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Neural network-based estimates of Southern Ocean net community production from in-situ O₂/Ar and satellite observation: a methodological study

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Received: 6 September 2013 – Accepted: 17 October 2013 – Published: 30 October 2013

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Published by Copernicus Publications on behalf of the European Geosciences Union.

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Abstract

Southern Ocean organic carbon export plays an important role in the global carbon cycle, yet its basin-scale climatology and variability are uncertain due to limited coverage of in situ observations. In this study, a neural network approach based on the self-organizing map (SOM) is adopted to construct weekly gridded ($1^\circ \times 1^\circ$) maps of organic carbon export for the Southern Ocean from 1998 to 2009. The SOM is trained with in situ measurements of O_2/Ar -derived net community production (NCP) that are tightly linked to the carbon export in the mixed layer on timescales of 1–2 weeks, and six potential NCP predictors: photosynthetically available radiation (PAR), particulate organic carbon (POC), chlorophyll (Chl), sea surface temperature (SST), sea surface height (SSH), and mixed layer depth (MLD). This non-parametric approach is based entirely on the observed statistical relationships between NCP and the predictors, and therefore is strongly constrained by observations.

A thorough cross-validation yields three retained NCP predictors, Chl, PAR, and MLD. Our constructed NCP is further validated by good agreement with previously published independent in situ derived NCP of weekly or longer temporal resolution through real-time and climatological comparisons at various sampling sites. The resulting November–March NCP climatology reveals a pronounced zonal band of high NCP roughly following the subtropical front in the Atlantic, Indian and western Pacific sectors, and turns southeastward shortly after the dateline. Other regions of elevated NCP include the upwelling zones off Chile and Namibia, Patagonian Shelf, Antarctic coast, and areas surrounding the Islands of Kerguelen, South Georgia, and Crozet. This basin-scale NCP climatology closely resembles that of the satellite POC field and observed air-sea CO_2 flux. The long-term mean area-integrated NCP south of $50^\circ S$ from our dataset, $14 \text{ mmol C m}^{-2} \text{ d}^{-1}$, falls within the range of $8.3\text{--}24 \text{ mmol C m}^{-2} \text{ d}^{-1}$ from other model estimates. A broad agreement is found in the basin-wide NCP climatology among various models but with significant spatial variations, particularly in the Patagonian Shelf. Our approach provides a comprehensive view of the Southern

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Ocean NCP climatology and a potential opportunity to further investigate interannual and intraseasonal variability.

1 Introduction

The Southern Ocean plays an important role in the global carbon cycle. The current annual global ocean uptake of atmospheric carbon dioxide (CO_2) is about 2 petagrams (Pg) of carbon, half of which is taken up by the vast Southern Ocean south of 30°S (Takahashi et al., 2012). Atmospheric CO_2 absorbed by the ocean can be transferred from the surface to the deep ocean via various physical, chemical and biological mechanisms associated with the solubility and biological pumps (Volk and Hoffert, 1985; Carlson et al., 2010).

Biological carbon export from the ocean surface is a function of various processes, including net community production (NCP), which reflects the metabolic balance between gross primary production (GPP) and community respiration (Codispoti et al., 1986; Minas et al., 1986). It describes the net rate at which CO_2 is transformed to particulate and dissolved organic carbon (POC and DOC). For the present study, we use NCP estimates derived from in situ measurements of the elemental ratio of O_2/Ar . The O_2/Ar method measures biological O_2 supersaturation in the mixed layer (Craig and Hayward, 1987), and yields NCP estimates over the O_2 residence timescale (1–2 weeks) (Reuer et al., 2007; Cassar et al., 2007, 2009, 2011). On this timescale, the NCP derived from this method is tightly linked to the export of organic carbon from the mixed layer at steady state, under the assumptions that both vertical mixing of O_2 -depleted waters from below and accumulation of POC and DOC in the mixed layer are negligible (Cassar et al., 2009, 2011; Jonsson et al., 2013). Although we use NCP and carbon export production interchangeably in this study, it should be noted that under some circumstances, the assumption of steady-state is violated (Hamme et al., 2012; Jonsson et al., 2013).

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While in situ O₂/Ar measurements shed new light on the NCP distribution and variability, the Southern Ocean remains seriously undersampled. The difficulty in obtaining a large-scale picture of the carbon export owes to the unavailability of direct satellite measurements. In addition, NCP is highly variable in space and time and cannot be derived from linear interpolation between in situ measurements. Field experiments also reveal that the plankton ecosystem and CO₂ flux variability are not dominated by just one single mechanism but by a confluence of several processes that shift in relative importance over time and space (Banse, 1996; Abbott et al., 2000, 2001; Cassar et al., 2011; Tortell et al., 2012), which are difficult to capture in biogeochemical models.

An alternative strategy is to use a data-driven modeling approach. We may achieve a more comprehensive characterization of temporal and spatial variability of NCP by examining the statistical relationships between NCP and physical as well as biogeochemical properties that potentially have impacts on carbon export. In addition to mixed layer depth (MLD) and light (i.e., photosynthetically available radiation, PAR) (Cassar et al., 2011), POC, Chl, sea surface temperature (SST), and sea surface height (SSH) are likely important factors regulating or correlated with NCP in the Southern Ocean. POC production is the dominant form of NCP in the Southern Ocean (Ogawa et al., 1999; Wiebinga and de Baar, 1998; Kaehler et al., 1997; Hansell and Carlson, 1998; Sweeney et al., 2000; Schlitzer, 2002; Ishii et al., 2002; Allison et al., 2010), and Chl concentration is commonly used to estimate net primary production (NPP) from satellites (Behrenfeld and Falkowsky, 1997; Moore and Abbott, 2000; Campbell et al., 2002; Carr et al., 2006; Bissinger et al., 2008; Friedrichs et al., 2009; Saba et al., 2011; Friedland et al., 2012; Nevison et al., 2012; Olonscheck et al., 2013). SST has been used to derive export and export efficiency based on the relationship with NPP and through its influence on heterotrophic activity (Laws et al., 2000; Laws 2004; Laws et al., 2011). SSH yields information on oceanic eddies, fronts, and nutrient transport that are crucial to spatial variation of biological activity (Abbott et al., 2000, 2001; Glorioso et al., 2005; Kahru et al., 2007; Gruber et al., 2011).

vides a description of the SOM methodology for generating weekly NCP maps and for calculating error estimates. In Sect. 4 we present our results, noting some of the most salient features from the constructed NCP dataset. Section 5 provides a discussion and conclusions.

2 Data

We make extensive use of gridded data products and cruise measurements in the Southern Ocean domain poleward of 20° S and for the period between 1998 and 2009. The gridded and research cruise data are described below.

