have also been observed in the equatorial Pacific (Feely et al., 2006; Ishii et al., 2009). Based on their measurements from 1983 to 2003, Midorikawa et al. (2006) have suggested that the interannual variation of $p\text{CO}_2^{\text{sea}}$ in the western subtropical North Pacific is also related to the ENSO. Although the extent of the ENSO influence on oceanic and atmospheric variables is known to be global (Trenberth and Caron, 2000), the impact of the ENSO

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on the distribution of $p\text{CO}_2^{\text{sea}}$ over the entire area of the North Pacific is not well understood. Figure 9 depicts the estimated distributions of the de-trended $p\text{CO}_2^{\text{sea}}$, SST, and MLD anomalies during the winters of 2003 (i.e. El Niño) and 2008 (i.e. La Niña). Anomalies in Fig. 9 are deviations from the monthly climatology for the period of 2002–

2008. El Niño/La Niña periods were chosen in accordance with JMA's definition based on the five-month running mean SST deviation for the NINO.3 region (5°S to 5°N , 150°E to 90°E). The patterns of SST anomalies in Fig. 9 are typical of El Niño and La Niña winters (Trenberth and Caron, 2000). The $p\text{CO}_2^{\text{sea}}$ anomaly related to ENSO events is easily discernible in the western-central subtropical region, in the eastern subarctic region, and in the eastern mid-latitude region south of 30°N . For example, a negative $p\text{CO}_2^{\text{sea}}$ anomaly is apparent in the western-central subtropical region in 2003 (El Niño), when the SST anomaly was negative; whereas a positive $p\text{CO}_2^{\text{sea}}$ anomaly is apparent in 2008 (La Niña), when the SST anomaly is positive. The opposite pattern is observed for the eastern mid-latitude region south of 30°N . The amplitudes of the associated $p\text{CO}_2^{\text{sea}}$ anomalies are about $15\ \mu\text{atm}$, and their SST amplitudes are 1°C . The $p\text{CO}_2^{\text{sea}}$ change closely tracked the SST change in accordance with the iso-chemical temperature dependency of Takahashi et al. (1993).

A negative relationship between $p\text{CO}_2^{\text{sea}}$ and SST is apparent in the eastern subarctic North Pacific, where the signal of thermodynamic changes on variations of $p\text{CO}_2^{\text{sea}}$ was opposite to that seen in the subtropics. As indicated in Fig. 9, the MLD anomaly clearly showed the pattern typical of ENSO events (Alexander et al., 2002). In contrast, the MLD was deeper in 2008 than in 2003 in the eastern subarctic region. This result indicates that more CO_2 -rich subsurface water was entrained into surface waters during the La Niña period than during the El Niño period.

4 Summary

In this study we used the SOM technique of Telszewski et al. (2009) to examine the temporal and spatial variations of $p\text{CO}_2^{\text{sea}}$ in the North Pacific during the period 2002–2008. To improve the $p\text{CO}_2^{\text{sea}}$ estimates, we used SSS as an additional training parameter and assumed a trend of increasing $p\text{CO}_2^{\text{sea}}$ to take into account the effect of anthropogenic CO_2 emissions on $p\text{CO}_2^{\text{sea}}$. The estimated results revealed that the SOM technique could satisfactorily reconstruct variations of $p\text{CO}_2^{\text{sea}}$ associated with bio-geophysical processes expressed by the variability in four proxy parameters: SST, MLD, CHL and SSS. We calculated the uncertainty of the $p\text{CO}_2^{\text{sea}}$ estimation to be 17.6 μatm . The fact that the uncertainty was reduced by about 12 % by inclusion of SSS in the training dataset suggests that SSS can be a useful parameter for the estimation of temporal and spatial variation of $p\text{CO}_2^{\text{sea}}$. We also found that $p\text{CO}_2^{\text{sea}}$ estimates were improved by taking account of the temporal trend associated with anthropogenic CO_2 emissions.

