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Decision letter and referee reports: first round

16th Jan 24

Dear Professor Li,

Your manuscript titled "Melting sea ice will weaken carbon sinks in the Southern Ocean" has now been seen by 2 reviewers, whose comments are appended below. You will see that they find your work of some potential interest. However, they have raised quite substantial concerns that must be addressed. In light of these comments, we cannot accept the manuscript for publication, but would be interested in considering a revised version that fully addresses these serious concerns.

In addition, we are including some editorial thresholds: i) please include and explain in-depth the use of predictors in the main text, ii) include a comparison to traditional approaches, and iii) consider including additional pCO<sub>2</sub> datasets in their analysis (if available).

We hope you will find the reviewers' comments useful as you decide how to proceed. Should additional work allow you to address these criticisms, we would be happy to look at a substantially revised manuscript. If you choose to take up this option, please either highlight all changes in the manuscript text file, or provide a list of the changes to the manuscript with your responses to the reviewers.

Please bear in mind that we will be reluctant to approach the reviewers again in the absence of substantial revisions.

If the revision process takes significantly longer than three months, we will be happy to reconsider your paper at a later date, as long as nothing similar has been accepted for publication at Communications Earth & Environment or published elsewhere in the meantime.

We are committed to providing a fair and constructive peer-review process. Please do not hesitate to contact us if you wish to discuss the revision in more detail.

Please use the following link to submit your revised manuscript, point-by-point response to the reviewers' comments with a list of your changes to the manuscript text (which should be in a separate document to any cover letter), a tracked-changes version of the manuscript (as a PDF file) and any completed checklist:

[redacted]

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Please do not hesitate to contact us if you have any questions or would like to discuss the required revisions further. Thank you for the opportunity to review your work.

Best regards,

Jose Luis Iriarte Machuca, PhD  
Editorial Board Member

Communications Earth & Environment

Clare Davis, PhD  
Senior Editor  
Communications Earth & Environment

#### EDITORIAL POLICIES AND FORMAT

If you decide to resubmit your paper, please ensure that your manuscript complies with our editorial policies and complete and upload the checklist below as a Related Manuscript file type with the revised article:

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For your information, you can find some guidance regarding format requirements summarized on the following checklist: (<https://www.nature.com/documents/commsj-phys-style-formatting-checklist-article.pdf>) and formatting guide (<https://www.nature.com/documents/commsj-phys-style-formatting-guide-accept.pdf>).

#### REVIEWER COMMENTS:

Reviewer #3 (Remarks to the Author):

The manuscript describes an approach to reduce the uncertainty/discrepancy in data products and model outputs for surface ocean pCO<sub>2</sub> in the Southern Ocean. The authors state that this is mainly due to the lack of in situ observations during winter (compared to summer).

They have applied the boosting ensemble learning feed forward neural networks (BEL FFNNs) method using a gridded version of SOCAT data, and data from the Southern Ocean flux station (SOFS, 142.0°E, 46.8°S), south of Tasmania (Australia) for validation.

Question: Aren't there any other pCO<sub>2</sub> observing time series in other sector of the S. Ocean? Or only for summer periods?

My main question for the methods section concerns the following (l. 76-78):

"The surface ocean pCO<sub>2</sub> converted from the Surface Ocean CO<sub>2</sub> Atlas version 2023 (SOCAT v2023) dataset was used for pCO<sub>2</sub> mapping by fitting the non-linear relationship between pCO<sub>2</sub> and environmental variables"

To which environmental variables?

Additionally, the list of predictors appears in the supplementary material only, and it is hard for the reader to understand why the winter predictors were chosen for each latitude area.

In the conclusion section, my concern is about the statement on lines 502-506:

Is there an estimate for this in the future? In figure 9 we see the decrease in the S. Ocean carbon sink

in the scenarios where 50% or 100% of the sea ice melts - but within the period ~1992-2022 considered in this study. What are the modelled predictions (please cite the models, like in figure 7, for instance), despite the discrepancy in the ocean carbon sink?

How does the calculated uncertainty in sea-air CO<sub>2</sub> fluxes (section "uncertainty") affect the estimates of the decreasing C sink from this manuscript?

# Melting sea ice will weaken carbon sinks in the Southern Ocean

Guorong Zhong<sup>1,2,3,4</sup>, Xuegang Li<sup>1,2,3,4\*</sup>, Jinming Song<sup>1,2,3,4\*</sup>, Baoxiao Qu<sup>1,3,4</sup>, Fan Wang<sup>1,2,3,4</sup>, Yanjun Wang<sup>1,4</sup>, Bin Zhang<sup>1,4</sup>, Jun Ma<sup>1,3,4</sup>, Huamao Yuan<sup>1,2,3,4</sup>, Liqin Duan<sup>1,2,3,4</sup>, Qidong Wang<sup>1,3,4</sup>, Jianwei Xing<sup>1,3,4</sup>, and Jiajia Dai<sup>1,3,4</sup>

(1. Institute of Oceanology, Chinese Academy of Sciences, Qingdao 266071, China;

2. University of Chinese Academy of Sciences, Beijing 101407, China;

3. Laoshan Laboratory, Qingdao 266237, China;

4. Center for Ocean Mega-Science, Chinese Academy of Sciences, Qingdao 266071, China)

Correspondence to: Xuegang Li ([lixuegang@qdio.ac.cn](mailto:lixuegang@qdio.ac.cn)) and Jinming Song ([jmsong@qdio.ac.cn](mailto:jmsong@qdio.ac.cn))

**Abstract:** Employing machine learning methods for mapping surface ocean  $p\text{CO}_2$  has reduced the uncertainty in estimating sea-air  $\text{CO}_2$  flux. However, a general discrepancy exists between the Southern Ocean carbon sinks derived from  $p\text{CO}_2$  products and those from biogeochemistry models. By performing a boosting ensemble learning feed-forward neural networks (BEL FFNNs) method, we have identified an underestimation of the surface Southern Ocean  $p\text{CO}_2$  due to notably uneven density of  $p\text{CO}_2$  measurements between summer and winter, which resulted in about 16% overestimating of Southern Ocean carbon sink over the past three decades. In particular, the Southern Ocean carbon sink since 2010 was notably overestimated by approximately 29%. This overestimation can be mitigated by a winter correction in algorithms, with the average Southern Ocean carbon sink during 1992-2021 corrected to  $-0.87 \text{ PgC yr}^{-1}$  from the original  $-1.01 \text{ PgC yr}^{-1}$ . Furthermore, the most notable underestimation of surface ocean  $p\text{CO}_2$  mainly occurred in regions south of  $60^\circ\text{S}$  and was hiding under ice cover. If sea ice melts completely, there could be a further reduction of about  $0.14 \text{ PgC yr}^{-1}$  in the Southern Ocean carbon sink due to exposure of high  $p\text{CO}_2$  seawater to the atmosphere in winter.

**Keywords:** Carbon sink, Southern Ocean,  $\text{CO}_2$  flux,  $p\text{CO}_2$ , machine learning

## 1 Introduction

The increasing concentration of atmospheric  $\text{CO}_2$  since the onset of the industrial era has been affecting the natural climate due to the greenhouse effect. This effect is partially mitigated by the global ocean  $\text{CO}_2$  uptakes, which account for about one-quarter of the anthropogenic  $\text{CO}_2$  emissions (Sabine et al., 2004). Natural climate

33 variability and anthropogenic climate change also feedback to influence the sea-air CO<sub>2</sub>  
34 exchange (Rödenbeck et al., 2022). It is essential to quantify the global ocean carbon  
35 sink and its temporal variability to understand further the response of the carbon cycle  
36 to future global change. The surface ocean partial pressure of CO<sub>2</sub> (*p*CO<sub>2</sub>)  
37 measurements from the SOCAT dataset were widely used and mapped into continuous  
38 gridded data to estimate the sea-air CO<sub>2</sub> flux (Bakker et al., 2016). Due to a lower  
39 spatial decorrelation length scale of hundreds of kilometers in the surface ocean than  
40 that of thousands of kilometers in the atmosphere (Wanninkhof et al., 2013), surface  
41 ocean *p*CO<sub>2</sub> has more notable spatial variability than atmospheric *p*CO<sub>2</sub>. Considerable  
42 variability and sparse measurements of surface ocean *p*CO<sub>2</sub> indicate insufficient  
43 observations to estimate CO<sub>2</sub> flux in most ocean areas directly. Significant uncertainty  
44 in carbon sink estimation arises from sparse and uneven *p*CO<sub>2</sub> measurements, the gas  
45 transition velocity, and the cool skin effect (Woolf et al., 2016; Woolf et al., 2019;  
46 Watson et al., 2020). Recent application of machine learning algorithms in *p*CO<sub>2</sub>  
47 mapping methods increased data availability and further reduced the uncertainty in  
48 *p*CO<sub>2</sub>-based carbon sink estimates (Gregor et al., 2021; Chau et al., 2022; Gloege et al.,  
49 2022; Zhong et al., 2022). The average net global ocean carbon sink during the last  
50 three decades was documented as -1.40~-2.45 PgC yr<sup>-1</sup> (Zeng et al., 2014; Landschützer  
51 et al., 2016; Watson et al., 2020; Iida et al., 2021; Rödenbeck et al., 2022). The  
52 differences between results were caused by differences in algorithms, division of global  
53 biogeochemical provinces, and selection of *p*CO<sub>2</sub> predictors. The accuracy of *p*CO<sub>2</sub>  
54 mapping based on machine learning methods remains to be improved, especially in  
55 polar regions with sparser *p*CO<sub>2</sub> measurements.

56 The Southern Ocean south of 30°S was a strong carbon sink and has contributed  
57 to about 40% of global ocean anthropogenic CO<sub>2</sub> uptakes (Sabine et al., 2004; Fletcher,  
58 S. E. M. et al., 2006; Frölicher et al., 2015; Landschützer et al., 2015). Changes in the  
59 Southern Ocean carbon sink strongly affect the global ocean CO<sub>2</sub> uptake. However, the  
60 Southern Ocean carbon sink estimated by *p*CO<sub>2</sub>-based machine learning methods was  
61 about 0.4 PgC yr<sup>-1</sup> stronger than the result from global ocean biogeochemical models  
62 since 2012 (Friedlingstein et al., 2022; Mayot et al., 2023). A notable seasonal  
63 variability of surface ocean *p*CO<sub>2</sub> was reported in the Southern Ocean, mainly south of  
64 50°S, with high *p*CO<sub>2</sub> levels and carbon sources observed in winter (Takahashi et al.,  
65 2009; Landschützer et al., 2016). The strongly seasonally uneven surface ocean *p*CO<sub>2</sub>  
66 measurements with missing winter observations may result in an overestimation of the  
67 Southern Ocean carbon sink from *p*CO<sub>2</sub> products (Bushinsky et al., 2019; Hauck et al.,

68 2020; Gloege et al., 2021; Friedlingstein et al., 2022). Besides supplying more  
69 measurements from sailboats or floats (Landschützer et al., 2023), whether this  
70 overestimation can be solved by improving algorithms is worth investigating. Thus, we  
71 reestimated the Southern Ocean carbon sink using a different machine learning method  
72 and investigated the influence of seasonally uneven SOCAT  $p\text{CO}_2$  measurements on  
73 the  $p\text{CO}_2$  mapping and carbon sink estimate.

## 74 **2 Data and methods**

### 75 **2.1 $p\text{CO}_2$ mapping and winter correction**

76 The surface ocean  $p\text{CO}_2$  converted from the Surface Ocean  $\text{CO}_2$  Atlas version  
77 2023 (SOCAT v2023) dataset was used for  $p\text{CO}_2$  mapping by fitting the non-linear  
78 relationship between  $p\text{CO}_2$  and environmental variables (Bakker et al., 2016). The  
79 relationship fitting was based on a boosting ensemble learning feed-forward neural  
80 networks (BEL FFNNs) consisting of three FFNNs. The first FFNN (FFNN I in Figure  
81 1) outputs will be used as a  $p\text{CO}_2$  predictor in the second and the last FFNN (FFNN II  
82 and FFNN III in Figure 1). All FFNNs in this work used 10 neurons in each hidden  
83 layer, and the number of hidden layers was adjusted to achieve an optimal FFNN size  
84 based on a change in predictor errors. The average of several FFNN outputs with  
85 changing initial states was taken as the final  $p\text{CO}_2$  prediction value. The  $p\text{CO}_2$   
86 predictors used in this work were selected by the stepwise FFNN algorithm based on  
87 the variation of  $p\text{CO}_2$  predicting error caused by each predictor (Zhong et al., 2022).  
88 However, due to the lack of winter measurements, the  $p\text{CO}_2$  predictors in the Southern  
89 Ocean selected by the stepwise FFNN algorithm were more relevant to the drivers of  
90  $p\text{CO}_2$  in summer than winter. By increasing the weightings of winter measurements  
91 in calculating the predicting error (equation S1), the  $p\text{CO}_2$  predictors in the Southern  
92 Ocean were corrected for the winter period (Table S1). Furthermore, another winter  
93 correction was also carried out by changing the temporal period of measurements used  
94 for training networks.