2.1 Gridded predictor data

We consider six gridded data products, PAR, POC, Chl, SST SSH, and MLD, as potential predictors of NCP for use in the SOM analysis and for the generation of weekly NCP maps, as described more thoroughly in Sect. 3.

We utilize satellite PAR and POC from the Moderate Resolution Imaging Spectroradiometer flown on the Aqua satellite (MODIS-Aqua) 8 day mean 9 km for the period 10 July 2002–30 December 2009. The weekly averaged Chl are constructed from the daily 9 km maps of Sea-viewing Wide Field-of-view Sensor (SeaWiFS), version 5.2 for the period 7 January 1998–26 December 2007 (O'Reilly et al., 1998). For SST, we use NOAA Optimum Interpolation 0.25° Daily SST Blended with Advanced Very High Resolution Radiometer (AVHRR) and AMSR version 2 data (OI SST) (Reynolds et al., 2007) for the period 7 January 1998–19 August 2009. The weekly SSH anomaly maps are obtained from the Archiving, Validation and Interpretation of Satellite Oceanographic Data (AVISO) on about a 1/3° × 1/3° grid (Ducet et al., 2000) from 7 January 1998 to 22 July 2009. To determine the absolute SSH, we added the AVISO SSH anomaly to the sea level climatology of Niiler and Maximenko (Niiler et al., 2003; Maximenko

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et al., 2009). We choose this particular SSH climatology because it has high spatial resolution (Sokolov and Rintoul, 2007).

Because the coverage of Argo float profiles is not homogenous (Akoi et al., 2007a), and the available gridded Argo data are either of coarser resolutions or shorter time periods (http://www.argo.ucsd.edu/Gridded_fields.html), we choose the MLD of the high resolution OGCM for the Earth Simulator (OFES) (Masumoto et al., 2004; Sasaki et al., 2006, 2008). The OFES is an eddy-resolving quasi-global (75° N–75° S) ocean model based on the Geophysical Fluid Dynamics Laboratory Modular Ocean Model version 3 (GFDL MOM3) with 0.1° horizontal resolution and 54 vertical levels. The model captures realistic upper ocean dynamics, including eddies and heat balance (Sasaki and Nonaka, 2006; Taguchi et al., 2007; Scott et al., 2008; Zhuang et al., 2010; Yoshida et al., 2010; Sasaki et al., 2011; Chang et al., 2012), and has been used to investigate the Southern Ocean dynamical variability (Aoki et al., 2007a, b, 2010; Sasaki and Schneider, 2008; Thompson et al., 2010; Thompson and Richards, 2011). In the present study, we use the MLD from the OFES simulation forced by the QuikSCAT satellite wind field from 28 July 1999 to 28 October 2009.

For the interpolation of the predictor data to the daily ship track locations, all gridded data are first interpolated to daily resolution. For the generation of weekly NCP maps, all gridded predictor data are interpolated to a common 1° × 1° latitude–longitude grid poleward of 20° S at weekly temporal resolution.

2.2 Research cruise data

In the SOM analysis described below, the predictand of interest is an estimate of NCP from an extensive set of published data obtained from 41 research cruises in the Southern Ocean between 1998 and 2009 (Reuer et al., 2007; Cassar et al., 2007, 2011). Figure 1a shows our ship tracks with time of the cruises color-coded in months. We see that the ship tracks mainly cover regions of high chlorophyll (see Fig. 2c) during the growing season between November and March. The histogram of the ship track NCP distribution is shown in Fig. 1b. From visual inspection, we also exclude spuriously large

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(SOMs), similar to that used by Friedrich and Oschlies (2009) and Telszewski et al. (2009) for generating maps of the North Atlantic $p\text{CO}_2$. The method of self-organizing maps combines elements of cluster analysis with nonlinear, nonparametric regression (Kohonen, 2001). This particular approach is advantageous for the present purpose because the methodology does not assume a pre-defined functional form between predictor and predictand; rather, the methodology relies on an *unsupervised learning* procedure whereby the potentially complex predictor/predictand relationships are determined entirely by the data used to construct the SOM through a process called training. In addition, the methodology readily handles one or more missing predictors when generating NCP maps, which is a useful property given the limited coverage of satellite predictor data over the Southern Ocean for some periods. The approach used here differs from previous SOM studies (Friedrich and Oschlies, 2009; Telszewski et al., 2009) in that we perform a thorough validation analysis to determine an optimal combination of SOM parameters and predictors and to provide estimates of error for weekly NCP predictions. Below we include a brief description of the SOM methodology and descriptions of the procedures for generating NCP maps and calculating error estimates. Additional discussion is found in the Supplementary Methods section of the supporting material, and a more thorough description of the SOM methodology can be found in the appendix of Johnson et al. (2008).

3.1 Self-organizing map methodology and NCP dataset construction

In the present application, the SOM is trained with the seven-dimensional (six predictors and the predictand, NCP) daily ship track data, where each daily observation is treated as a seven-dimensional data vector. The NCP mapping is accomplished in two steps: (1) SOM training with ship track data to determine the predictor/NCP clusters, and (2) assignment of weekly gridded predictor data to the best-matching SOM clusters and the concomitant assignment of the associated cluster NCP values to the corresponding grid. The first step generates K clusters, where the user specifies the number K , that describe prototypical combinations of predictor and NCP values (the

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method for determining K is described below in Sect. 3.2). In the second stage, for each grid and week the available predictor data are combined into a data vector of up to six dimensions; then this data vector is mapped to the best-matching SOM cluster on the basis of minimum Euclidean distance. The NCP value associated with that best-matching cluster, which is determined in step 1, is then assigned to that particular grid and week. This process is repeated for each available grid and week to construct weekly NCP maps.

As mentioned above, the SOM approach has the advantage of readily handling data even when one or more predictors are missing during both the training and NCP mapping stages. Due to limitations of satellite data coverage and differences in the starting and ending dates of the predictor datasets, most ship track days and weekly grids have at least one missing predictor value. In particular, the large cloud cover over the Southern Ocean, which typically exceeds 70 % south of 40° S during the growing season (Warren et al., 1988), significantly impairs satellite retrieval of POC and Chl. Table 1 shows the availability of each variable in both the ship track data used to train the SOM and the gridded weekly data used to construct the NCP maps. Some variables such as SST, MLD, and SSH have good spatial and temporal coverage, whereas others are more sparse. Even though POC and Chl are among those of the lower data availability, an improvement is apparent from their relatively high coverage of 40–60 %, in contrast to the large cloud cover (> 70 % on average), which is a result of interpolation of the predictor data (7 or 8 day $1^\circ \times 1^\circ$) onto daily ship track locations as well as the weekly grids. Overall, only approximately 30 % of all ship track days have all six predictor values available. For cases when one or more predictor values are missing, the SOM algorithm finds the best-matching clusters on the basis of minimum Euclidean distance, just as in the usual case, except that all dimensions corresponding to missing data are ignored. In the process of assigning NCP values to the weekly gridded data, the cluster dimension corresponding to NCP is ignored in every case of cluster assignment because NCP is excluded from the predictor data. The NCP value of the best-matching cluster is then assigned to the corresponding grid. Thus, this particular

3.3 Bootstrap NCP dataset constructions

In addition to measurement error and random NCP variability unaccounted by the predictors, which are captured in the error estimates in Sect. 3.2, another important source of error for the long-term mean is the limited data coverage used to construct the SOM.