The calculated $p\text{CO}_2^{\text{sea}}$ variations in six ocean areas generally agreed well not only with the NIES VOS program $p\text{CO}_2^{\text{sea}}$ data used for the labeling process but also with other in situ $p\text{CO}_2^{\text{sea}}$ datasets. Seven-year (2002–2008) averaged monthly $p\text{CO}_2^{\text{sea}}$ distributions were similar to 35-yr climatology $p\text{CO}_2^{\text{sea}}$ distributions (Takahashi et al., 2009). However, the SOM-based $p\text{CO}_2^{\text{sea}}$ mapping with its high spatial resolution reflected oceanic conditions with more accuracy. The estimated inter-annual $p\text{CO}_2^{\text{sea}}$ variability revealed a difference in the spatial pattern of $p\text{CO}_2^{\text{sea}}$ during the winter of the El Niño period in 2003 and the La Niña period in 2008. A negative $p\text{CO}_2^{\text{sea}}$ anomaly was apparent in 2003 in the western subtropical North Pacific and in the eastern subarctic North Pacific off the coast of Alaska, whereas a positive anomaly was apparent in 2008 in the same regions. In the western subtropical and eastern mid-latitude regions, the correlation of the $p\text{CO}_2^{\text{sea}}$ variability with ENSO events seemed to be related mainly to changes in the thermodynamic properties of seawater. In contrast, similar correlation

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in the subarctic North Pacific seemed to be related to changes in vertical transport of CO₂ rich subsurface waters.

Further improvement of $p\text{CO}_2^{\text{sea}}$ estimates will require an increase in the number of data points used for labeling to reduce the $p\text{CO}_2^{\text{sea}}$ error. We plan to undertake a longer-term study using the community quality controlled (Pfeil et al., 2012) SOCAT collection as the labeling dataset. The number of neurons is also crucial for accurate $p\text{CO}_2^{\text{sea}}$ estimation. In this study we used three times as many neurons as Telszewski et al. (2009) to achieve adequate reproducibility of the $p\text{CO}_2^{\text{sea}}$ estimates. However, the number of neurons used in this study was determined not by scientific analysis, but was based on the available computing power. More sensitivity studies are needed to determine the relationship between the estimated error and the number of neurons. It might also be possible to improve the $p\text{CO}_2^{\text{sea}}$ estimate by inclusion of more ocean parameters. Sea surface height is a potential training parameter with basin-wide coverage. Even if sea surface height cannot be directly related to $p\text{CO}_2^{\text{sea}}$ variations, a combination of parameters can be used to identify location and time more precisely.

In addition to estimates in the North Pacific, long-term global $p\text{CO}_2^{\text{sea}}$ mapping based on such measurements is also important for understanding inter-annual variations of air-sea CO₂ exchanges. Although $p\text{CO}_2^{\text{sea}}$ variations related to climate changes such as the PDO have been reported (Valsala et al., 2012), the overall impact of such changes on global $p\text{CO}_2^{\text{sea}}$ variations is not well understood. In the present study, the study area was confined to the North Pacific. However, the SOM technique used in the present study has the potential to estimate $p\text{CO}_2^{\text{sea}}$ in regions where there are insufficient numbers of observations, and such regions will be our next target. It is axiomatic to say that further $p\text{CO}_2^{\text{sea}}$ measurements are critical, especially in the South Pacific, where few $p\text{CO}_2^{\text{sea}}$ measurements have been made (Sabine et al., 2012).

Supplementary material related to this article is available online at:
<http://www.biogeosciences-discuss.net/10/4575/2013/bgd-10-4575-2013-supplement.pdf>.

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Table 1. Summary of NIES surface ocean CO_2 measurements made by four volunteer observing ships in the Pacific Ocean.