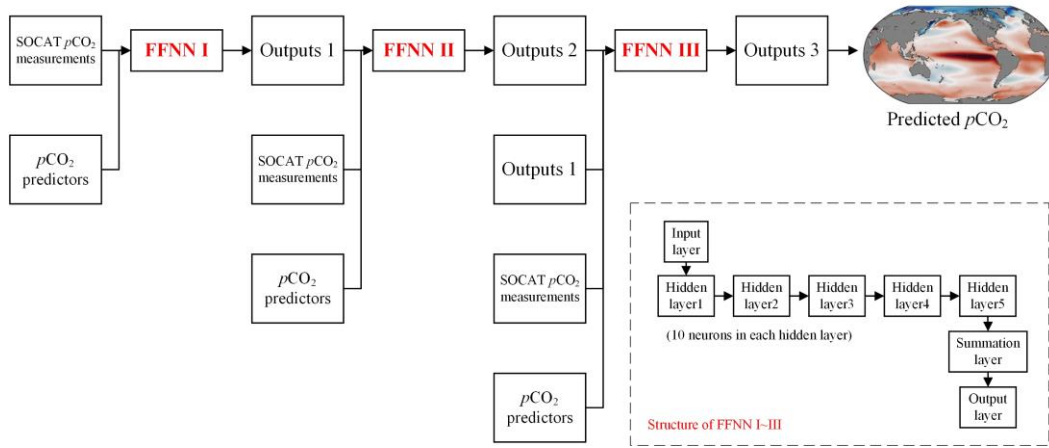


Figure 1. The procedure of the Boosting Ensemble Learning Method

To eliminate the influence of FFNN structure on correction validity, the performances of the individual FFNN and BEL FFNNs were compared under different training strategies: one based on SOCAT  $p\text{CO}_2$  measurements of all months and others based on sectional winter measurements. The predicted  $p\text{CO}_2$ , root mean square error (RMSE), and bias with different training strategies and  $p\text{CO}_2$  predictors were compared to evaluate the influence of seasonally uneven  $p\text{CO}_2$  measurements and to determine which training strategy will be used. The predictor error was calculated using a K-fold cross validation method, where the  $p\text{CO}_2$  measurements were divided into four groups by year, and each one was predicted by the other three groups (Gregor et al., 2019; Zhong et al., 2022). Then, the results were further compared to the observations from the Southern Ocean Flux station (SOFS) time series stations for validation (Sutton et al., 2019). The final  $p\text{CO}_2$  product includes two types of data: 1) the  $p\text{CO}_2$  from October to April based on SOCAT measurements of all seasons, and 2) the  $p\text{CO}_2$  from May to September based on sectional SOCAT winter measurements and corrected predictors.

## 2.2 CO<sub>2</sub> flux estimate

The sea-air CO<sub>2</sub> flux was estimated based on the  $p\text{CO}_2$  difference across the interface (Woolf et al., 2016; Watson et al., 2020):

$$F = k \cdot (a_{\text{subskin}} \cdot p\text{CO}_{2\text{w}} - a_{\text{skin}} \cdot p\text{CO}_{2\text{atm}}) \quad (1)$$

where  $p\text{CO}_{2\text{w}}$  represents surface ocean  $p\text{CO}_2$  and  $p\text{CO}_{2\text{atm}}$  represents atmospheric  $p\text{CO}_2$ . The  $p\text{CO}_{2\text{atm}}$  was calculated from the  $x\text{CO}_2$  of the NOAA Greenhouse Gas Marine Boundary Layer Reference product (Lan et al., 2023) and sea level pressure from the ERA5 monthly averaged data (Hersbach et al., 2019), with the water vapor correction (Dickson et al., 2007).  $a_{\text{skin}}$  and  $a_{\text{subskin}}$  are the solubility of CO<sub>2</sub> at the skin and subskin layers (Woolf et al., 2016), calculated from temperature and salinity (Weiss, 1974).  $k$  is the CO<sub>2</sub> transfer velocity as a function of wind speed (Wanninkhof, 1992):



$$K = \Gamma(660/Sc)^{0.5}U^2 \quad (2)$$

where  $Sc$  is the Schmid number of  $CO_2$  in seawater, and  $U$  is the average wind speed using the ERA5 product (Hersbach et al., 2020). The transfer velocity was scaled by the scale factor ( $\Gamma$ ) 0.27 for ERA5 wind products to match the  $^{14}C$  constraint (Sweeney et al., 2007).

### 2.3 uncertainty

The uncertainty of sea-air  $CO_2$  flux estimate includes mainly three parts: the uncertainty of transfer velocity, the cool skin impact, and the uncertainty in the surface ocean  $pCO_2$  reconstruction. The uncertainty of transfer velocity  $k$  was related to the wind product and considered about 5-30% (Takahashi et al., 2009; Ho et al., 2011; Woolf et al., 2019), and here we used 10%. Recent research suggested an underestimate of  $0.35 \text{ PgC yr}^{-1}$  in the global ocean carbon sink caused by the cool skin impact (Woolf et al., 2019). The uncertainty caused by the temperature and salinity gradient was considered 3% and 1.7% after the subskin correction, respectively (Woolf et al., 2016; Watson et al., 2020). The last uncertainty term came from the reconstruction of gridded surface ocean  $pCO_2$  data, including the uncertainty of the  $pCO_2$  measurement, averaging to  $1^\circ \times 1^\circ$  grids, and the  $pCO_2$  interpolation. Thus, the total uncertainty in the  $pCO_2$  reconstruction was calculated on average (Wang et al., 2014): where the measurement uncertainty  $\sigma(\text{meas})$  was about 2-5  $\mu\text{atm}$  (Pfeil et al., 2013; Wanninkhof et al., 2013b), which was lower than the others and can be neglected (Landschützer et al., 2014). The uncertainty of averaging to  $1^\circ \times 1^\circ$  grids,  $\sigma(\text{grid})$ , used 5  $\mu\text{atm}$  from the previous research (Sabine et al., 2013). For the  $pCO_2$  interpolation uncertainty  $\sigma(\text{map})$ , we used the predicting error of 7-25  $\mu\text{atm}$  in different regions (Zhong et al., 2022). The uncertainty in each area was calculated as the following (Landschützer et al., 2014):

$$\sigma(\langle pCO_2 \rangle)^2 = \frac{\sigma(\text{grid})^2}{N_{\text{eff}}(\text{grid})} + \frac{\sigma(\text{map})^2}{N_{\text{eff}}(\text{map})} \quad (3)$$

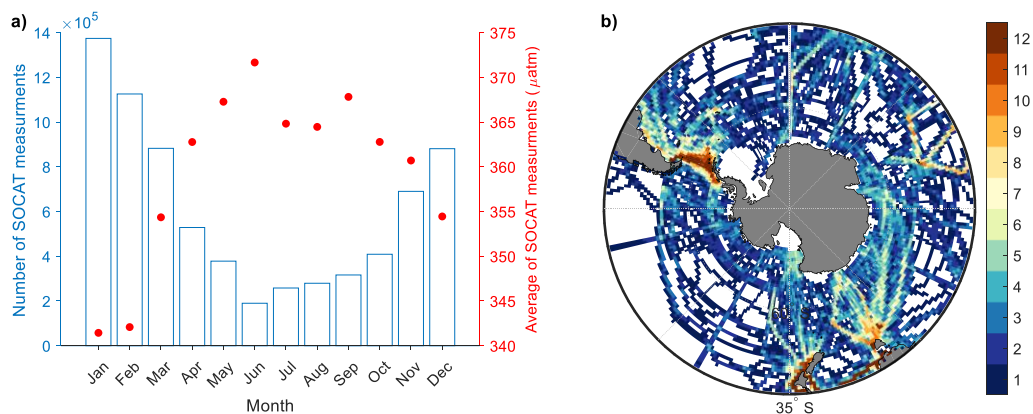
The  $\sigma(\langle pCO_2 \rangle)$  calculated from the  $pCO_2$  interpolation uncertainty ranges from 1.7 to 6.6  $\mu\text{atm}$  in each region. Based on the average  $CO_2$  transfer velocity of  $0.07 \text{ mol C m}^{-2} \text{ yr}^{-1}$  in the Southern Ocean, the uncertainty  $\sigma(pCO_2)$  caused by the  $pCO_2$  interpolation errors in different regions range from  $\pm 0.05$  to  $\pm 0.10 \text{ PgC yr}^{-1}$ . The total uncertainty of  $pCO_2$  interpolation estimated by the sum of squares of  $\sigma(pCO_2)$  in each province was  $\pm 0.13 \text{ PgC yr}^{-1}$ , corresponding to roughly 15% of the average Southern Ocean carbon sink estimated below. Thus, combining the uncertainties stemming from transfer velocity, cool skin influences, and  $pCO_2$  interpolation, the final uncertainty was  $\pm 10\%$  ( $= \sqrt{10\%^2 + 3\%^2 + 1.7\%^2 + 15\%^2}$ ), using the square root of the sum squares

156 propagation, corresponding to  $\pm 0.16 \text{ PgC yr}^{-1}$  ( $1\sigma$ ).

### 157 **3 Result and Discussion**

#### 158 **3.1 Influence of uneven measurements on the Southern Ocean $p\text{CO}_2$ mapping**

159 Various machine learning methods were applied in the surface ocean  $p\text{CO}_2$   
160 mapping and  $\text{CO}_2$  flux estimating (Landschützer et al., 2016; Gregor et al., 2021; Iida  
161 et al., 2021; Wang et al., 2021; Chau et al., 2022; Zhong et al., 2022), where a majority  
162 of methods are based on non-linear relationship fitting between SOCAT  $f\text{CO}_2$   
163 measurements, or converted  $p\text{CO}_2$ , and environmental variables (Bakker et al., 2016).  
164 However, the number of SOCAT measurements is uneven between different seasons in  
165 the Southern Ocean. The SOCAT measurements in the Southern Ocean are concentrated  
166 in summer with low surface ocean  $p\text{CO}_2$  (Figure 2a). ~~While in winter~~, the number of  
167 measurements with high surface ocean  $p\text{CO}_2$  was only about one-fifth of that in summer.  
168 In most Southern Ocean areas, the SOCAT measurements covered less than four unique  
169 months from 1992 to 2021 (Figure 2b). Meanwhile, ~~the~~ high surface ocean  $p\text{CO}_2$  was  
170 observed during the winter in the Southern Ocean, according to the research based on  
171 either  $p\text{CO}_2$  measurements or gridded products. The lack of measurements during high  
172 surface ocean  $p\text{CO}_2$  seasons in most Southern Ocean areas may notably influence the  
173 non-linear relationship fitting and  $p\text{CO}_2$  mapping, particularly in the months from June  
174 to September with the sparsest measurements. The seasonally unbalanced distribution  
175 of measurements may be a potential reason for the higher  $p\text{CO}_2$  predicting error of the  
176 Southern Ocean than the neighboring areas in previous research (Landschützer et al.,  
177 2016; Chau et al., 2022; Zhong et al., 2022).



178  
179 Figure 2. The number of a) SOCAT  $f\text{CO}_2$  measurements in each month and b) unique months  
180 covered by SOCAT measurements in the Southern Ocean south of  $35^\circ\text{S}$  from 1992 to 2021. SOCAT:  
181 the Surface Ocean  $\text{CO}_2$  Atlas dataset version 2023 (Bakker et al., 2016).

182 To evaluate the influence of seasonal-uneven SOCAT measurements on  $p\text{CO}_2$   
183 mapping, the RMSE and bias from May to September were compared between different

184 validation groups, with the only difference in training strategy (Table 1). The  
 185 comparison of  $p\text{CO}_2$  predicting error between different training strategies reveals a  
 186 substantial influence of uneven measurements on the accuracy of machine learning  
 187  $p\text{CO}_2$  predicting method. Training neural networks with SOCAT measurements only  
 188 from April to October instead of all months resulted in a notable decrease of 0.5~1.4  
 189  $\mu\text{atm}$  in RMSE. This decrease in RMSE caused by the change of training strategies was  
 190 even more effective than the decrease of less than 0.4  $\mu\text{atm}$  caused by the improvement  
 191 of the FFNN structure (BEL FFNNs in Table 1). In the areas south of 50°S, the BEL  
 192 FFNNs and the individual FFNN trained with sectional winter measurements resulted  
 193 in significantly lower RMSE during winter than those trained with all-month  
 194 measurements. The bias during May-September between predicted  $p\text{CO}_2$  and SOCAT  
 195 measurements of more than -3  $\mu\text{atm}$  was notably different from the range of -1~1  $\mu\text{atm}$   
 196 in other months, indicating a significant underestimation of surface seawater  $p\text{CO}_2$  in  
 197 the areas south of 50°S. In particular, the  $p\text{CO}_2$  from May to September in the area  
 198 south of 60°S, as predicted by BEL FFNNs using measurements from all months, was  
 199 underestimated by an average of 5.77  $\mu\text{atm}$ . Meanwhile, the  $p\text{CO}_2$  predicted by the  
 200 individual FFNN in the Southern Ocean south of 60°S was also notably lower than  
 201 SOCAT data in winter due to missing winter measurements. When training with  
 202 measurements only from April to October, the BEL FFNNs reached the lowest RMSE  
 203 in winter, and the bias was only -1.38  $\mu\text{atm}$ . Similarly, the predicted  $p\text{CO}_2$  by the  
 204 individual FFNN was only 1.47  $\mu\text{atm}$  lower than measurements on average, indicating  
 205 a significant improvement in the underestimation of  $p\text{CO}_2$  during winter. In the 50-60°S  
 206 region, training BEL FFNNs and the individual FFNN with sectional winter  
 207 measurements can also reduce the predicting bias. By training BEL FFNNs only with  
 208 measurements from April to September, the winter RMSE in the 50-60°S area was the  
 209 lowest among different training strategies, with a bias of only -0.36  $\mu\text{atm}$ .