5 Because we are constructing a gridded NCP dataset over a large domain based on a limited number of research cruise measurements, a small number of measurements may have a disproportionate influence on the regional NCP constructions. To provide a quantitative measure of how this limitation impacts the uncertainty in the NCP climatology constructions, we use a bootstrap approach to construct 100 additional NCP
10 datasets. From these 100 datasets, the NCP climatology variance for a particular location provides an indication of the sensitivity of the NCP estimates to this particular, limited ship track dataset used to train the SOM.

For each of these 100 bootstrap NCP datasets, we perform the NCP construction in the same way as described above but with one distinction: the SOM is trained with
15 resampled ship track data. The resampling procedure, which follows conventional bootstrap procedures, is performed as follows. A bootstrap ship track dataset is constructed by randomly selecting research cruise numbers from 1 through 41 with replacement, and then placing the ship track data from the randomly chosen cruise number into the bootstrap dataset. This process of randomly choosing cruise numbers and placing the
20 corresponding data into the bootstrap ship track dataset is repeated until the bootstrap ship track dataset has the same number of daily NCP and predictor observations as in the original ship track dataset. The SOM is then trained on the bootstrap ship track data with the same parameter and predictor combination as discussed above, and then the bootstrap NCP dataset is constructed based on this modified SOM.

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4 Results

In this section, the basin-scale features in the constructed NCP dataset are first described. In the absence of the basin-scale NCP observation, we compare the spatial pattern of the constructed NCP with the satellite-measured POC and Chl, because the former accounts for 80–90 % of NCP in the Southern Ocean (Hansell and Carson 1998; Allison et al., 2010), and the latter is often used to derive phytoplankton biomass and NPP. Secondly, we examine the regional values of constructed NCP by comparison with those reported in the literature. We also include the 95 % bootstrap confidence intervals and seasonal standard deviation to indicate the uncertainty and temporal variability, respectively. For comparison with the in situ data that are not on our data grids, a 1–2° spatial average is taken of the constructed NCP surrounding the point of observation. We note that exact agreement is not expected, given that the in situ derived NCP used for comparison were obtained by various methods that access different temporal and spatial scales of carbon export and that sometimes include different processes. Because our data are resolved on weekly timescales, we only perform comparisons with measurements of weekly or longer temporal resolution.

Thirdly, we show a dominant basin-scale NCP distribution emerged from various models, with discussion of the discrepancies. In addition, because the biological pump is the main mechanism that drives atmospheric CO₂ into the ocean (e.g., Volk and Hoffert, 1985; Carlson et al., 2010) we compare our NCP to the observed air–sea CO₂ flux of the Southern Ocean. To convert from annual means to daily range, we assume that the growing season varies from 90 to 120 days (Heywood and Whitaker, 1984; Sweeny et al., 2000; Reuer et al., 2007; Racault et al., 2012) because of the large spatial and temporal variability in its duration for the Southern Ocean (Lizotte, et al., 2001; Racault et al., 2012; Borrione and Schlitzer 2013). The total area south of 50° S is approximated to be $45.7 \times 10^6 \text{ km}^2$ (Moore and Abbot, 2000).

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4.1 Southern Ocean NCP climatology

Figure 2a shows the spatial distribution of 12 yr growing season NCP climatology (1998–2009), superimposed with the major Southern Ocean fronts (Orsi et al., 1995). An elongated zonal band of high NCP ($\geq 20 \text{ mmol C m}^{-2} \text{ d}^{-1}$) is seen approximately following the Subtropical Front (STF $\sim 40^\circ \text{ S}$), where macronutrient-rich subantarctic water converges with the macronutrient-poor subtropical water (Takahashi et al., 2012). It stretches from the southwest Atlantic, across the south Indian Ocean to the western South Pacific, then splits with the STF east of the dateline around 170° W , and turns southeastward to about 120° W . A sharp NCP gradient exists north of the front, with very low NCP throughout most of the subtropics except near large landmasses. Elevated NCP is seen along the Southern Boundary (SBdy), the southernmost limit of the Antarctica Circumpolar Circulation (ACC), and along the Antarctic coast, including the Ross Sea and Amundsen Sea, where strong CO_2 sinks have recently been observed (Arrigo et al., 2008; Tortell et al., 2012). Between the STF and SBdy, we also see high NCP ($\geq 20 \text{ mmol C m}^{-2} \text{ d}^{-1}$) in the complex region off the southeastern South America between the Río de la Plata and the Falkland Island, including the Patagonian Shelf and Brazil-Malvinas Confluence (BMC) zone, and in the vicinity of the Crozet Islands ($48\text{--}60^\circ \text{ E}$, $42\text{--}49^\circ \text{ S}$), Kerguelen Island ($67\text{--}95^\circ \text{ E}$, $45\text{--}55^\circ \text{ S}$), and South Georgia ($34\text{--}42^\circ \text{ W}$, $50\text{--}55^\circ \text{ S}$).

As discussed in the previous section, one of the limitations of this study is the limited availability and spatial coverage of NCP observations used in the SOM analysis for generalizing the relationships between NCP and each of the predictors. As a quantitative indication of how this limitation may impact the constructed NCP climatology, Fig. 3 shows the standard deviation, σ_{boot} , of the growing season mean NCP from the one hundred bootstrap NCP datasets (Sect. 3.3), superimposed with the locations of each ship track. Largest uncertainties ($\sigma_{\text{boot}} \sim 6 \text{ mmol C m}^{-2} \text{ d}^{-1}$) are found over the subtropical oceans, where ship track coverage does not exist. These locations are generally low productivity regions with ocean surface characteristics not generally targeted by the

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field campaigns. In regions of dense ship track coverage, the uncertainty is generally lower ($\sigma_{\text{boot}} \leq 4 \text{ mmol C m}^{-2} \text{ d}^{-1}$). The regions of high NCP bootstrap climatology standard deviation provide an indication of where targeted measurements in future studies may help to reduce the uncertainty of Southern Ocean NCP estimates.