Vessel name	Period	Observed area	NDIR analyzer
<i>M/S Skaugran</i>	Mar 1995–Sep 1999	North Pacific	Rosemount Analytical Model 880A
<i>M/S Alligator Hope</i>	Nov 1999–Mar 2001	North Pacific	Licor 6262
<i>M/S Pyxis</i>	Jul 2002–present	North Pacific	Licor 6262 (–Apr 2006) Licor 7000 (Apr 2006–)
<i>M/S Trans Future 5</i>	Jul 2006–present	Western North/ South Pacific	Licor 6262

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Table 2. Ranges of SST, MLD, CHL and SSS in the training dataset, the labeling dataset and the trained neurons. Percentages of the training data within the range of the labeling dataset and the neurons are given for each parameter.

	SST ($^{\circ}\text{C}$)			MLD (m)			CHL (mg m^{-3})			SSS (psu)		
	Min	Max	cover (%)	Min	Max	cover (%)	Min	Max	cover (%)	Min	Max	cover (%)
Training data	-1.8	32.7		1	> 500		0.00	10		30.15	35.69	
Labeling data	-1.1	31.5	99.940	1	416	99.995	0.00	10	100	30.15	35.69	100
Neurons	-0.6	29.4	96.651	1	194	99.807	0.00	3.2	99.778	31.79	35.58	99.886

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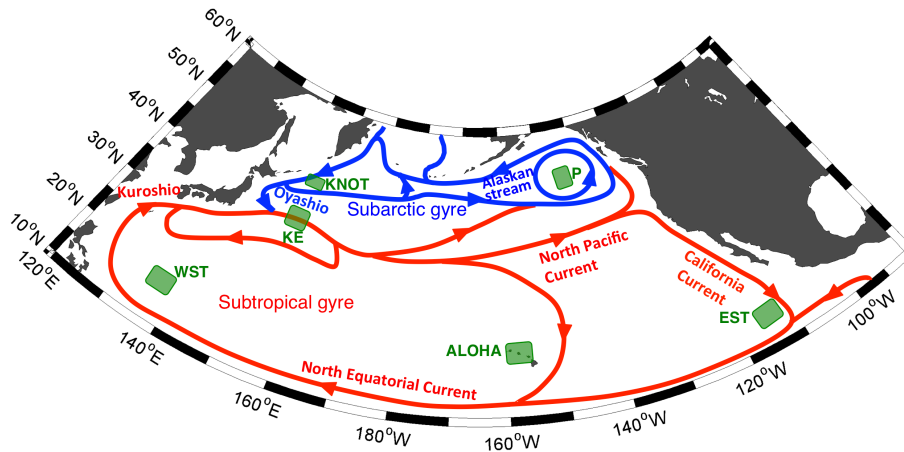


Fig. 1. Schematic map of the current system in the North Pacific rewritten from Schmitz (1996) with the areas of three ocean time-series stations and three areas for comparison of seasonal and interannual variations of $p\text{CO}_2^{\text{sea}}$ and related oceanic parameters “KNOT”, “P”, and “ALOHA” denote ocean time-series station areas in the North Pacific, and “WST”, “KE”, and “EST” denote ocean areas of the western subtropics, Kuroshio extension, and eastern subtropics, respectively.

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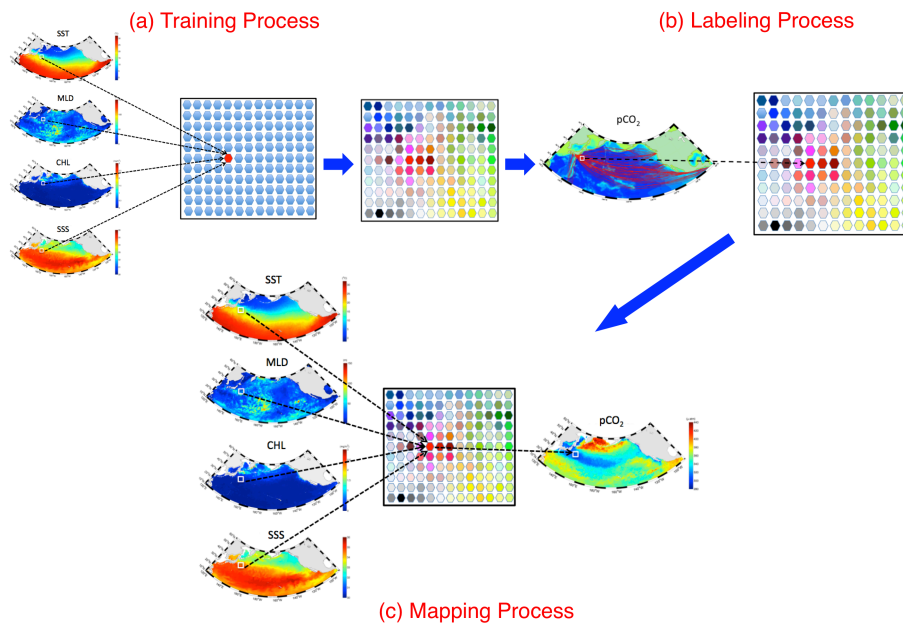