210

211 Table 1. Comparison of  $p\text{CO}_2$  predicting error in the Southern Ocean during May-  
 212 September among different training strategies

Validation group	Training period	35-50° S		50-60° S		S of 60° S	
		RMSE ( $\mu\text{atm}$ )	bias ( $\mu\text{atm}$ )	RMSE ( $\mu\text{atm}$ )	bias ( $\mu\text{atm}$ )	RMSE ( $\mu\text{atm}$ )	bias ( $\mu\text{atm}$ )
BEL FFNNs	May-Sep	12.01	+0.61	11.97	+0.22	14.76	+0.33
	Apr-Sep	10.70	+0.38	11.88	-0.36	14.87	-0.90
	May-Oct	11.39	-0.36	12.07	-0.66	14.50	-0.07
	Apr-Oct	11.10	-0.68	12.09	-1.16	14.20	-1.38

	Mar-Nov	11.32	-1.26	12.51	-2.13	15.50	-4.47
	All Months	<b>9.86</b>	<b>-0.39</b>	13.27	-3.13	16.09	-5.77
<b>BEL FFNNs with corrected predictors</b>	May-Sep	12.24	+0.74	11.93	+0.17	14.44	+1.17
	Apr-Sep	10.76	+0.30	11.26	+0.09	13.49	-0.06
	May-Oct	12.81	-0.28	11.44	+0.04	14.27	-0.20
	Apr-Oct	11.83	-0.79	<b>10.93</b>	<b>-0.46</b>	<b>13.29</b>	<b>-0.74</b>
	Mar-Nov	11.69	-1.49	13.07	-0.46	14.07	+0.02
	All Months	9.88	-0.29	11.49	-1.08	14.61	-0.90
Individual FFNN	May-Sep	12.05	+0.50	11.99	+0.07	15.15	0.36
	Apr-Sep	10.58	+0.30	12.02	-0.52	15.04	-1.14
	May-Oct	11.43	-0.59	12.21	-0.75	14.92	-0.32
	Apr-Oct	11.19	-0.83	12.29	-1.49	14.86	-1.47
	Mar-Nov	11.64	-1.43	12.82	-2.56	15.76	-3.95
	All Months	9.95	-0.34	13.31	-3.33	17.14	-5.38
Individual FFNN with corrected predictors	May-Sep	12.57	+0.50	12.30	+0.37	14.54	+0.83
	Apr-Sep	10.72	+0.27	11.45	+0.14	13.79	-0.27
	May-Oct	13.09	-0.45	11.52	-0.07	14.46	-0.23
	Apr-Oct	11.35	-0.92	11.06	-0.09	13.63	-0.27
	Mar-Nov	12.02	-1.55	11.55	-0.09	17.86	+0.50
	All Months	9.95	-0.28	12.06	-1.04	15.85	-0.05

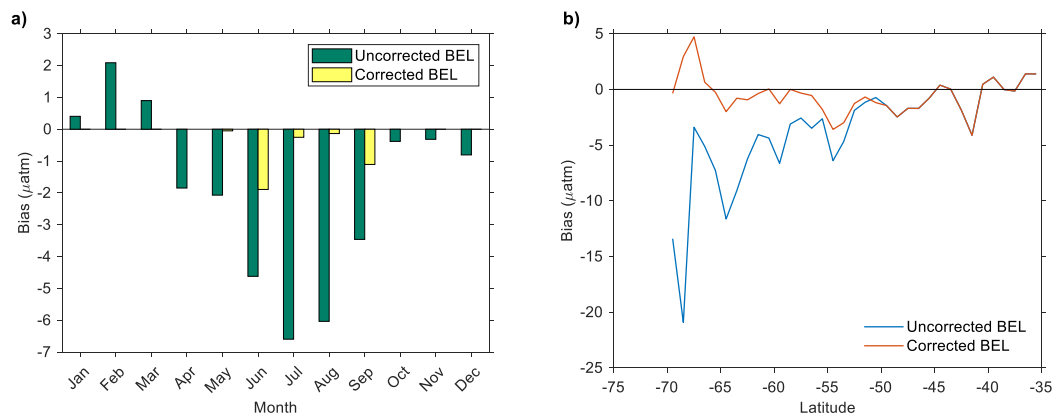
213 (BEL FFNNs: boosting ensemble learning based on three FFNNs constructed in this work;  
214 Individual FFNN: one FFNN with the same structure used in the BEL; Training Period: a period of  
215 SOCAT samples used for training neural networks to predict  $p\text{CO}_2$  during May-September; RMSE  
216 and bias: calculated from the difference between predicted  $p\text{CO}_2$  and SOCAT measurements during  
217 May-September based on the K-fold cross validation method. Corrected predictors:  $p\text{CO}_2$  predictors  
218 selected by a stepwise BEL FFNNs algorithm based on increasing weightings of winter  
219 measurements, see supplementary S1.)

220 In contrast, there is no significant underestimation of winter surface ocean  $p\text{CO}_2$  in  
221 the Southern Ocean  $35\text{-}50^\circ\text{S}$ . The RMSE by training BEL FFNNs with sectional winter  
222 measurements was larger than that by training with all measurements, and the  
223 improvement of bias was also not observed when using sectional winter measurements.  
224 On the other hand, corrected  $p\text{CO}_2$  predictors may better reflect the drivers of surface  
225 ocean  $p\text{CO}_2$  in the Southern Ocean during winter. By using the month as a predictor,  
226 the correction of  $p\text{CO}_2$  predictors can also effectively mitigate the underestimation of  
227 winter  $p\text{CO}_2$  in the Southern Ocean. Simply changing  $p\text{CO}_2$  predictors without  
228 correcting the training period, the RMSE of BEL FFNNs with weighted predictors  
229 during winter in the  $50\text{-}60^\circ\text{S}$  region decreases to  $11.49 \mu\text{atm}$ , and the bias reduces to -


230 1.08  $\mu\text{atm}$  compared to BEL FFNNs with original predictors (see predictors listed in  
231 Table S1). The same decrease in RMSE was also observed in the areas south of 60°S.  
232 Using both correction methods simultaneously, the RMSE can be minimized to 10.93  
233  $\mu\text{atm}$  and 13.29  $\mu\text{atm}$  in the 50-60°S and regions south of 60°S, respectively. The bias  
234 also fell within an acceptable range of -1 to 1  $\mu\text{atm}$ , close to the bias level in other  
235 months without notable underestimation or overestimation.

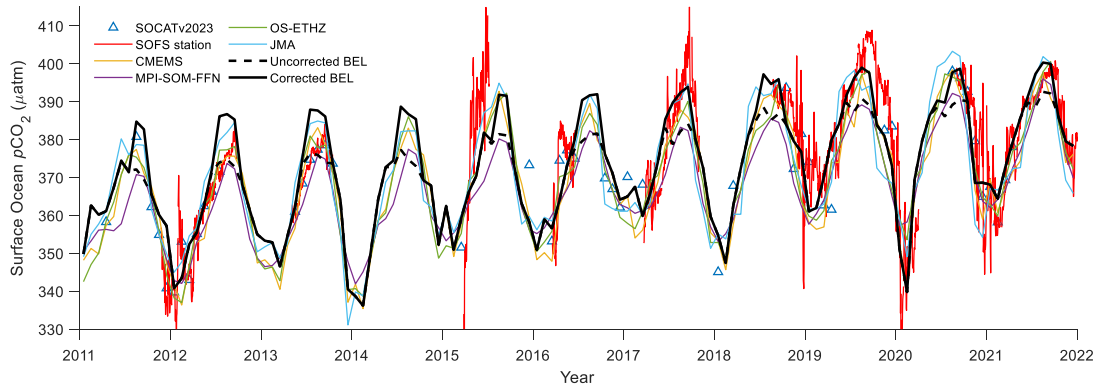
236 The BEL FFNNs and individual FFNN both showed an underestimated surface  
237 seawater  $p\text{CO}_2$  in the Southern Ocean south of 50°S in winter, indicating that the  
238 underestimation of surface seawater  $p\text{CO}_2$  was not caused by the structure of FFNN but  
239 rather by the seasonally uneven  $p\text{CO}_2$  measurements. Training networks with sectional  
240 winter measurements and correction of  $p\text{CO}_2$  predictors can mitigate the  
241 underestimation of surface Southern Ocean  $p\text{CO}_2$  in winter. Considering that the BEL  
242 FFNNs have a lower RMSE compared to the individual FFNN, the BEL FFNNs using  
243 corrected  $p\text{CO}_2$  predictors and training with measurements only from April to October  
244 have better accuracy of the  $p\text{CO}_2$  mapping in the Southern Ocean during winter.

245 With the correction of the training period and  $p\text{CO}_2$  predictors, the bias of predicted  
246  $p\text{CO}_2$  from May to September was notably smaller than the uncorrected result (Figure  
247 3a). In July, the  $p\text{CO}_2$  predicted by the BEL FFNNs was notably lower than SOCAT  
248 measurements, with a considerable bias of 6.6  $\mu\text{atm}$ . In contrast, the bias from October  
249 to April was generally within the range of -1 to 1  $\mu\text{atm}$ , indicating a non-significant  
250 overestimation or underestimation of surface seawater  $p\text{CO}_2$  in the Southern Ocean.  
251 With the winter correction, the bias from May to September decreased notably to near  
252 zero. Even in the most biased July, the bias of corrected BEL FFNNs fell to only -0.3  
253  $\mu\text{atm}$ , significantly mitigating the underestimation of winter surface ocean  $p\text{CO}_2$  in the  
254 Southern Ocean. The bias at different latitudes reveals that the underestimation of  
255 surface seawater  $p\text{CO}_2$  in the Southern Ocean due to seasonally uneven measurements  
256 becomes more significant at higher latitudes (Figure 3b). In the region south of 50°S,  
257 the uncorrected average deviation is negative, reaching approximately -20.92  $\mu\text{atm}$  at  
258 around 68.5°S. The difference in the effect of the winter correction may be related to  
259 the density of measurements, as the decrease in bias was more notable in sparsely  
260 sampled high-latitude areas.



261  
 262 Figure 3. Distribution of bias between predicted  $p\text{CO}_2$  and SOCAT measurements in the Southern  
 263 Ocean south of  $35^\circ\text{S}$ . a): monthly bias in the Southern Ocean south of  $50^\circ\text{S}$  (predicted  $p\text{CO}_2$  minus  
 264 SOCAT measurements); b): zonal bias during May-Sep; Uncorrected BEL: based on training sample  
 265 of all seasons; Corrected BEL: based on training sample only from April to October. BEL: Boosting  
 266 ensemble learning FFNNs used in this study.

267 Compared to the observation from the SOF  time series station (Sutton et al., 2019),  
 268 the  $p\text{CO}_2$  values from May to September from different methods were lower due to the  
 269 lack of SOCAT winter data for training (Figure 4). During years that winter SOCAT  
 270 data are available, such as 2012, 2013, and 2018, the  $p\text{CO}_2$  values from different  
 271 methods were close to the observations from the SOFS time series station  
 272 (Landschützer et al., 2016; Gregor et al., 2021; Iida et al., 2021; Chau et al., 2022;). The  
 273 surface ocean  $p\text{CO}_2$  of BEL FFNNs product after correction in winter was about 10  
 274  $\mu\text{atm}$  higher than the uncorrected BEL FFNNs results. It was much closer to the time  
 275 series observation, suggesting a better accuracy of corrected BEL FFNNs  $p\text{CO}_2$  than  
 276 the uncorrected results. Both the validation based on the SOCAT dataset and the  
 277 validation based on time-series observations from the SOFS station suggest that  
 278 correction of the training period and  $p\text{CO}_2$  predictors can effectively mitigate the  
 279 underestimation due to seasonally uneven measurements. Therefore, the final  $p\text{CO}_2$   
 280 product constructed in this study consists of  $p\text{CO}_2$  data from October to April based on  
 281 all measurements and  $p\text{CO}_2$  data from May to September based on corrected  $p\text{CO}_2$   
 282 predictors and measurements only from April to October.