The climatologies of POC (2002–2009) and Chl (1998–2007) are shown in Fig. 2b and c for comparison. Chl is in log scale due to its strong positive skewness. Overall, the regions of high mean NCP (Fig. 2a) correspond well with regions of high mean POC and Chl. The area-weighted, centered pattern correlation coefficients are 0.66 and 0.33 for climatological NCP vs. POC and vs. $\log_{10}(\text{Chl})$, respectively. On the basis of these pattern correlations, the climatological POC and Chl fields are able to explain, in a linear sense, 44 % and 11 % of the climatological NCP field, respectively. However, the temporal correlation between NCP and POC and \log_{10} Chl in the daily ship track data are only 0.20 and 0.23, respectively, which suggests that POC and Chl alone only explain a small percentage of the NCP variability on daily and shorter timescales. The low correlation between NCP and Chl on shorter timescales is consistent with Reuer et al. (2007). Despite this weak linear relationship in the ship track data, we seem to be able to tease out a clear link in the Southern Ocean climatology.

4.2 Regional NCP evaluation

In the following, we compare the regional NCP between the constructed data and independent in situ estimates available in the literature. For the NCP values reported for the period prior to our data availability, we provide the climatological values from our data at the sites and calendar days of the measurements. For those reported for the period overlapping our data period (1998–2009), we carry out a real-time comparison.

First we compare our NCP climatology with that off the southeast coast of the South Island of New Zealand, derived from the Munida time series (171.5° E 45.85° S) using a ^{13}C -based diagnostic box model (Brix et al., 2013). Their reported NCP climatology, 14.6–22.3 $\text{mmol C m}^{-2} \text{ d}^{-1}$, is in strong agreement with our constructed climatology of 20.8 $\text{mmol C m}^{-2} \text{ d}^{-1}$, with a 95 % bootstrap confidence in-

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side the bloom) and downstream (inside the bloom) values are listed in Table 3c. Our data capture the upstream and downstream differences in all three island regions. The downstream (inside the bloom) values, however, are smaller than those reported for the Kerguelen Island and South Georgia, possibly due in part to area averaging over a coarse grid in our dataset.

4.3 Basin-scale climatology comparison

4.3.1 Model comparison

Figures 4 and 5b show the basin-scale export rate estimates from two different models, one based on inverse modeling (GCM fitting to observation) (Schlitzer, 2002), and the other from a satellite NPP-export model calibrated to atmospheric O_2/N_2 measurements (Nevison et al., 2012). Because only the January climatology is available from Nevison et al. (2012), we include our January map in Figure 5a for comparison. We see that the spatial patterns in these two models are in broad agreement with the climatology of our data (Figs. 2a and 5a), including regions of high carbon export along the zonal band between 40° S and 60° S, in the coastal upwelling zones off Chile and Namibia, as well as on the Patagonian Shelf. The main difference between the present study (Fig. 2a) and the inverse modeling result of Schlitzer (2002) (Fig. 4) is that in the latter, the climatology is smoother, the zonal band of high export rate is displaced more to the south, and the high export region off the coast of Chile is more spread out. The broader and smoother features in Schlitzer (2002) are likely due to the coarser spatial resolutions available at the time of the study.

The two January climatologies generally differ by less than $20 \text{ mmol C m}^{-2} \text{ d}^{-1}$ throughout the Southern Ocean, except a large discrepancy greater than $100 \text{ mmol C m}^{-2} \text{ d}^{-1}$ over the Patagonian Shelf (Fig. 5c). Closer inspection reveals a wide range of NCP values in this region among models: $28\text{--}30 \text{ mmol C m}^{-2} \text{ d}^{-1}$ in our January map (Fig. 5a), $150\text{--}400 \text{ mmol C m}^{-2} \text{ d}^{-1}$ in that of Nevison et al. (2012) (Fig. 5b), $40\text{--}140 \text{ mmol C m}^{-2} \text{ d}^{-1}$ in Westberry et al. (2012) (not shown), and 50--

60 mmol C m⁻² d⁻¹ in Schlitzer's annual mean (2002) (Fig. 4). High daily NCP of 70–90 mmol C m⁻² d⁻¹ has been measured over periods of 3–4 days in this region (Schloss et al., 2007), although it is unclear if such high values over short time periods are representative of the monthly climatology.

The Patagonian Shelf region is known to exhibit highly variable biological activity owing to its uncertain relationships between phytoplankton communities and NCP (Schloss et al., 2007), complicated bathymetry, complex ocean dynamics (Bianchi et al., 2005; Romero et al., 2006; Rivas, 2006; Garcia et al., 2008), and multiple sources of iron, including atmospheric dust (Erickson et al., 2003; Gassó et al., 2010; Signorini et al., 2009; Boyd et al., 2012) and ocean upwelling, sediment resuspension, and shelf transport (Garcia et al., 2008; Signorini et al., 2009; Painter et al., 2010). However, the scarcity of in situ measurements of longer timescales has hindered the progress in establishing a reliable regional climatology and has made model validation challenging.

4.3.2 Air–sea CO₂ flux

We now compare our NCP with the air–sea CO₂ flux obtained from the monthly climatological maps of Takahashi et al. (2009) for the growing season. In Fig. 6a, a zonal band of high CO₂ flux is seen between 40° S and 60° S, similar to the zonal belt of CO₂ flux reported for the February climatology (Takahashi et al., 2012). Albeit with a much coarser resolution (5° lon × 4° lat), the pattern of high CO₂ flux is in good agreement with the high NCP band (see Fig. 2a), outlined by the contour of NCP = 16 mmol C m⁻² d⁻¹ in Fig. 6a. The small CO₂ flux compared with NCP could result from CO₂ outgassing due to warming during the growing season, dampening the biologically-driven CO₂ uptake (Takahashi et al., 2012).

Figure 6b shows the monthly mean of the area-integrated NCP, CO₂ flux, and SST south of 50° S from October to March. The NCP starts to increase steadily from 0.6 Pg C yr⁻¹ in October until it reaches a peak around 1 Pg C yr⁻¹ in December and January, with a quick decline in February and March. Similarly, the CO₂ flux changes

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from $-0.2 \text{ Pg C yr}^{-1}$ (out of the ocean) in October to $+0.2 \text{ Pg C yr}^{-1}$ in December, peaks at $0.4\text{--}0.5 \text{ Pg C yr}^{-1}$ in January and February, lagging the NCP peak by one month, and declines thereafter. We see that the large difference between the CO_2 flux and NCP seems coincident with the fast increase in SST from October to January. This difference becomes smaller as the SST increase slows down from January to March. Overall, this large imbalance in the early growing season is suggestive of the dominance of the warming-induced CO_2 outgassing, but further investigation is warranted.