Fig. 2. Visualization of the processes that make up the procedure for SOM analysis.

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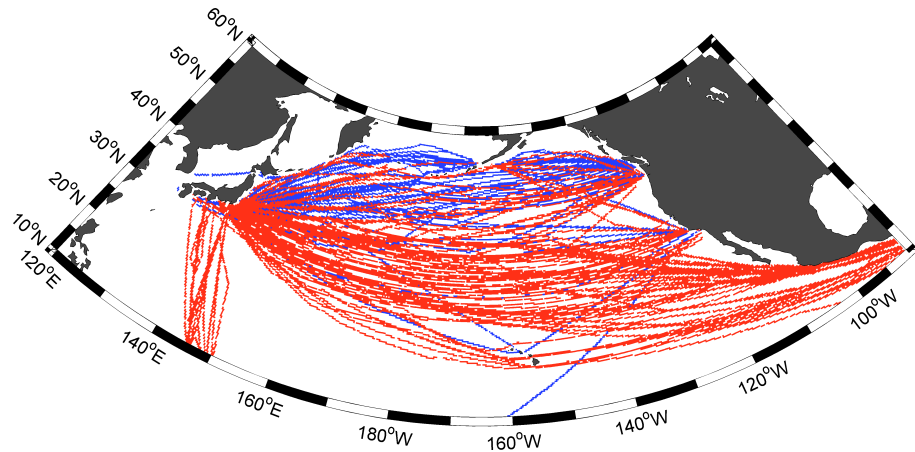


Fig. 3. Composite cruise tracks from 1998 to 2008. Blue lines represent the cruises from 1998 to 2001 and red lines show the cruises after 2002.

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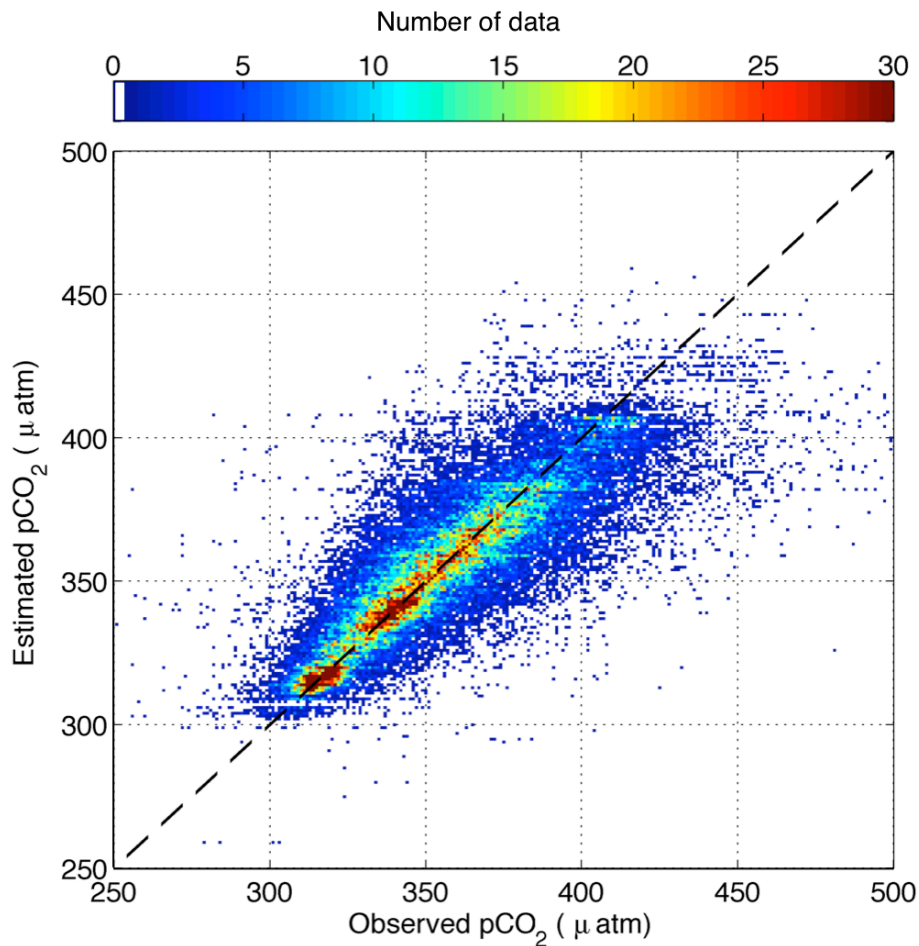