283

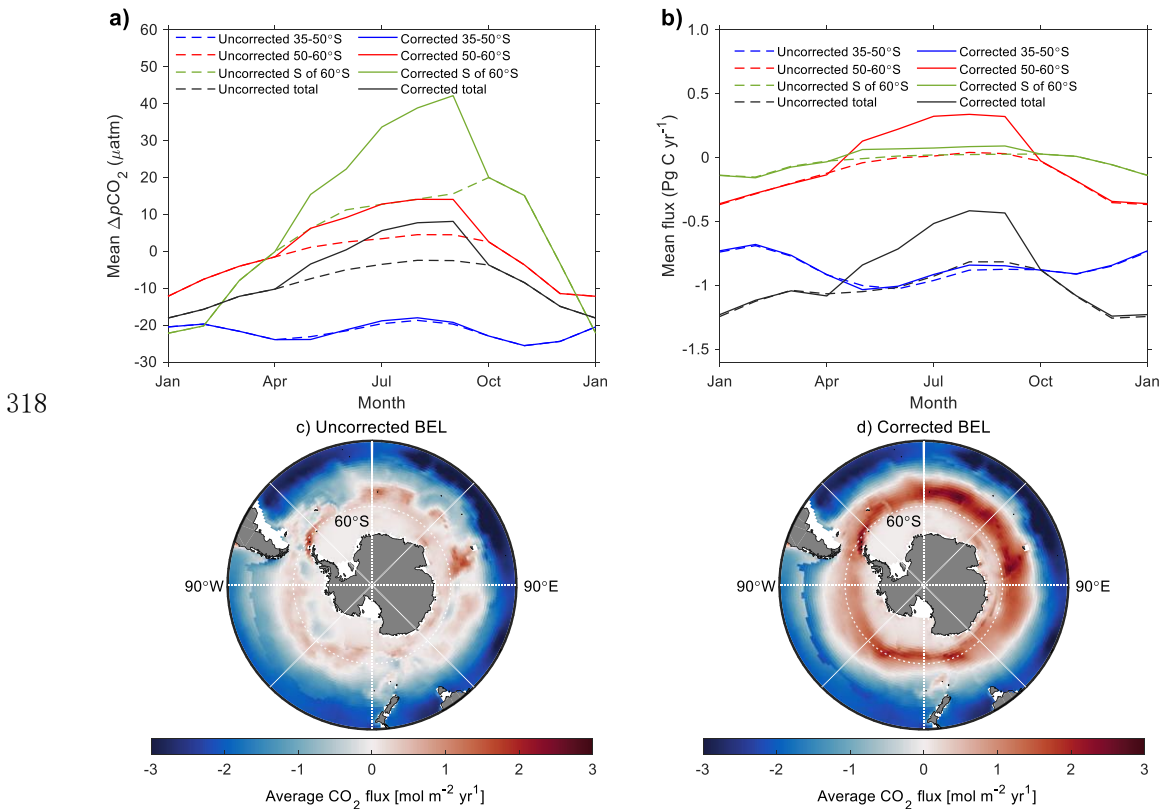
284 Figure 4. Comparison between corrected and uncorrected ensemble learning  $p\text{CO}_2$  product in the  
 285 SOFS station. CMEMS: Chau et al., 2022; MPI-SOM-FFN: Landschützer et al., 2016; OS-ETHZ:  
 286 Gregor et al., 2021; JMA: Iida et al., 2021; Uncorrected BEL: boosting ensemble learning FFNNs  
 287 based on training sample of all seasons; Corrected BEL:  $p\text{CO}_2$  during May-September were  
 288 predicted based on corrected predictors and training samples only from April to October.

### 289 **3.2 Overestimated Southern Ocean carbon sink due to biased $p\text{CO}_2$** 290 **mapping**

291 The validation based on SOCAT measurements and SOFS time series observations  
 292 reveals that the  $p\text{CO}_2$  products constructed using FFNN with the entire monthly  $p\text{CO}_2$   
 293 measurements from the SOCAT dataset may significantly underestimate the winter  
 294 surface ocean  $p\text{CO}_2$  in the Southern Ocean south of  $50^\circ\text{S}$ . Due to upwelling derived  
 295 from the wind driving a strong surface divergence through the Ekman transport (Gruber  
 296 et al., 2019), the surface seawater  $p\text{CO}_2$  in the winter of the Southern Ocean is  
 297 significantly higher than in the summer, with strong carbon source regions in winter  
 298 (Landschützer et al., 2016; Gruber et al., 2019; Wang et al., 2021). The previous studies  
 299 may have underestimated the strength of carbon sources in the winter of the Southern  
 300 Ocean, leading to an overestimation of the overall carbon sink intensity in the Southern  
 301 Ocean. Our results demonstrate that the variations in surface seawater  $p\text{CO}_2$  before and  
 302 after the winter correction significantly impact the  $p\text{CO}_2$  difference and  $\text{CO}_2$  flux across  
 303 the air-sea interface (Figure 5). The surface seawater  $p\text{CO}_2$  in the Southern Ocean south  
 304 of  $50^\circ\text{S}$  is higher than atmospheric  $p\text{CO}_2$  from May to September, and the  $p\text{CO}_2$   
 305 difference after correction became larger, particularly in the region south of  $60^\circ\text{S}$ .  
 306 However, due to the influence of sea ice coverage, the  $p\text{CO}_2$  flux in the area south of  
 307  $60^\circ\text{S}$  is nearly zero from May to September, and the difference in  $\text{CO}_2$  flux between  
 308 uncorrected and corrected BEL FFNNs was not significant. In the  $35\text{-}50\text{S}$  area with  
 309 relatively more measurements, the seasonal variation pattern of  $p\text{CO}_2$  differs from that



310 south of 50S, and there is almost no change in the  $p\text{CO}_2$  difference and  $\text{CO}_2$  flux  
 311 between uncorrected and corrected BEL FFNNs. Overall, although the south of 60S  
 312 shows the most considerable change in winter  $\Delta p\text{CO}_2$  before and after correction, the  
 313 underestimation of surface seawater  $p\text{CO}_2$  in the 50-60 area unaffected by sea ice  
 314 coverage is the main reason for the overestimation of the carbon sink intensity in the  
 315 Southern Ocean. The corrected average Southern Ocean carbon sink from May to  
 316 September is  $-0.58 \text{ PgC yr}^{-1}$ , decreasing by  $0.34 \text{ PgC}$  compared to the uncorrected  
 317 results.



320 Figure 5. Distribution of average sea-air  $p\text{CO}_2$  difference and  $\text{CO}_2$  flux from May to September  
 321 during 1992-2021. a) sea-air  $\Delta p\text{CO}_2$  in different regions: surface ocean  $p\text{CO}_2$  minus atmospheric  
 322  $p\text{CO}_2$ ; b) sea-air  $\text{CO}_2$  flux in different regions; c) distribution of  $\text{CO}_2$  flux from uncorrected BEL  
 323 FFNNs product; d) distribution of  $\text{CO}_2$  flux from corrected BEL FFNNs product; uncorrected BEL  
 324 FFNNs: constructed from SOCAT measurements of all month, corrected BEL FFNNs: data from  
 325 May to September constructed based on corrected predictors and only SOCAT measurements during  
 326 Apr-Oct.

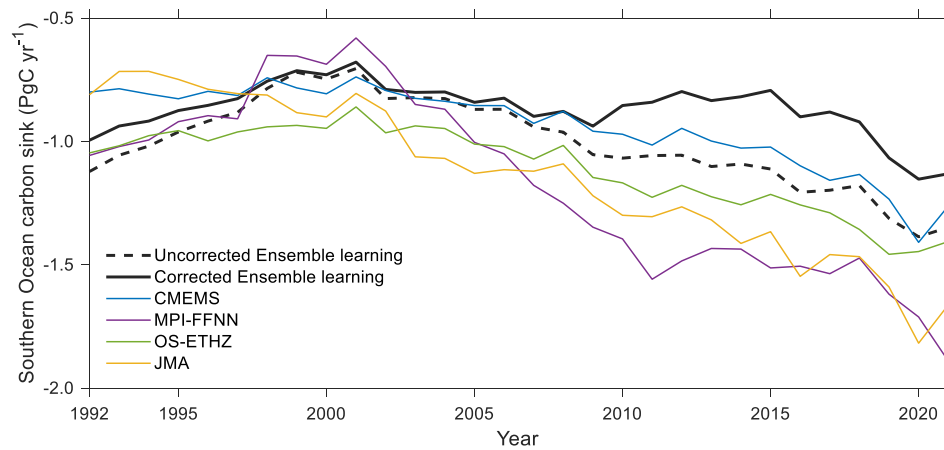
327 Over the past 30 years, the corrected average Southern Ocean carbon sink was  $-$   
 328  $0.87 \pm 0.16 \text{ PgC yr}^{-1}$ , which is approximately  $0.14 \text{ PgC yr}^{-1}$  lower than before the  
 329 correction, suggesting an overestimation of about 16%. The overestimation of the  
 330 carbon sink intensity in the Southern Ocean is mainly observed after 2010, with a



331 decrease in the decadal average carbon sink from  $-1.20 \text{ PgC yr}^{-1}$  to  $-0.93 \text{ PgC yr}^{-1}$  after  
332 correction. This indicates that the seasonally uneven measurements led to an  
333 overestimation of the Southern Ocean carbon sink by approximately 29% compared to  
334 the corrected intensity during this period (Figure 6). Although the corrected Southern  
335 Ocean carbon sink was lower than uncorrected results in the 1990s, the variability  
336 pattern was similar before and after correction. Since 2001, the Southern Ocean carbon  
337 sink has generally strengthened, but the strengthening rate is relatively slower after the  
338 winter correction. The variability of the Southern Ocean carbon sink from our corrected  
339 BEL product was highly consistent with previous research based on models or  
340 observations, in which the Southern Ocean carbon sink receded significantly in the  
341 1990s, reaching a trough at the beginning of the 21st century (Le Quere et al., 2007;  
342 Lovenduski et al., 2008), and subsequently restrengthened to full intensity (Gregor et  
343 al., 2018; Landschützer et al., 2015; Munro et al., 2015). Compared to previous  
344 products, our estimation of the corrected Southern Ocean carbon sink shows a similar  
345 intensity in the 1990s and the lowest intensity since 2003. However, research based on  
346 SOCCOM buoy data also suggested a significantly weaker Southern Ocean carbon sink,  
347 challenging existing results from  $p\text{CO}_2$  products (Bushinsky et al., 2019), although the  
348 float  $p\text{CO}_2$  data calculated indirectly from pH and alkalinity seems to be overestimated  
349 in organic-rich freshwaters (Abril et al., 2015). Notably, there was almost no difference  
350 between the uncorrected and corrected carbon sink from 1999 to 2001, when the  
351 Southern Ocean carbon sink was at its weakest point in the past three decades. The  
352 relatively denser measurements in the SH winter than in other decades may be one  
353 important reason. Around 2000, the SOCAT winter measurements were close to half  
354 of the measurements in summer. Therefore, the influence of seasonally uneven  
355 measurements is relatively minor.

356 Both carbon sinks before and after the winter correction consistently show a rapid  
357 weakening of the Southern Ocean carbon sink during the 1990s. The corrected Southern  
358 Ocean carbon sink in this work weakened from  $-0.99 \pm 0.15 \text{ Pg C yr}^{-1}$  in 1992 to -  
359  $0.68 \pm 0.13 \text{ Pg C yr}^{-1}$  in 2001, and then strengthened back to  $-1.13 \pm 0.14 \text{ Pg C yr}^{-1}$  until  
360 2021. Such notable interannual changes were also found in other research based on  
361 observations covering the past two decades (Landschützer et al., 2016; Rödenbeck et  
362 al., 2014; Ritter et al., 2017; Gregor et al., 2021; Chau et al., 2022). The contribution of  
363 the Southern Ocean south of 35° on the global ocean  $\text{CO}_2$  uptakes decreased from  
364 approximately 63% in 1992 to 45% in 2021. The weakening of the Southern Ocean  
365 carbon sink in the 1990s was thought to be caused by the strengthening of the upper-

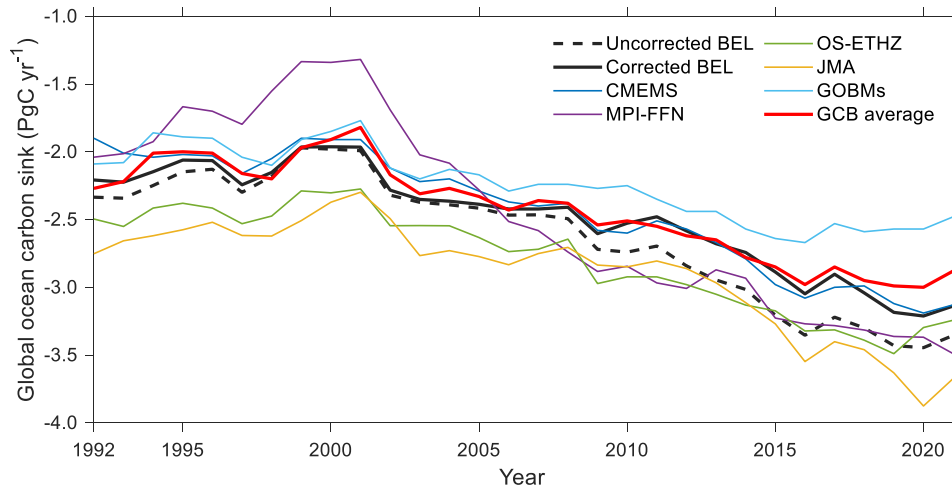
366 ocean overturning circulation and CO<sub>2</sub> release in source areas and the weakening of  
 367 CO<sub>2</sub> uptake in sink areas due to a southward shift of westerlies (Gillett et al., 2003;  
 368 Gruber et al., 2019; Landschützer et al., 2015; Miller et al., 2006; Rödenbeck et al.,  
 369 2015). The upwelling of the Southern Ocean increased by approximately 40% due to  
 370 enhanced wind-driven circulation. (DeVries et al., 2017). However, the weakening of  
 371 the upwelling since the beginning of the 21st century led to the reinvigoration of carbon  
 372 sink (Landschützer et al., 2015). Research based on an idealized upper ocean box model  
 373 also suggested that the slowed growth rate of atmospheric *p*CO<sub>2</sub> and the global sea  
 374 surface temperature response to the 1991 eruption of Mt Pinatubo volcanic were two  
 375 external forces to explain the global-scale reduction in the ocean carbon sink, and the  
 376 reinvigoration of carbon sink was **driven** by the acceleration of atmospheric *p*CO<sub>2</sub>  
 377 growth after 2001 (McKinley et al., 2020).