5 Discussion and conclusions

In this study we have described the methodology and general features of a 1998–2009 Southern Ocean NCP dataset constructed through a neural network approach. This effort represents the first attempt to construct such a dataset over the Southern Ocean or any large basin entirely on the basis of observed relationships between NCP measurements and NCP predictors. This approach is based on a self-organizing map analysis that assumes no parametric functional form between NCP and the predictors. Overall, we find that our constructed NCP dataset is in good agreement with previously published independent in situ derived NCP values of weekly or longer temporal resolution through real-time as well as climatological comparisons at different sampling sites (Tables 2–3). One exception is the region south of 75° S , where the predictor coverage is poor (Sect. 4.2).

The growing season climatology of our constructed NCP reveals a pronounced zonal band of high NCP that approximately follows the STF between 40° S and 60° S in the Atlantic, Indian and western Pacific sectors, and turns southeastward shortly after the dateline (Fig. 2a). Other regions of elevated NCP include area along the SBdy and Antarctic coast, the complex region of Patagonian Shelf and BMC zone, as well as the coastal upwelling zones off Chile and Namibia. This elongated zonal band resembles the observed air-sea CO_2 flux (Fig. 6a). The CO_2 flux is generally smaller than the NCP in early growing season (Fig. 6b). This difference may result from the rapid tempera-

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(Kara et al., 2000) for this calculation (<http://apdr.c.soest.hawaii.edu/>). We see that the overall pattern of POC inventory is similar to the NCP distribution.

Although the NCP and POC climatologies correspond well, some spatial variations of the POC–NCP relationship are evident. Such variations may result from true physical differences in the POC–NCP relationships and/or to errors related to the NCP estimates and satellite-derived POC estimates (Gardner et al., 2003; Stramski et al., 2008). To explore further, we show in Fig. 7b the scatter plot of NCP against POC, sorted by latitude bands, for each of the Southern Ocean grid points. This figure demonstrates that although there is a positive correlation between NCP and POC, the relationship appears not to be a simple linear relationship, with variations across different latitude bands. For example, the relationship between POC and NCP appears to be stronger for lower mean POC values at lower latitudes but weaker at higher latitudes poleward of 60° S. If this variation is not due to measurement artifacts, this plot suggests that there may be some regions with high mean POC but relatively low NCP, and vice versa.

Another possibility, however, is that there may be errors in the ship track NCP estimates in some regions characterized by strong vertical mixing of O₂-undersaturated waters to the surface, as pointed out by Reuer et al. (2007). Although we excluded all negative NCP estimates from the SOM analysis, which correspond to regions of upwelled, O₂-undersaturated water, it is possible that this vertical mixing effect still remains in some non-excluded, positive estimates of NCP if the biological productivity of O₂ is strong enough. When this effect occurs, some of the low NCP/high POC regions may have a negative bias from O₂-undersaturated upwelled water. Future investigations into these particular regions are needed to determine to what degree this anomalous low NCP/high POC behavior represents a physical process, a bias, or some combination of the two.

Strong correspondence between POC and NCP in the Southern Ocean on longer timescales suggests that as satellite POC observation becomes available for a longer time period, it can provide a direct view of carbon export variability with a reasonable amount of uncertainty. However, on shorter timescales, the correspondence between

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NCP and POC is weaker, as evidenced by the correlation of 0.20 in the daily ship track data (Sect. 4.1) and pattern correlations of less than 0.5 in the monthly snapshots (Supplement). In addition, a major obstacle in monitoring POC variability from satellite is cloud cover, as the Southern Hemisphere belt (between 30° S and 65° S) is among the cloudiest regions on the planet (Haynes et al., 2011). Therefore, evaluation of NCP variability across a range of timescales requires consideration of the relationships between NCP and multiple variables, as in the present dataset.

Although these results suggest promise in providing insight into Southern Ocean NCP mean state and variability, substantial uncertainty in the NCP construction remains. On weekly timescales, uncertainty due to NCP variance unexplained by the predictors likely dominates, as we estimated a MAE and RMSE of 6.76 and 11.4 mmol C m⁻² d⁻¹, respectively, based on the ship track data. For longer time averages, i.e. seasonal to decadal, errors in NCP measurements and limitations in ship track coverage likely dominate the uncertainty. As discussed above, efforts to remove possible biases related to the vertical mixing of O₂-undersaturated water would reduce NCP measurement errors.

Regarding the latter source of uncertainty, additional field campaigns to measure Southern Ocean NCP, particularly in several data sparse regions, possibly would lead to improved NCP constructions. Through a bootstrap approach to constructing several overlapping NCP datasets, we have quantified the variance in NCP climatology owing to the limitations of ship track coverage. This analysis has identified several regions where bootstrap climatology variance is high but the number of NCP observations is low or zero (see Fig. 3). This finding suggests that targeted measurements in these particular regions may help to constrain the relationships between NCP and each of the predictors, thus resulting in reduced uncertainty in the Southern Ocean NCP climatology and variability.

Notwithstanding these limitations, the dataset we present provides a new opportunity to investigate large-scale variability of NCP and its connections to the Southern Ocean carbon cycle in ways previously not possible in an observation-based dataset. A recent

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SSH climatology (<http://apdrc.soest.hawaii.edu/datadoc/mdot.php>), and production of ARGO MLD data (http://apdrc.soest.hawaii.edu/dods/public_data/Argo_Products); Japan Agency for Marine-Earth Science and Technology (JAMSTEC) for providing the OFES MLD data (<http://www.jamstec.go.jp/esc/ofes/eng/>); and Lamont-Doherty Earth Observatory (LDEO) for providing the air-sea CO₂ flux (http://cdiac.ornl.gov/oceans/LDEO_Underway_Database/). The SOM constructed NCP from 1998–2009 reported in this study will be available at <http://etta.renci.duke.edu/moncp/c/moncp.html>.

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Variable	Ship track availability (%)	Weekly gridded map availability (%)
SST	99.5	97.0
Chl	57.4	59.9
POC	43.3	40.4
PAR	75.8	45.9
MLD	98.5	83.7
SSH	82.4	78.9

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Table 2. Comparison of area-integrated NCP for the Southern Ocean south of 50° S.