Fig. 4. Scatter plot of estimated $p\text{CO}_2^{\text{sea}}$ with observed $p\text{CO}_2^{\text{sea}}$. Colors indicate the number of data in a $1 \mu\text{atm} \times 1 \mu\text{atm}$ bin.

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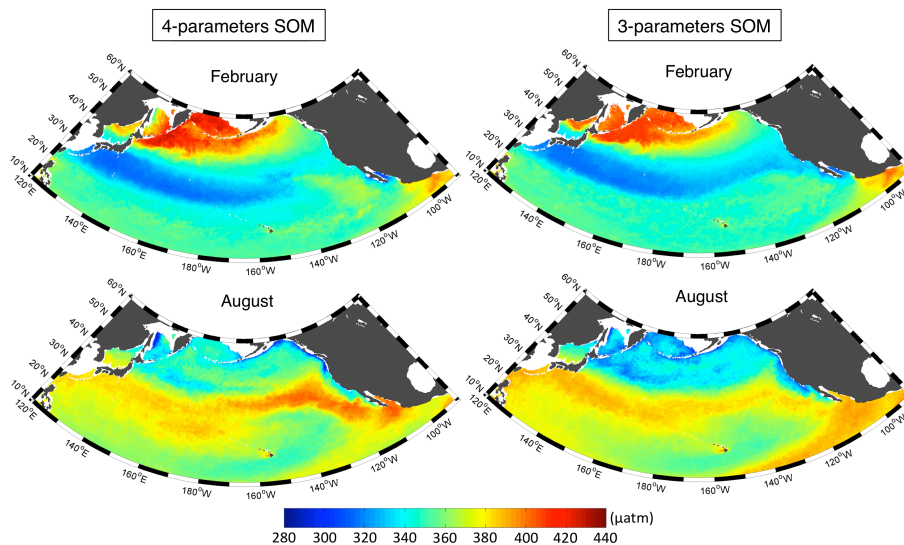


Fig. 5. Comparison of seven-year averaged monthly $p\text{CO}_2^{\text{sea}}$ distributions from 2002 to 2008 in February (upper) and August (bottom). Figures on the left are the $p\text{CO}_2^{\text{sea}}$ distributions estimated from the four-parameter SOM including SSS. Figures on the right were estimated from the three-parameter SOM without SSS.