378  
 379 Figure 6. Interannual variability of the Southern Ocean carbon sink from uncorrected and corrected  
 380 ensemble learning method and other products. CMEMS: Chau et al., 2022; MPI-SOM-FFNN:  
 381 Landschützer et al., 2016; OS-ETHZ: Gregor et al., 2021; JMA: Iida et al., 2021; Uncorrected BEL:  
 382 boosting ensemble learning based on training sample of all seasons; Corrected BEL: *p*CO<sub>2</sub> during  
 383 May-September were predicted based on training sample only from April to September.

384 After the winter correction for seasonally uneven measurements in the Southern  
 385 Ocean, the global ocean carbon sink estimated from the Stepwise FFNN product and  
 386 corrected Southern Ocean *p*CO<sub>2</sub> data was relatively lower than other *p*CO<sub>2</sub> products  
 387 (Figure 7). However, our estimates are more consistent with the average results from  
 388 the Global Carbon Budget study, based on 10 global ocean biogeochemistry models  
 389 and 7 *p*CO<sub>2</sub> products (Friedlingstein et al. 2022). The global ocean carbon sink  
 390 estimated from previous *p*CO<sub>2</sub> products was notably stronger than the result from  
 391 biogeochemical models, and the discrepancy mainly occurred in the Southern Ocean  
 392 carbon sinks (Friedlingstein et al. 2022). The corrected Southern Ocean carbon sink

393 decreased the discrepancy with model results, indicating that previous  $p\text{CO}_2$  products  
 394 using the SOCAT dataset may also experience an overestimation of the Southern Ocean  
 395 carbon sink due to seasonally uneven measurements.



396

397 Figure 7. Global ocean carbon sink over the past three decades after the Southern Ocean correction.  
 398 **GOBMs**: average results of global ocean biogeochemical models (Friedlingstein et al. 2022); GCB  
 399 average: average results of 10 global ocean biogeochemical models and 7  $p\text{CO}_2$  products in the  
 400 Global Carbon Budget 2022 (Friedlingstein et al. 2022); CMEMS: Chau et al., 2022; MPI-SOM-  
 401 FFNN: Landschützer et al., 2016; OS-ETHZ: Gregor et al., 2021; JMA: Iida et al., 2021;  
 402 Uncorrected BEL: boosting ensemble learning FFNNs based on training sample of all seasons;  
 403 Corrected BEL: Southern Ocean  $p\text{CO}_2$  during May-September were corrected for uneven  
 404 measurements.

405

### 406 3.3 Influence of sea ice cover on the Southern Ocean carbon sink

407 The significant differences in the Southern Ocean carbon sink before and after  
 408 correction were only observed in the last decade. However, the  $p\text{CO}_2$  difference across  
 409 the interface after the winter correction was much more notable, particularly in the  
 410 Southern Ocean south of  $60^\circ\text{S}$ , where the surface seawater  $p\text{CO}_2$  is much higher than  
 411 atmospheric  $p\text{CO}_2$  (Figure 8). The vertical mixing and biological activity were reported  
 412 as primary controlling factors of surface ocean  $p\text{CO}_2$  in continent shelf areas, leading  
 413 to more considerable uncertainty in  $\text{CO}_2$  flux estimate compared to the open ocean (Qu  
 414 et al., 2014; Laruelle et al., 2017; Song et al., 2018). However,  $\text{CO}_2$  exchange between  
 415 the seawater and the atmosphere in the Antarctic shelf is impeded due to the extensive  
 416 sea ice coverage in most areas south of  $60^\circ\text{S}$ . As a result, despite the high surface  
 417 seawater  $p\text{CO}_2$  in this region, the  $\text{CO}_2$  release to the atmosphere is limited, and the

418 carbon source intensity is close to zero. The sea ice coverage in the Southern Ocean  
 419 south of 60°S also eliminates the influence of seasonally uneven  $p\text{CO}_2$  measurements.  
 420 Therefore, although the  $p\text{CO}_2$  difference across the interface was more significant after  
 421 the winter correction in areas south of 60°S, the carbon source intensity and its  
 422 difference before and after correction remain close to zero. Recent research has reported  
 423 that the melting of sea ice in the Arctic Ocean exposes more sea surface, serving as one  
 424 of the essential factors of rapid acidification in the Arctic Ocean (Qi et al., 2022).  
 425 Similarly, in the Amundsen and Bellingshausen Seas of the Southern Ocean, which are  
 426 characterized by warm water intrusion from the open ocean, the highest basal ice shelf  
 427 melting rates have been observed (Jacobs et al. 2011; Nakayama et al. 2013; Hellmer  
 428 et al., 2017). The Antarctic shelf ocean warming accelerated by increasing El Niño  
 429 variability was hastening the ice shelf/sheet melt (Cai et al., 2023). Unlike the Arctic  
 430 Ocean, the surface ocean  $p\text{CO}_2$  under sea ice coverage in the winter Southern Ocean  
 431 was much higher than in the atmosphere. If the sea ice completely melts, a significant  
 432 amount of  $\text{CO}_2$  will be directly released into the atmosphere through the exposed sea  
 433 surface. Furthermore, sea ice melting can indirectly impact the surface ocean  $p\text{CO}_2$  and  
 434 carbon sink intensity in the Southern Ocean through various pathways, such as reducing  
 435 sea surface temperature and altering convective overturning rates (Merino et al., 2016).

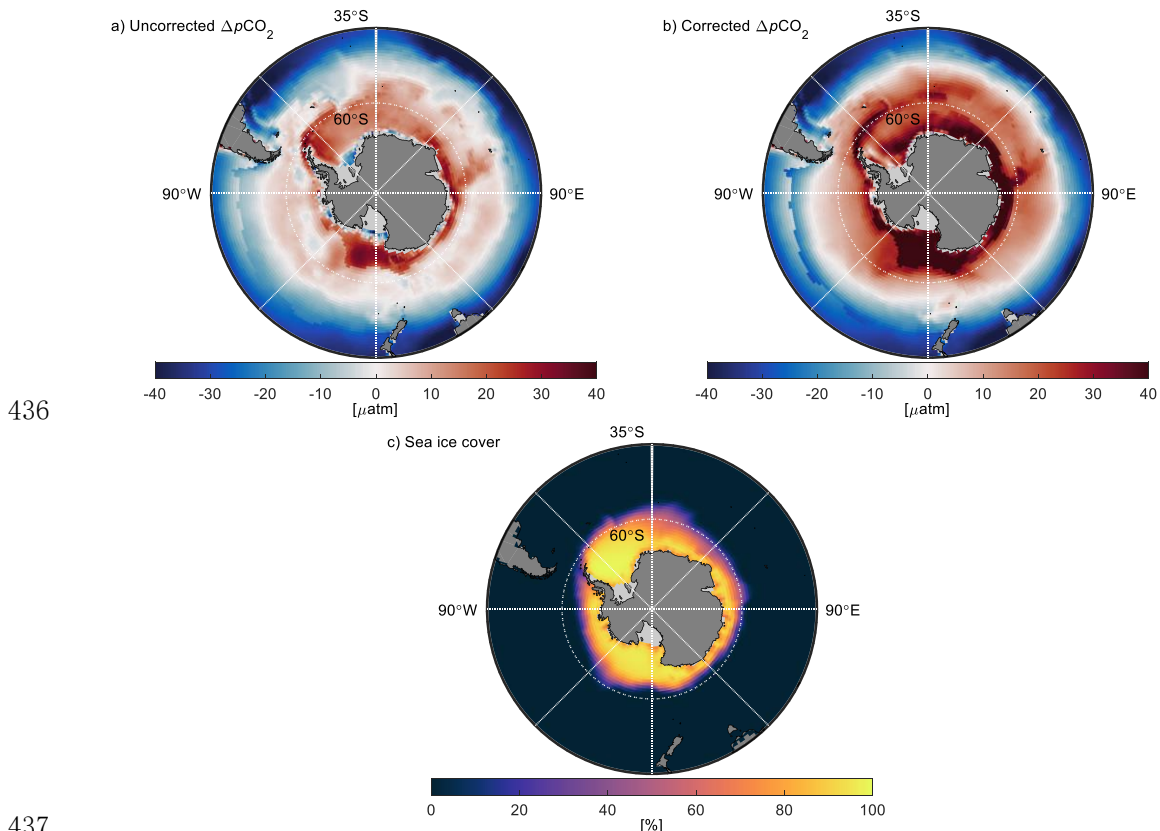
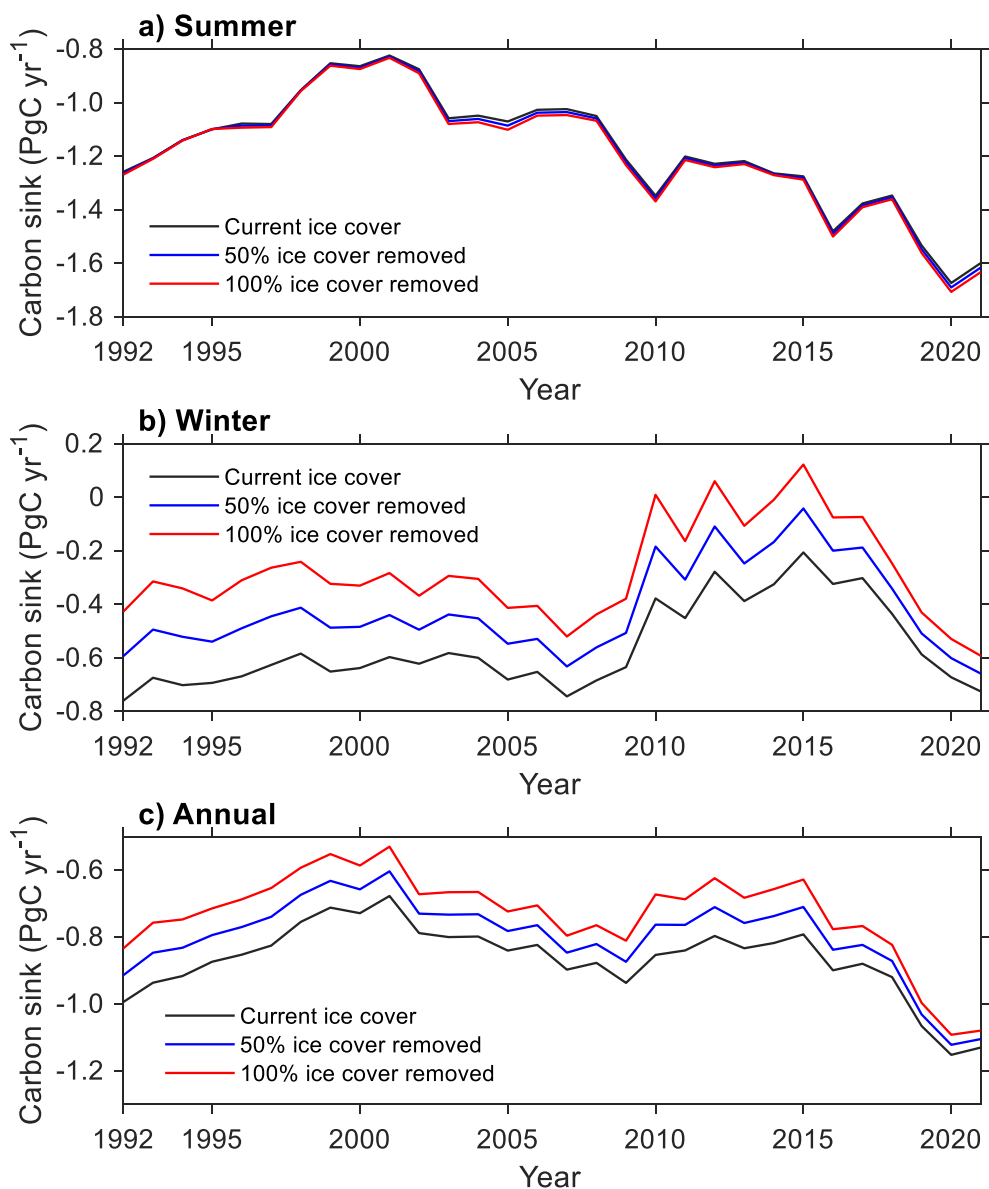


Figure 8. Distribution of average sea-air  $\Delta p\text{CO}_2$  and sea ice coverage during May-Sep in the

439 Southern Ocean. a)  $\Delta p\text{CO}_2$  calculated from uncorrected BEL product, b)  $\Delta p\text{CO}_2$  calculated from  
440 corrected BEL product, c) sea ice coverage from ERA5 product (Hersbach et al., 2020).  $\Delta p\text{CO}_2$ :  
441 surface ocean  $p\text{CO}_2$  minus atmospheric  $p\text{CO}_2$ .