Reference	Method	Period	NCP ($\text{mmolC m}^{-2} \text{d}^{-1}$)	
			Previous studies	this study (95% CI) ^a
Moore et al. (2013)	NCAR CMIP5 coupled carbon-climate simulation	1990s	12–15	
Westberry et al. (2012)	Carbon-based NPP model and empirical relationships of in vitro PvR ^b	2004	8.3	
Nevison et al. (2012)	VGPM NPP and export model	1998–2007	12–24	14 (12–21)
Dunne et al. (2007)	POC export from empirical equation based on in situ observation	1998–2004	11–14	1998–2009
Pollard et al. (2006)	Nutrient drawdown based on Ekman flux divergence	long-term	17–22	
Schlitzer (2002)	3-D inverse model	steady-state	15–20	

^a 95% bootstrap confidence interval.

^b PvR: photosynthesis vs. respiration.

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Table 3a. Climatological comparison of independent in situ NCP measurements and the constructed NCP.

Reference	Method	Location	Time	NCP (mmol C m ⁻² d ⁻¹)	
				Previous study	This study Climatology (σ) ^a (95 %) ^b
Indian sector					
Minas and Minas (1992)	Mass balance based on nutrient drawdown	(65° E, 40–62° S)	Aug/Sep–Feb/Mar 1976–1977	17	17 (± 14) (13–23) ^c
Ishii et al. (1998)	Seasonal Δ DIC (temporal difference)	(30–40° E, 67–68.2° S)	14–17 Feb 1993	14–19	12 (± 7.4) (8.5–20)
		(47.5–48.8° E, 66–66.5° S)	19 Feb 1993	22–29	11 (± 6.8) (7.9–22)
		(49.1–67.8° E, 65–65.7° S)	26–28 Feb 1993	13–17	8.7 (± 8.5) (6.7–18)
		(70.6–77.5° E, 67–69° S)	28 Feb–1 Mar 1993	24–32	16 (± 5.1) (12–25)
Indian and Pacific sectors					
		(80–150° E, 63–65° S)	4–13 Mar 1993	20–27	16 (± 4.7) (6–22)
Rubin et al. (1998)	Seasonal Δ DIC (vertical gradient)	(110–171° E, 67–70° S)	Winter–late Feb/ mid Mar 1992, 1994	6.5–24	15 (± 11) (12–19) ^c
Ishii et al. (2002)	Seasonal Δ DIC	(140° E, 64–65.5° S) (temporal difference)	19 Dec 1994–21 Jan 1995	2.5–28	18 (± 11) (11–22)
Ross Sea					
Sweeny et al. (2000)	Seasonal Δ DIC	(163–186° E, 74–78° S) (vertical gradient)	Mid Oct 1996–Mid Feb 1997	22–64	19 (± 9.7) (14–25)

^a Seasonal standard deviation.

^b 95 % bootstrap confidence interval.

^c November–March mean.

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Table 3b. Real-time comparison of independent in situ NCP measurements and the constructed NCP.

Reference	Method	Location	Time	NCP ($\text{mmolCm}^{-2}\text{d}^{-1}$)	
				Previous studies	This study (95%) ^a
		Scotia Sea			
Shim et al. (2006)	nutrient drawdown	(52° W, 57–60° S)	20 Nov– 31 Dec 2001	24–29	25 (15–33)
		Atlantic sector			
Hamme et al. (2012)	O ₂ /Ar	(37–38° W, 50–51° S)	2–9 Mar 2008 9–14 Mar 2008	11–22 5–13.8	15 (2.6–23) 6.6 (1.7–25)
Moore et al. (2011)	Mass balance based on ΔDIC and O ₂	(37–38° W, 50–51° S)	9–14 Mar 2008	3.2–6.7	6.6 (1.7–25)
		Atlantic-Indian sector			
Boutin and Merlivat (2009)	Based on mixed layer budget on diurnal time scale	(16.4–21.2° E, 46.8–47.8° S)	28 Nov– 30 Dec 2006	30–51	40 (15–50)

^a 95 % bootstrap confidence interval.

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Neural network-based estimates of Southern Ocean NCP

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Reference	Method	Location	Time	NCP ($\text{mmol C m}^{-2} \text{ d}^{-1}$)	
				Previous study	This study (95%) ^a
Kerguelen					
Jouandet et al. (2008)	seasonal Δ DIC (vertical gradient)	Nov 2004–	Inside bloom	49–98	30 (15–40)
		Feb 2005	(72° E, 50.5° S) Outside bloom (78° E, 52° S)	17–26	22 (15–34)
South Georgia					
Jones et al. (2012)	seasonal Δ DIC (vertical gradient)	Nov 2007–	Bloom	43	29 (17–31)
		Feb 2008	(39–40° W, 52° S) HNLC (42° W, 56–57° S)	12	17 (14–26)
Crozet					
Bakker et al. (2007)	Δ DIC in the upper 100 m	8 Nov 2004–	Bloom	33–45	31 (18–37)
		16 Jan 2005	(47–52° E, 43–45.5° S) HNLC (47.8–49° E, 51.5–52.9° S)	16–19	18 (13–27)

^a 95% bootstrap confidence interval.

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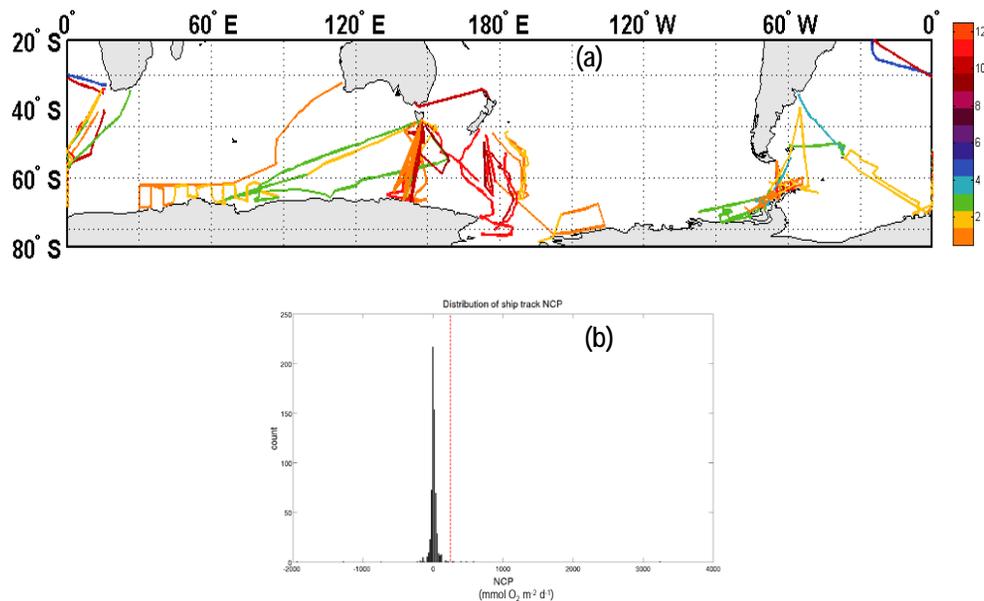


Fig. 1. (a) The ship tracks of the in situ NCP measurements used in this study. The time of the research cruises is color-coded in months. (b) The histogram of the ship track NCP distribution. The red dashed line marks $\text{NCP} = 250 \text{ mmol O}_2 \text{ m}^{-2} \text{ d}^{-1}$.