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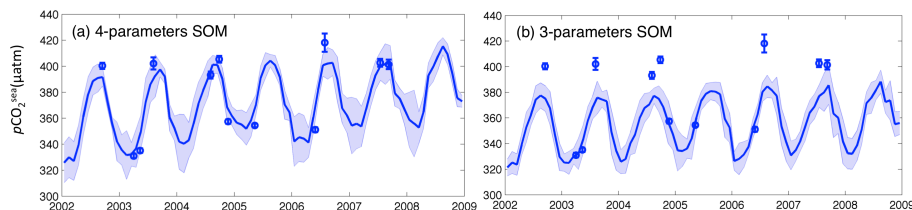


Fig. 6. The $p\text{CO}_2^{\text{sea}}$ variations in the area (36°N to 38°N , 138°W to 142°W) where the North Pacific current flows, estimated by the four-parameter SOM including SSS **(a)** and the three-parameter SOM without SSS **(b)**. The blue lines and the shaded areas indicate the mean values of the estimated $p\text{CO}_2^{\text{sea}}$ and the spatial variability ($2\text{-}\sigma$) calculated in the area, respectively. Blue circles are the in situ $p\text{CO}_2^{\text{sea}}$ values obtained from the NIES VOS program. The $p\text{CO}_2^{\text{sea}}$ observations in the target areas include several grid points binned by 0.25° latitude \times 0.25° longitude resolution, and the bar indicates the spatial variability ($1\text{-}\sigma$).

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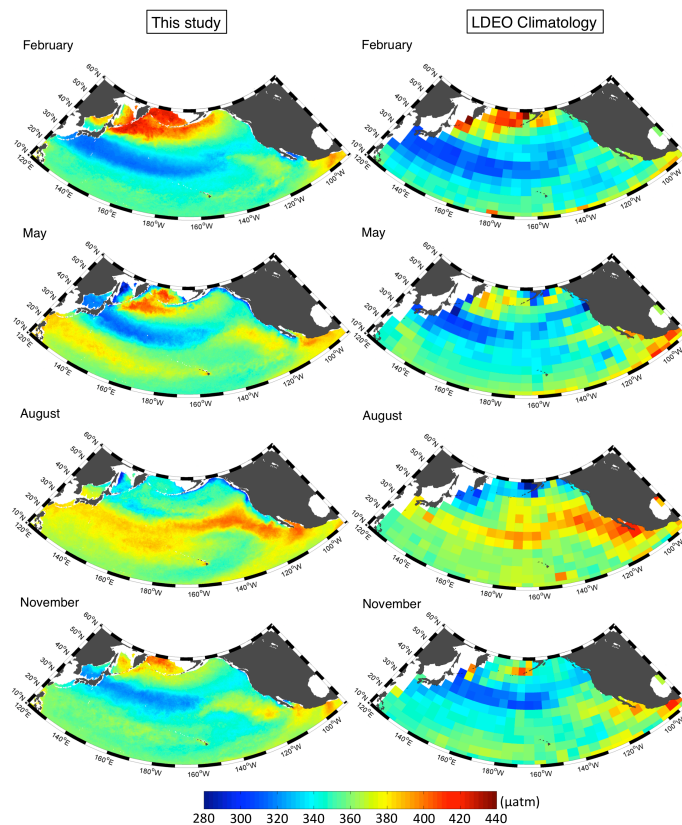


Fig. 7. Distributions of the seven-year averaged monthly mean $p\text{CO}_2^{\text{sea}}$ in this study (panels on left) and the LDEO monthly $p\text{CO}_2^{\text{sea}}$ climatology (panels on right, but with $8.8 \mu\text{atm}$ added to the maps to change the reference year from 2000 to 2005) for February, May, August, and November.

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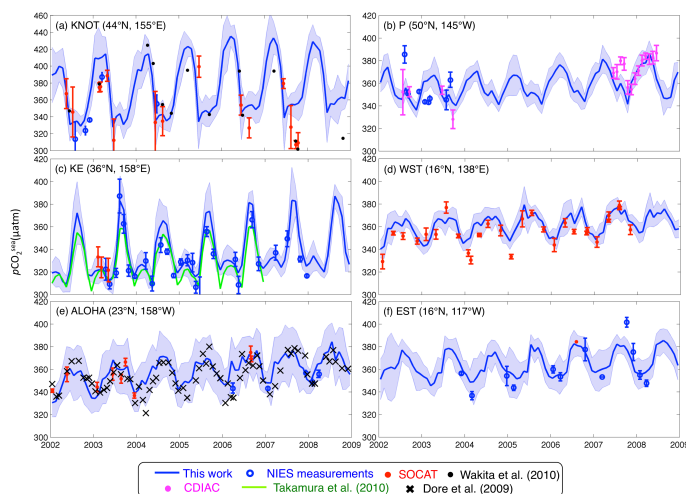