442 Figure 4 shows the simulated carbon sink intensity in the Southern Ocean under  
443 different sea ice coverage without considering indirect factors based on the recent sea-  
444 air  $p\text{CO}_2$  difference. During the summer period in the Southern Ocean, when sea ice  
445 coverage is limited, and the surface seawater  $p\text{CO}_2$  in the covered areas is lower than  
446 atmospheric  $p\text{CO}_2$ , it is assumed that the complete melting of the currently covered sea  
447 ice would have little impact on the summer carbon sink intensity. However, during the  
448 winter, when sea ice coverage is extensive, and the surface seawater  $p\text{CO}_2$  in the  
449 covered areas is much higher than atmospheric  $p\text{CO}_2$ , the complete melting of the  
450 currently covered sea ice would result in the release of  $\text{CO}_2$  from the exposed surface  
451 Southern Ocean at an average rate of  $0.28 \text{ PgC yr}^{-1}$  during winter. This would weaken  
452 the role of the Southern Ocean in the global ocean  $\text{CO}_2$  uptakes and the role of the  
453 global ocean in buffering the rise in atmospheric  $\text{CO}_2$  concentration. Additionally,  
454 unlike the relatively stable increasing trend in carbon sink intensity during summer over  
455 the past 20 years, the winter carbon sink intensity in the Southern Ocean has shown  
456 significant fluctuations in the last decade but with no significant long-term trend. Based  
457 on the current data, considering the presence of sea ice-covered carbon sink areas in  
458 spring and autumn, the complete disappearance of sea ice coverage would lead to an  
459 average reduction of  $0.14 \text{ PgC yr}^{-1}$  in the overall annual  $\text{CO}_2$  absorption in the Southern  
460 Ocean. The magnitude of this reduction depends on the  $p\text{CO}_2$  values of seawater  
461 covered by sea ice, and it is still uncertain how this will change in the future. However,  
462 it can be anticipated that sea ice melting will slow down the rate of carbon sink  
463 enhancement in the Southern Ocean for a considerable period until the continuously  
464 rising atmospheric  $p\text{CO}_2$  exceeds the surface ocean  $p\text{CO}_2$  beneath the winter sea ice.



465

466 Figure 9. Southern Ocean carbon sink on different scenarios of sea ice melt. a)  $\text{CO}_2$  flux from  
 467 December to February in each year; b)  $\text{CO}_2$  flux from June to August in each year; c) annual  $\text{CO}_2$   
 468 flux. Current ice cover: ice coverage data from the ERA5 product (Hersbach et al., 2020); 50% ice  
 469 cover removed: assuming that 50% of current ice cover melts; 100% ice cover removed: assuming  
 470 that all ice cover melts.

#### 471 **4 Summary and conclusions**

472 As one of the most important carbon sink regions, the Southern Ocean experienced  
 473 higher uncertainties of carbon sink estimation than other adjacent regions due to the  
 474 sparse and seasonally uneven measurements. By comparing the performance of the

475 BEL FFNNs with different training strategies in the Southern Ocean from May to  
476 September, it was found that using data from all months for training the neural network  
477 resulted in higher RMSE and bias than using only sectional winter measurements for  
478 training. The predicted  $p\text{CO}_2$  from May to September was significantly lower than the  
479 observed values when measurements of all months were used due to missing winter  
480 data, which was less than a fifth of summer measurements. As a result, the neural  
481 network significantly underestimated the surface seawater  $p\text{CO}_2$  in the Southern Ocean  
482 during winter. However, training the neural network using sectional winter  
483 measurements and correcting the  $p\text{CO}_2$  predictors could effectively alleviate the  
484 underestimation of winter Southern Ocean  $p\text{CO}_2$ . The underestimation of winter  
485 Southern Ocean  $p\text{CO}_2$  further led to an overestimation of the carbon sink intensity by  
486 about 16%. This may be a key factor contributing to the general discrepancy between  
487 carbon sink intensity estimated from  $p\text{CO}_2$  products and biogeochemical models.  
488 Especially in the last decade, the corrected average Southern Ocean carbon sink was  
489 only  $-0.93 \text{ PgC yr}^{-1}$ , significantly lower than the original intensity of  $-1.20 \text{ PgC yr}^{-1}$ ,  
490 indicating an overestimation of the Southern Ocean carbon sink by about 29% in the  
491 last decade. The winter correction in the Southern Ocean carbon sink has reduced the  
492 discrepancy between  $p\text{CO}_2$  products and biogeochemical models and brought the  
493 estimated global ocean carbon sink intensity closer to the average results obtained from  
494 the Global Carbon Budget 2022.

495 Furthermore, although the  $p\text{CO}_2$  difference after correction was more notable in  
496 the Southern Ocean south of  $60^\circ\text{S}$ , the extensive sea ice coverage almost eliminates the  
497  $\text{CO}_2$  flux and mitigates the underestimation of winter surface ocean  $p\text{CO}_2$ . Therefore,  
498 the difference in carbon sink intensity before and after correction in the Southern Ocean  
499 was mainly observed in the  $50\text{-}60^\circ\text{S}$  region. If sea ice melts and exposes all currently  
500 covered surface Southern Oceans, the high  $p\text{CO}_2$  seawater will release an additional  
501  $0.28 \text{ PgC yr}^{-1}$  of  $\text{CO}_2$  to the atmosphere in winter of each year, leading to an average  
502 reduction of  $0.14 \text{ PgC yr}^{-1}$  in the overall annual Southern Ocean carbon sink. Over a  
503 considerable period, sea ice melting will lead to  $\text{CO}_2$  release from the sea ice-covered  
504 regions, slowing down the enhancement rate of the Southern Ocean carbon sink until  
505 the continuously rising atmospheric  $p\text{CO}_2$  surpasses the surface ocean  $p\text{CO}_2$  in the  
506 winter sea ice areas.

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512 Science Data Center and Public Technical Service Center, Institute of Oceanology,  
513 Chinese Academy of Sciences. The dataset of  $1^{\circ}\times 1^{\circ}$  gridded surface ocean  $p\text{CO}_2$  and  
514 sea-air  $\text{CO}_2$  flux is available from the Institute of Oceanology of the Chinese Academy  
515 of Sciences Marine Science Data Center at <https://doi.org/10.12157/iocas.2021.0022>.  
516 We thank SOCAT for sharing the  $p\text{CO}_2$  observation data. The Surface Ocean  $\text{CO}_2$  Atlas  
517 (SOCAT) is an international effort, endorsed by the International Ocean Carbon  
518 Coordination Project (IOCCP), the Surface Ocean Lower Atmosphere Study (SOLAS)  
519 and the Integrated Marine Biosphere Research (IMBeR) program, to deliver a  
520 uniformly quality-controlled surface ocean  $\text{CO}_2$  database. The many researchers and  
521 funding agencies responsible for the collection of data and quality control are thanked  
522 for their contributions to SOCAT.

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699 Reconstruction of global surface ocean *p*CO<sub>2</sub> using region-specific predictors  
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This article describes the impact of melting sea ice on carbon sink. The paper addresses boosting ensemble learning feed-forward neural networks to underestimation of the surface Southern Ocean  $p\text{CO}_2$ . The main issue regards sparse measurements of surface ocean  $p\text{CO}_2$ . The sea-air  $\text{CO}_2$  flux was estimated based on the  $p\text{CO}_2$  difference across the interface. The major claim of the article regards the fact that when using all months for training the neural network resulted in higher RMSE and bias than using only sectional winter measurements for training. Also the winter correction in the Southern Ocean carbon sink has reduced the bias in the  $p\text{CO}_2$  estimation with notable difference South of 60S.

Even if promising the author should add additional analysis to the results and correct the following:

- The github link to the code is missing, that is necessary
- The author in the method should highlight more why they choose feedforward neural network with 10 layers. Can the author provide a plot of their loss function?
- The paper is missing a comparison with a classic regression approach which would highlight why choosing the feedforward neural network can be a good choice. I highly recommend adding it.
- In line 99 the author has used the SOCAT  $p\text{CO}_2$  measurements, the authors should talk more about the dataset including the time range of it.
- In line 104 the author mentioned K-fold cross validation with a number of folds equal 4. Is the number 4 arbitrary?
- In line 188 the authors train a neural network with SOCAT measurements only from April to October. The resulting RMS is lower in this case. The author should emphasize more why it should be the case. This section 188-200 needs further confirmation.

The predictors used for the neural network have been put in supplemental materials. I would encourage to talk more in the text about these predictors and why they are important.

In the conclusion part the authors should emphasize more about the broader impacts of their findings and how these methods can be beneficial to the scientific community.

Given the interested topic covered by the article I would recommend major revision to the editor in order to address the changes written above.

(**Bold black: Reviewer comments; thick red: Response to comments; thick black: changes in manuscript**)

**Reviewer #1:**

**This article describes the impact of melting sea ice on carbon sink. The paper addresses boosting ensemble learning feed-forward neural networks to underestimation of the surface Southern Ocean  $p\text{CO}_2$ . The main issue regards sparse measurements of surface ocean  $p\text{CO}_2$ . The sea-air  $\text{CO}_2$  flux was estimated based on the  $p\text{CO}_2$  difference across the interface. The major claim of the article regards the fact that when using all months for training the neural network resulted in higher RMSE and bias than using only sectional winter measurements for training. Also the winter correction in the Southern Ocean carbon sink has reduced the bias in the  $p\text{CO}_2$  estimation with notable difference South of 60S.**

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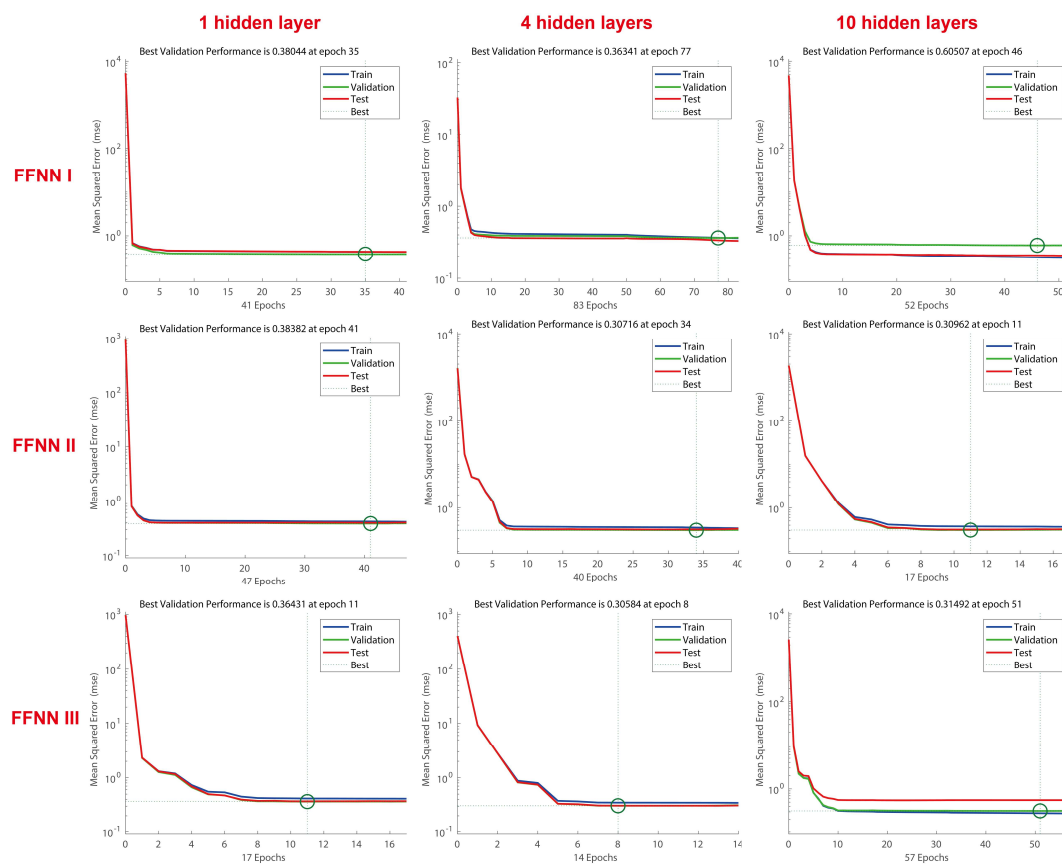
**Response:** The MATLAB codes have been uploaded to the GitHub repository at <https://github.com/GuorongZhong/Stepwise-BEL-FFNN-code-for-MATLAB.git>, and the link has been added in a Data Availability section.

**2) The author in the method should highlight more why they choose feedforward neural network with 10 layers. Can the author provide a plot of their loss function?**

**Response:** We used a few hidden layers with 10 neurons in each layer, and the number of hidden layers was adjusted based on  $p\text{CO}_2$  predicting errors to avoid underfitting caused by too less neurons and overfitting caused by too many neurons. One another way is using only one hidden layer and adjusting the number of inner neurons. These two structures were commonly used in previous research. However, to achieve the same predicting error, neural networks with more hidden layers require far fewer neurons compared to shallower neural networks. Therefore, we used a deeper structure and changed the number of hidden layers instead of directly changing the number of neurons in each layer. We used the mean squared error as the loss function and compared the performance of FFNNs with different numbers of hidden layers, to determine how many layers should be used. Although we evaluated the performance based on RMSE rather than the loss function, the RMSE and loss function both suggested the best performance when we used a proper number of hidden layers. For



example, we used FFNNs with 4 hidden layers in the areas between 50–60°S based on changes in RMSE with the number of hidden layers. The loss function also suggested the best performance when using 4 hidden layers. Here is the loss function plot of the BEL FFNNs when using one hidden layer, 4 hidden layers, and 10 hidden layers. The FFNNs with one hidden layer are slightly underfitting, while the FFNNs with 10 hidden layers are overfitting, and both of them have a higher mean squared error and RMSE. In other regions, we also compared the RMSE when using different numbers of hidden layers to determine the structure. Since the loss functions are not used to validate the FFNNs performance in our work, the figure of loss functions is not put in the main text or supplemental materials.