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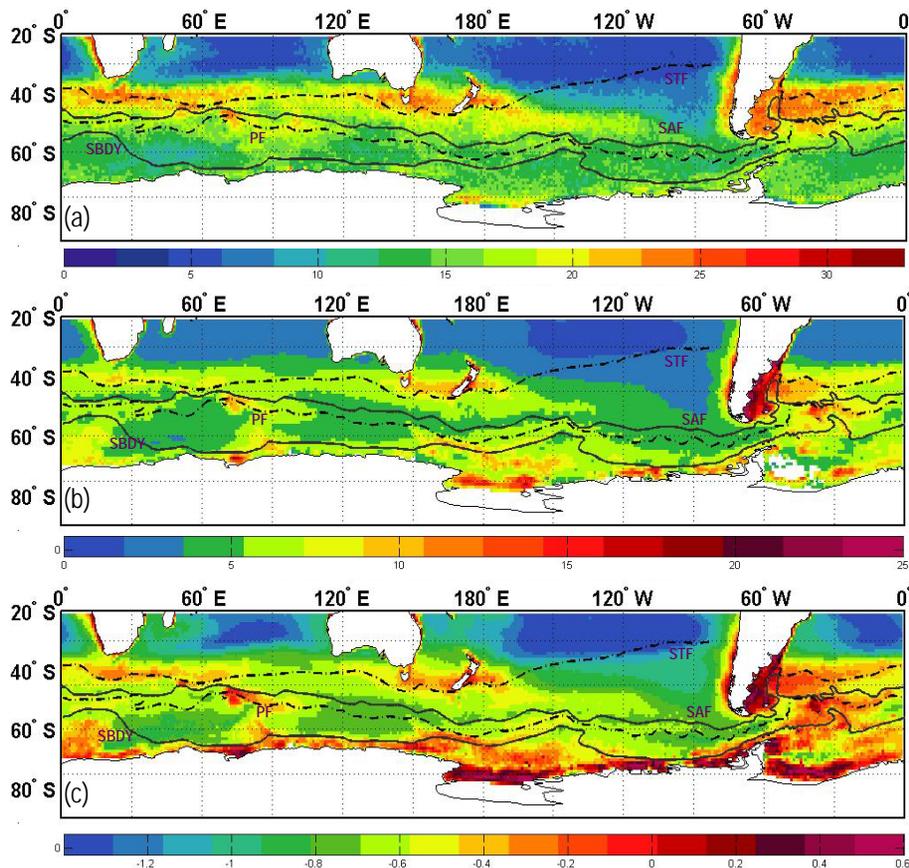
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Fig. 2. Growing season (November–March) climatologies (in color) of **(a)** NCP ($\text{mmol C m}^{-2} \text{d}^{-1}$) for 1998–2009, **(b)** POC (mmol C m^{-3}) for 2002–2009, and **(c)** \log_{10} Chl (mg m^{-3}) for 1998–2007. The major Southern Ocean fronts (Orsi et al., 1995) are superimposed (from the north): the Subtropical Front (STF), the Subantarctic Front (SAF), the Polar Front (PF), and the Southern Boundary (SBdy).

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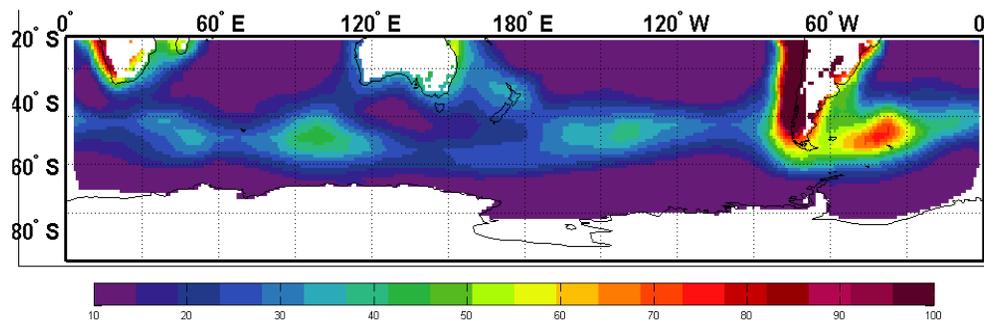


Fig. 4. Long-term mean annual POC export of Schlitzer (2002) ($\text{mmol C m}^{-2} \text{d}^{-1}$).

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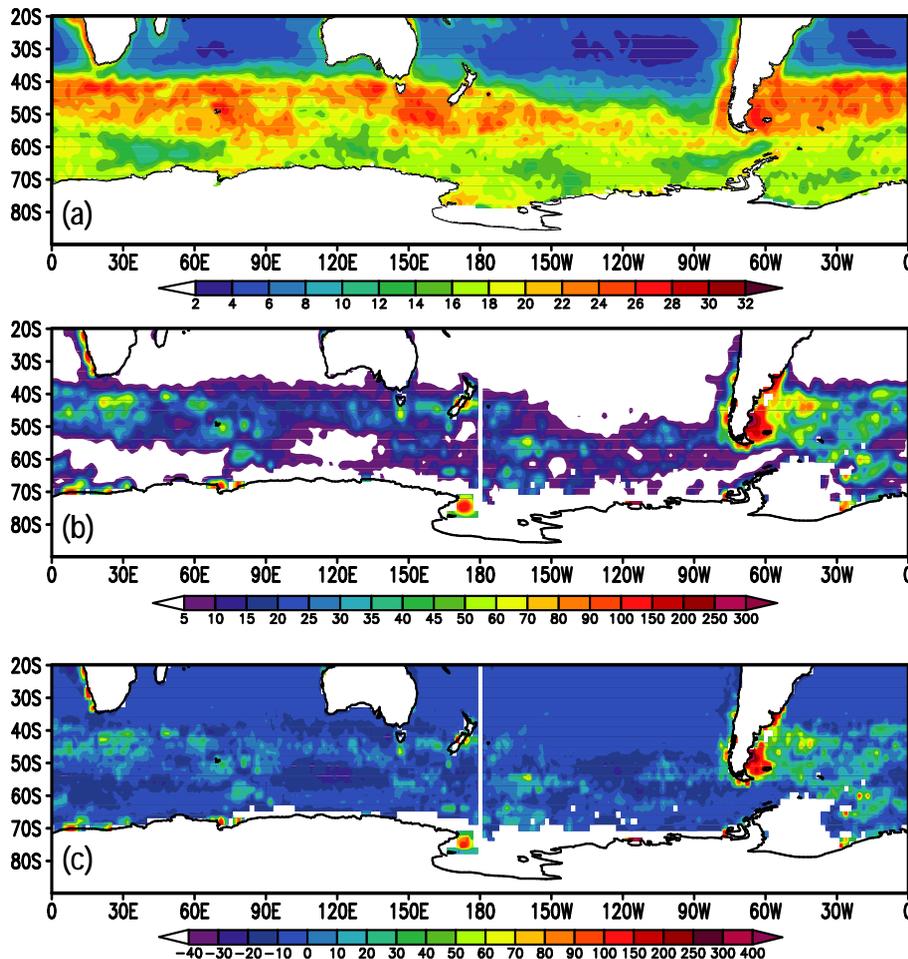
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Fig. 5. January NCP climatologies: **(a)** our constructed NCP (1998–2009); **(b)** Nevison et al. (2012) (1998–2007); **(c)** difference between two climatologies (**b**–**a**). (Unit: $\text{mmol C m}^{-2} \text{d}^{-1}$.)