Fig. 8. Interannual variation of $p\text{CO}_2^{\text{sea}}$ (μatm) within time-series station areas and within ocean areas. The blue solid lines and shaded areas show the monthly $p\text{CO}_2^{\text{sea}}$ values and the spatial variability ($2\text{-}\sigma$) calculated in the respective areas. The grid size of all the averaged areas except in the Station KNOT area is set to 4° latitude \times 5° longitude, whereas the Station KNOT area is set to 43.5°N to 45.5°N , 153°E to 157°E . Blue circles and red dots are in situ $p\text{CO}_2^{\text{sea}}/f\text{CO}_2^{\text{sea}}$ values obtained from NIES measurements and the SOCAT database, respectively. Black dots and crosses on panel (a) and (c) are the $p\text{CO}_2^{\text{sea}}$ values calculated from measurements of DIC and TA reported by Wakita et al. (2010) and Dore et al. (2009). Purple dots on panel (b) are the $p\text{CO}_2^{\text{sea}}$ values observed by Wong and Johansen (2010) and Sabine et al. (2010). In panel (c), the solid green line denotes the $p\text{CO}_2^{\text{sea}}$ values during the 2002–2006 period estimated by Takamura et al. (2010). Note that the range of the ordinate in the Station KNOT area is larger than those of other station areas.

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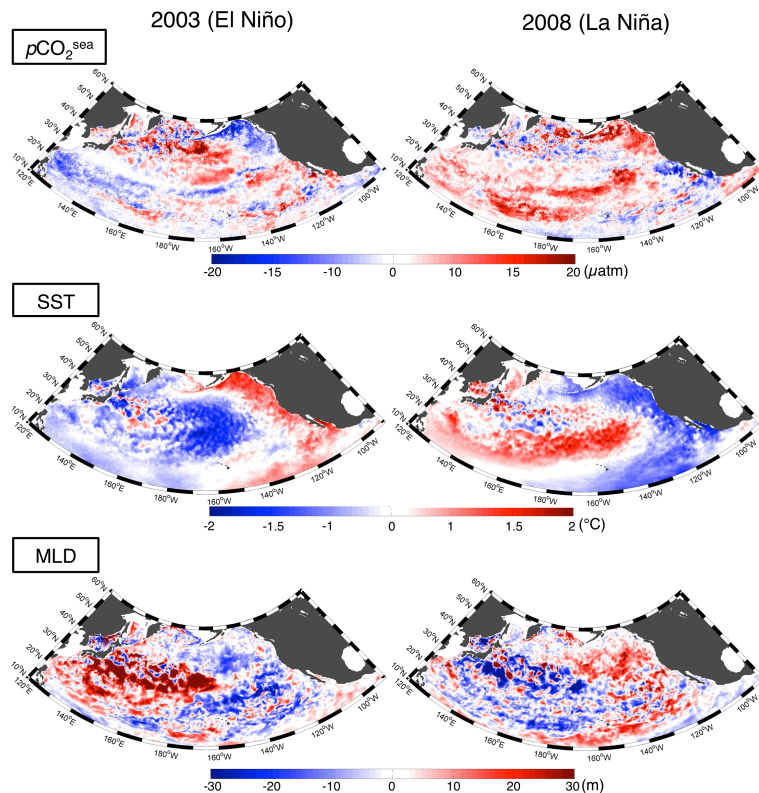


Fig. 9. Anomalies from the monthly climatology for the period 2002–2008 for de-trending $p\text{CO}_2^{\text{sea}}$ (upper), SST (middle), and MLD (bottom) distributions during the winter of 2003 (panels on left) and 2008 (panels on right).

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