The loss function of the BEL FFNNs in region 50–60°S when using one hidden layer, 4 hidden layers, and 10 hidden layers

**3) The paper is missing a comparison with a classic regression approach which would highlight why choosing the feedforward neural network can be a good choice. I highly recommend adding it.**

Response: The  $p\text{CO}_2$  predicting error from two classic approaches has been added for comparison, including a multiple linear regression (MLR) and a multiple non-linear

regression (MNLR). The classic approaches suggested a higher RMSE and a more severe underestimation of Southern Ocean  $p\text{CO}_2$  than the FFNN methods (Table 2). The newly added contents are as follows:

In addition, we also test the  $p\text{CO}_2$  RMSE and bias of traditional regression methods for comparison, including a multiple linear regression (MLR) and a multiple non-linear regression (MNLR). As expected, the traditional regression methods are more susceptible to seasonal uneven measurements, showing higher RMSE and more severe underestimation of Southern Ocean  $p\text{CO}_2$ . In particular, the MLR using measurements from all months resulted in a winter RMSE of 34.02  $\mu\text{atm}$  in the region south of 60°S, and output  $p\text{CO}_2$  values lower than the real measurements by an average of 17.29  $\mu\text{atm}$ . This result is barely acceptable, and it also explains why traditional regression methods in previous research were generally limited to specific seasons. Although the MNLR performs better than the MLR, its RMSE was still much higher than that of the FFNN methods, and the MNLR output  $p\text{CO}_2$  during winter was also significantly lower than measurements in regions south of 50°S. Similar to the treatment of the training period of the two FFNN methods, a lesser underestimation of Southern Ocean  $p\text{CO}_2$  in winter was found when using only partial winter measurements for regression. In the 35-50°S region, the RMSE of traditional regression methods was still higher than the two FFNN methods, and the influence of seasonal uneven measurements was not significant.

Table 2. Comparison of  $p\text{CO}_2$  predicting error in the Southern Ocean during May-September among different methods and regression periods

Regression Method	Regression Period	35-50° S		50-60° S		S of 60° S	
		RMSE ( $\mu\text{atm}$ )	bias ( $\mu\text{atm}$ )	RMSE ( $\mu\text{atm}$ )	bias ( $\mu\text{atm}$ )	RMSE ( $\mu\text{atm}$ )	bias ( $\mu\text{atm}$ )
BEL	May-Sep	12.01	+0.61	11.97	+0.22	14.76	+0.33
FFNNs	Apr-Sep	10.70	+0.38	11.88	-0.36	14.87	-0.90
	May-Oct	11.39	-0.36	12.07	-0.66	14.50	-0.07
	Apr-Oct	11.10	-0.68	12.09	-1.16	14.20	-1.38
	Mar-Nov	11.32	-1.26	12.51	-2.13	15.50	-4.47
	All Months	<b>9.86</b>	<b>-0.39</b>	13.27	-3.13	16.09	-5.77
<b>BEL</b>	May-Sep	12.24	+0.74	11.93	+0.17	14.44	+1.17
<b>FFNNs</b>	Apr-Sep	10.76	+0.30	11.26	+0.09	13.49	-0.06
<b>with</b>	May-Oct	12.81	-0.28	11.44	+0.04	14.27	-0.20
<b>corrected</b>	Apr-Oct	11.83	-0.79	<b>10.93</b>	<b>-0.25</b>	<b>13.29</b>	<b>-0.74</b>

<b>predictors</b>	Mar-Nov	11.69	-1.49	13.07	-0.46	14.07	+0.02
	All Months	9.88	-0.29	11.49	-1.08	14.61	-0.90
Individual	May-Sep	12.05	+0.50	11.99	+0.07	15.15	0.36
FFNN	Apr-Sep	10.58	+0.30	12.02	-0.52	15.04	-1.14
	May-Oct	11.43	-0.59	12.21	-0.75	14.92	-0.32
	Apr-Oct	11.19	-0.83	12.29	-1.49	14.86	-1.47
	Mar-Nov	11.64	-1.43	12.82	-2.56	15.76	-3.95
	All Months	9.95	-0.34	13.31	-3.33	17.14	-5.38
	May-Sep	12.57	+0.50	12.30	+0.37	14.54	+0.83
FFNN	Apr-Sep	10.72	+0.27	11.45	+0.14	13.79	-0.27
with	May-Oct	13.09	-0.45	11.52	-0.07	14.46	-0.23
corrected	Apr-Oct	11.35	-0.92	11.06	-0.09	13.63	-0.27
predictors	Mar-Nov	12.02	-1.55	11.55	-0.09	17.86	+0.50
	All Months	9.95	-0.28	12.06	-1.04	15.85	-0.05
MLR with	May-Sep	16.34	-2.33	13.67	-1.71	21.12	+1.09
corrected	Apr-Sep	15.48	-0.67	14.51	-2.29	22.21	-3.00
predictors	May-Oct	16.98	-4.55	16.29	-4.83	23.46	-0.89
	Apr-Oct	15.87	-2.93	16.39	-5.56	24.79	-6.69
	Mar-Nov	16.09	-2.53	16.75	-6.22	29.21	-13.40
	All Months	17.70	-2.30	19.01	-6.11	34.02	-17.29
MNLR	May-Sep	14.37	-0.83	12.17	-0.62	17.04	+2.41
with	Apr-Sep	13.51	+0.67	11.20	-0.95	17.70	-2.86
corrected	May-Oct	14.55	-4.06	13.18	-3.47	17.70	+2.41
predictors	Apr-Oct	14.35	-3.45	13.53	-3.76	20.21	-6.64
	Mar-Nov	14.21	-1.72	12.72	-4.70	18.81	-8.01
	All Months	15.02	+0.90	13.92	-5.35	25.68	-13.41

(BEL FFNNs: boosting ensemble learning based on three FFNNs constructed in this work; Individual FFNN: one FFNN with the same structure used in the BEL; MLR: multiple linear regression; MNLR: multiple non-linear regression, see Supplementary Note 2; Regression period: a period of SOCAT samples used for training neural networks or performing classic regression to predict  $p\text{CO}_2$  during May-September; RMSE and bias: calculated from the difference between predicted  $p\text{CO}_2$  and SOCAT measurements during May-September based on the K-fold cross validation method. Corrected predictors:  $p\text{CO}_2$  predictors selected by a stepwise BEL FFNNs algorithm based on increasing weightings of winter measurements, see Table 1. Bold numbers:

the regression period with the lowest RMSE adopted in the final  $p\text{CO}_2$  product construction.)

**4) In line 99 the author has used the SOCAT  $p\text{CO}_2$  measurements, the authors should talk more about the dataset including the time range of it.**

**Response:** Thanks for the suggestion. We have added a description of the SOCAT dataset in the method section as follows:

The SOCAT dataset includes quality controlled global observations of in-situ surface ocean fugacity of carbon dioxide ( $f\text{CO}_2$ ), sea surface temperature, and salinity on ships, moorings, autonomous and drifting surface platforms for the global oceans and coastal seas from 1957 to 2023. This dataset is provided as a synthesis version and a gridded version, with an estimated  $f\text{CO}_2$  accuracy of better than  $5 \mu\text{atm}$ . The gridded  $f\text{CO}_2$  was converted to  $p\text{CO}_2$  using in-situ sea surface temperature and atmospheric pressure (Landschützer et al., 2013), and then the converted  $p\text{CO}_2$  was used in training neural networks:

$$p\text{CO}_2 = f\text{CO}_2 \cdot \exp\left(P_{atm}^{surf} \frac{B+2\cdot\delta}{R\cdot T}\right)^{-1} \quad (1)$$

where  $P_{atm}^{surf}$  is the atmospheric pressure using ERA5 sea level pressure product (Hersbach et al., 2020),  $B$  and  $\delta$  are virial coefficients calculated from temperature (Weiss, 1974),  $R$  is the gas constant and  $T$  is the absolute temperature.

**5) In line 104 the author mentioned K-fold cross validation with a number of folds equal 4. Is the number 4 arbitrary?**

**Response:** Setting  $K$  equal to 4 is not arbitrary but reasonable to be consistent with previous research. We set the  $K$  value to 4 in order to retain 25% measurements as an independent validation set during the validation process. In previous research, it has been common practice to set aside 20-25% of the measurements for independent validation to assess the accuracy of the neural network outputs. The  $K$ -fold cross-validation method used in this work is repeating this usual validation process for  $K$  times, to eliminate the influence of validation set selection.

**6) In line 188 the authors train a neural network with SOCAT measurements only from April to October. The resulting RMSE is lower in this case. The author should emphasize more why it should be the case. This section 188-200 needs further confirmation.**

Response: Thanks for the suggestion. This is mainly because of the effect of imbalanced data with data-rich summer and data-sparse winter. When training with imbalanced data, the neural network tends to perform better in data-rich seasons and significantly worse in data-sparse seasons. Recent studies suggested the effect of imbalanced data can be mitigated through data distribution re-balancing, control of loss function, and using transfer-learning based methods (Kang et al., 2020). Training a neural network with measurements only from April to October is a data distribution re-balancing method, which can effectively mitigate the influence of imbalanced data. The description of why RMSE is lower in the case using sectional winter measurements has been added in section 188-200 as follows:

This is because the quantity of  $p\text{CO}_2$  measurements is significantly imbalanced among different seasons, with data in winter much less than in summer. T When training with such seasonal imbalanced data, the neural network tends to perform better in data-rich summer, while the performance is significantly worse in data-sparse winter. This effect of imbalanced data can be mitigated through re-balancing data distribution and using re-balancing design in the loss function or learning algorithm of neural networks (Kang et al., 2020). Training the neural networks with partial winter measurements is a data distribution re-balancing method, as the number of measurements is less unbalanced after the data-rich summer was removed from the training set. As a result, in the areas south of  $50^\circ\text{S}$ , the BEL FFNNs and the individual FFNN trained with sectional winter measurements suggested a significantly lower RMSE during winter than those trained with all-month measurements.

Kang, B., Xie, S., Rohrbach, M., Yan, Z., Gordo, A., Feng, J., & Kalantidis, Y. (2020). Decoupling representation and classifier for long-tailed recognition. In *8th International Conference on Learning Representations, ICLR 2020*.

**7) The predictors used for the neural network have been put in supplemental materials. I would encourage to talk more in the text about these predictors and why they are important.**

Response: Thanks for the suggestion. We have added a new section in the method part to interpret the importance of  $p\text{CO}_2$  predictors and how they are selected. The predictors reflect the drivers that affect  $p\text{CO}_2$  and its variability, and directly influence the  $p\text{CO}_2$  predicting error of neural network methods. However, the factors driving  $p\text{CO}_2$  and its variability differ significantly among different regions. Therefore, it is important to

select a combination of  $p\text{CO}_2$  predictors that are most relevant to the  $p\text{CO}_2$  drivers in different regions for improving neural network performance. We have moved the context in supplemental materials to the main text, and added a section describing the data source of used data products for  $p\text{CO}_2$  predictors in supplemental materials. The newly added section is as follows:

## *2.2 Selection and correction of $p\text{CO}_2$ predictors*

The  $p\text{CO}_2$  predictors input into the FFNN reflect the drivers of surface ocean  $p\text{CO}_2$  and its variability. When changing the input  $p\text{CO}_2$  predictors, both the FFNN predicted  $p\text{CO}_2$  value and the predicting error significantly change, and these changes can be even greater than those caused by altering the FFNN structure. However, the environmental factors driving  $p\text{CO}_2$  and its variability differ significantly among different regions. The surface ocean  $p\text{CO}_2$  is largely affected by the upwelling and biological drawdown in the Antarctic region, and is affected by meridional overturning circulation in the subantarctic region (DeVries et al., 2017; Gruber et al., 2019). This means that using different predictors in different latitude regions can better reflect the regional influencing factors of  $p\text{CO}_2$  and its variability. To find the best combination of  $p\text{CO}_2$  predictors in different regions, we have proposed a Stepwise FFNN algorithm in previous work, where the changes in predicting error are fed back to the selection of input  $p\text{CO}_2$  predictors (Zhong et al., 2022). This algorithm allows for the objective selection of  $p\text{CO}_2$  predictors in different regions that result in the lowest  $p\text{CO}_2$  predicting error. The procedure of the Stepwise FFNN algorithm is determining  $p\text{CO}_2$  predictors one by one until no further reduction in predicting error is achieved by either adding or removing any predictors. Specifically, the first  $p\text{CO}_2$  predictor is selected by comparing predicting errors when individually using each collected environmental variable (listed in Table S1) as input of the FFNN. The variable with the lowest error is determined as the first  $p\text{CO}_2$  predictor, which is also the predictor that has the greatest impact on the distribution or variability of regional surface ocean  $p\text{CO}_2$ . Subsequently, leaving the first predictor unchanged, the predicting errors are compared when using each environmental variable as the second input of the FFNN. The environmental variable with the lowest error is determined as the second  $p\text{CO}_2$  predictor. In the same way, new predictors are continuously determined one after another, until the predicting error no longer continues to decrease regardless of which one variable is added as a  $p\text{CO}_2$  predictor. Meanwhile, whenever a new predictor is determined, the algorithm also tests if the predicting error will decrease when sequentially removing each determined predictor, in order to eliminate co-correlation and prevent overfitting. For example,

when the fourth predictor is determined, the model tests the change in predicting error by individually removing each one from the previously determined three predictors. If the error decreases after removing a previously determined predictor, this predictor is highly correlated with other determined predictors. By adding and removing variables in the input of the FFNN one by one in this way, the algorithm ultimately identifies a set of  $p\text{CO}_2$  predictors that minimize the  $p\text{CO}_2$  predicting error. In this work, the single FFNN structure used in the previous Stepwise FFNN algorithm has been replaced with a structure of ensemble learning FFNNs with stronger fitting capabilities (see Figure 1), referred to as the Stepwise BEL algorithm.