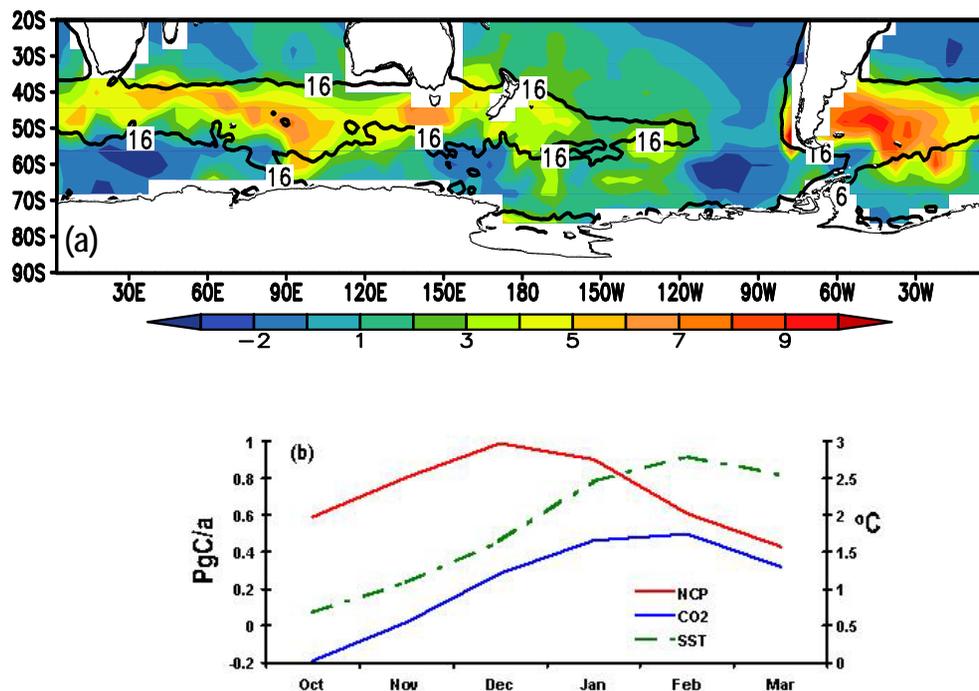


Fig. 6. Comparison with air–sea CO₂ flux (+: into the ocean). **(a)** November–March climatology of air–sea CO₂ flux (Takahashi et al., 2009) (mmolC m⁻² d⁻¹, in color) superimposed with the contour of NCP = 16 mmolC m⁻² d⁻¹. **(b)** Evolution of monthly mean area-integrated (> 50° S) NCP (red), CO₂ flux (blue), and SST (green) from October to March. The left y axis corresponds with the NCP and CO₂ (PgC a⁻¹) and the right y axis corresponds with SST (°C).

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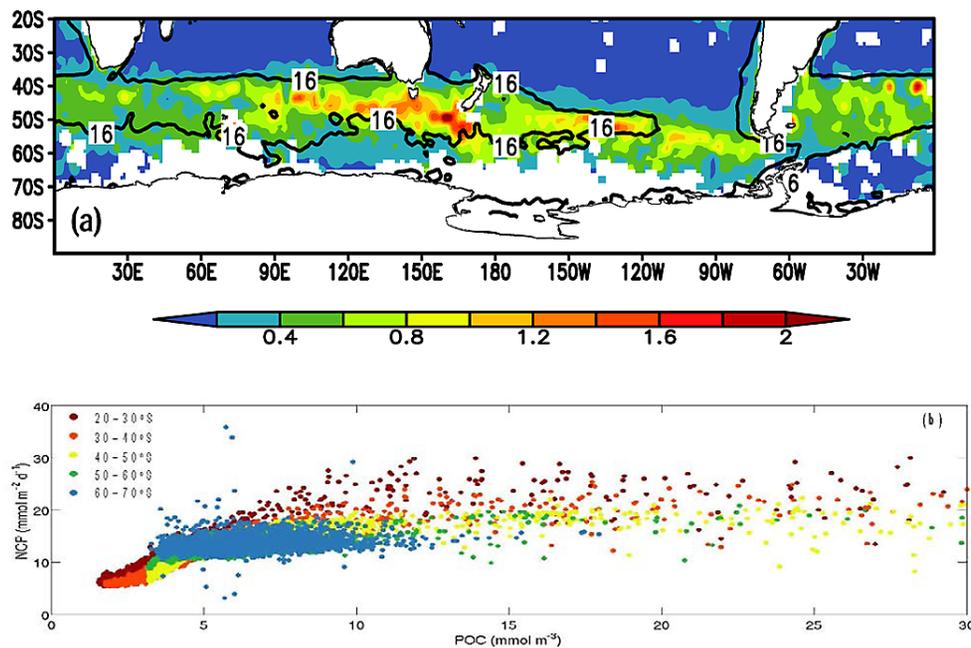


Fig. 7. (a) November–March climatology of POC inventory, defined as $\text{POC} \times \text{MLD}$ (mmol C m^{-2} , in color), superimposed with the contour of $\text{NCP} = 16 \text{ mmol C m}^{-2} \text{ d}^{-1}$. (b) The scatter plot of NCP ($\text{mmol C m}^{-2} \text{ d}^{-1}$, y axis) against POC (mmol C m^{-3} , x axis), sorted by latitudinal bands (color).