However, the Stepwise BEL algorithm relies on predicting errors for determination of  $p\text{CO}_2$  predictors, and the number of SOCAT  $p\text{CO}_2$  measurements in the Southern Ocean during the winter season is much lower than in the summer, leading to a lower weighting on winter predicting errors compared to summer in the determination. As a result, the selected predictors are more reflective of factors influencing  $p\text{CO}_2$  distribution in the summer (such as biological drawdown) while neglecting those in the winter (such as enhanced vertical mixing). Therefore, we increased the weighting of winter data to be nearly equal to that of summer, to carry out a winter correction of  $p\text{CO}_2$  predictors in the Southern Ocean:

$$RMSE = \sqrt{\frac{3*\sum(\Delta p\text{CO}_2 \text{ May-Sep})^2 + \sum(\Delta p\text{CO}_2 \text{ Oct-Apr})^2}{3*N_{\text{May-Sep}} + N_{\text{Oct-Apr}}}} \quad (2)$$

where the  $\Delta p\text{CO}_2$  was the difference between predicted  $p\text{CO}_2$  and SOCAT  $p\text{CO}_2$  measurements, and  $N$  was the number of monthly SOCAT measurements ( $3*N_{\text{May-Sep}} \approx N_{\text{Oct-Apr}}$ ). Based on a self-organization map method, the Southern Ocean was divided into different regions according to the similarity of  $p\text{CO}_2$  drivers, including two belt regions and three sectors connecting to major basins (Zhong et al., 2022). Therefore, the selection of  $p\text{CO}_2$  predictors and reconstruction of  $p\text{CO}_2$  in this work was based on three latitude areas: 35-50°S, 50-60°S, and south of 60°S (Table 1). Since there were no observed effects of uneven seasonal distribution on the neural network training in the 35-50°S region connecting the major basins, the correction of  $p\text{CO}_2$  predictors is only conducted in the area south of 50°S.

**Table 1 Winter correction of  $p\text{CO}_2$  predictors.**

Area	$p\text{CO}_2$ predictors
35-50°S Pacific sector	SST, sin(Longitude), $x\text{CO}_2$ , Latitude, SSS, Photosynthetically Available Radiation, Chlorophyll, Mixed layer depth, cos(Longitude), Mixed layer depth <sub>anom</sub> , Remote sensing reflectance at 531nm and 555nm

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Indian sector	SST, Total absorption at 645nm, Number of months since January 1992, Mixed layer depth, SSS, W velocity of ocean currents at 105m, Surface pressure, Total absorption at 678nm, W velocity of ocean currents at 195m, Total backscattering at 667nm, Nitrate, Total absorption at 555nm, Mixed layer depth <sub>anom</sub> , Particulate organic carbon, DIC, W velocity of ocean currents at 65m, Remote sensing reflectance at 488nm, Total backscattering at 443nm
Atlantic sector	Latitude, SSS, Dry air mixing ratio of atmospheric CO <sub>2</sub> , Particulate organic carbon, Total backscattering at 488nm, Mixed layer depth, Diffuse attenuation coefficient, Total backscattering at 412nm, Sea surface height, cos(Longitude), SST, Remote sensing reflectance at 460nm, Total backscattering at 547nm, Bathymetry, Total absorption at 678nm, Total backscattering at 469nm, Remote sensing reflectance at 678nm
50-60°S uncorrected	SSS <sub>anom</sub> , SST, Mixed layer depth, Dry air mixing ratio of atmospheric CO <sub>2</sub> <sub>anom</sub> , Bathymetry, Sea surface height <sub>anom</sub> , W velocity of ocean currents at 105m, DIC, Dissolved oxygen, Nitrate
50-60°S corrected	Dry air mixing ratio of atmospheric CO <sub>2</sub> , Mixed layer depth, SST, DIC, month, SSS, Bathymetry, Latitude, W velocity of ocean currents at 105m, Dissolved oxygen, W velocity of ocean currents at 5m, Dry air mixing ratio of atmospheric CO <sub>2</sub> <sub>anom</sub> , Mixed layer depth <sub>anom</sub>
S of 60°S uncorrected	DIC, Bathymetry, SSS, Alkalinity, cos(Longitude), SST, Sea surface height <sub>anom</sub> , W velocity of ocean currents at 195m, 5m, and 65m, SSS <sub>anom</sub>
S of 60°S corrected	Bathymetry, SSS, Alkalinity, SST, month, W velocity of ocean currents at 65m, 105m, and 195m, Dissolved oxygen, cos(Longitude), Sea surface height, Latitude, SSS <sub>anom</sub>

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(Uncorrected predictors were selected by a Stepwise BEL algorithm updated from Zhong et al., 2022, corrected predictors were selected using the same algorithm but increasing the weighting of winter SOCAT measurements; The sort order of  $p\text{CO}_2$  predictors indicated a relative contribution on decreasing predicting errors. The predictors denoted by subscript "anom" represent the monthly anomaly obtained by subtracting the monthly climatology. Data sources of used products are listed



in Supplementary Table 1.)

**Section added in the supplement:**

*Note 1 Products of pCO<sub>2</sub> predictors*

We have collected gridded products of different environmental variables as potential pCO<sub>2</sub> predictors (Table S1), and the selection of these products was based on two reasons. The first reason was their potential association with physical, chemical, and biological ocean processes which may affect the surface ocean pCO<sub>2</sub>. Another reason was the sufficient availability in time and spatial coverage and their potential association with the unavailable interannual variability of some climatological products used.

Most predictor products were obtained with a monthly and 1°×1° resolution, which can be directly used without any treatments. Differently, products with higher resolutions were integrated into the same monthly and 1°×1° resolution by averaging, before they can be used in the relationship fitting. For instance, the mixed layer depth product, originally obtained with a resolution of 0.25°×0.25°, was converted to a 1°×1° resolution by averaging 16 0.25° grids into one 1° grid. Similarly, predictor products obtained with daily or weekly resolutions were converted to the monthly resolution by directly averaging all values within the same month, such as the ocean currents product.

Supplementary Table 1. Data products used as pCO<sub>2</sub> predictors.

Predictor	Data product	Reference	Resolution
Sine of latitude		-	-
Sine of longitude		-	-
Cosine of longitude		-	-
Number of months since January 1992		-	-
Year		-	-
Month		-	-
SST and monthly anomaly	ECCO2 cube92	Menemenlis et al., 2008	0.25°, 1992-2022
SSS and monthly anomaly	ECCO2 cube92	Menemenlis et al., 2008	0.25°, 1992-2022
Climatological alkalinity	<a href="#">AT_NNGv2_climatology</a>	Broullón et al., 2019	1°
Climatological	<a href="#">TCO2_NNGv2LD</a>	Broullón et al.,	1°

dissolved inorganic carbon	<a href="#">EO climatology</a>	2020		
Climatological dissolved oxygen	WOA18	Garcia et al., 2019a	1°	
Climatological nitrate	WOA18	Garcia et al., 2019b	1°	
Climatological phosphate	WOA18			
Climatological silicate	WOA18			
Mixed layer depth and monthly anomaly	ECCO2 cube92	Menemenlis et al., 2008	0.25°, 1992-2022	
Sea surface height and monthly anomaly	ECCO2 cube92			
W velocity of ocean currents at 5 m, 65m, 105m, 195m, and in-situ depth	ECCO2 cube92			
Sea level pressure	ERA5	Hersbach et al., 2020	1°, 1979-2022	
Surface pressure	ERA5			
dry air mixing ratio of atmospheric CO <sub>2</sub> and monthly anomaly	NOAA Greenhouse Gas Marine Boundary Layer Reference	Lan et al., 2023	0.25°, 1979-2022	
Oceanic Nino Index	bi-monthly Multivariate El Niño/Southern Oscillation index	Wolter et al., 2011	1979-2023	
Arctic Oscillation index	Climate Prediction Center Daily Arctic Oscillation Index	CPC, 2002	1950-2023	
Southern Oscillation Index	Climate Prediction Center Southern Oscillation Index	CPC, 2005	1951-2023	
Bathymetry	GEBCO_2022 Grid	GEBCO, 2022	15 arc-second	
10 m Wind speed and monthly anomaly	ERA5	Hersbach et al., 2020	1°, 1979-2022	

Climatology of	MPI-ULB-	Landschützer et al., 2020	0.25°
Surface Ocean $p\text{CO}_2$	SOM_FFN_clim		
Chlorophyll concentration and monthly anomaly*	MODIS-Aqua Chlorophyll Data	NASA, 2022	9km, 2002-2023
Surface particulate organic carbon concentration	MODIS-Aqua Particulate Organic Carbon Data		
Photosynthetically Available Radiation	MODIS-Aqua Photosynthetically Available Radiation Data		
Diffuse attenuation coefficient at 490 nm	MODIS-Aqua Downwelling Diffuse Attenuation Coefficient Data		
Remote sensing reflectance at 412-678 nm	MODIS-Aqua Remote-Sensing Reflectance Data		
Total absorption at 412-678 nm	MODIS-Aqua Inherent Optical Properties Data		
Total backscattering at 412-678 nm	MODIS-Aqua Inherent Optical Properties Data		

(\*: products from Chlorophyll concentration to Total backscattering are satellite remote sensing products; Remote sensing reflectance, total absorption, and total backscattering both include 10 wavelengths: 412nm, 443nm, 469nm, 488nm, 531nm, 547nm, 555nm, 645nm, 667nm, and 678nm, with each wavelength regarded as one individual predictor.)

**8) In the conclusion part the authors should emphasize more about the broader impacts of their findings and how these methods can be beneficial to the scientific community.**

**Response: Thanks for the suggestion. We have modified the conclusion part as follows:**

Our method provides a feasible solution for handling the impact of uneven

measurements on the performance of neural networks. It also helps to improve the high uncertainty in  $p\text{CO}_2$ -based carbon sink estimates for special regions with limited and unevenly distributed data, such as polar regions. Furthermore, although the  $p\text{CO}_2$  difference after correction was more notable in the Southern Ocean south of  $60^\circ\text{S}$ , the extensive sea ice coverage almost eliminates the  $\text{CO}_2$  flux and mitigates the underestimation of winter surface ocean  $p\text{CO}_2$ . Therefore, the difference in carbon sink intensity before and after correction in the Southern Ocean was mainly observed in the  $50\text{-}60^\circ\text{S}$  region. If sea ice melts and exposes all currently covered surface Southern Oceans, the high  $p\text{CO}_2$  seawater will release an additional  $0.28 \text{ PgC yr}^{-1}$  of  $\text{CO}_2$  to the atmosphere in winter of each year, leading to an average reduction of  $0.14 \text{ PgC yr}^{-1}$  in the overall annual Southern Ocean carbon sink. This means that in the future, as global warming causes the melting of sea ice in the Southern Ocean, a portion of  $\text{CO}_2$  trapped under the sea ice may be released into the atmosphere. Additionally, as the seawater warms, it can lead to an increase in surface ocean  $p\text{CO}_2$  levels. The combined effects of global warming would limit the ocean's capacity to absorb atmospheric  $\text{CO}_2$ , which in turn could exacerbate global warming, potentially accelerating the pace of global climate change.

**Given the interested topic covered by the article I would recommend major revision to the editor in order to address the changes written above.**

**Reviewer #2:**

**The manuscript describes an approach to reduce the uncertainty/discrepancy in data products and model outputs for surface ocean  $p\text{CO}_2$  in the Southern Ocean.**

**The authors state that this is mainly due to the lack of in situ observations during winter (compared to summer).**

**They have applied the boosting ensemble learning feed forward neural networks (BEL FFNNs) method using a gridded version of SOCAT data, and data from the Southern Ocean flux station (SOFS, 142.0°E, 46.8°S), south of Tasmania (Australia) for validation.**

**Question:**

**1) Aren't there any other  $p\text{CO}_2$  observing time series in other sector of the S. Ocean? Or only for summer periods?**

**Response:** There are a few other  $p\text{CO}_2$  observing time series stations in the Southern Ocean, such as the Drake time series across the Drake Passage and the KERFIX time series in the Indian sector. The Drake time series station consists primarily of 15 stations across the Drake Passage in the Southern Ocean from 2002 to 2018. However, the mooring measurements are ship-based and moving across the Drake Passage between 55-70°W and 55-65°S, and the winter period was less sampled. It is difficult to validate the winter  $p\text{CO}_2$  from our method using these data, so the Drake time series was not used. In addition, there is a KERFIX station located in the Indian sector of the Southern Ocean (50.6°S, 68.4°E), but it is only from 1990 to 1995. The measurements of DIC and Alkalinity are only available from 1992 to 1993, and the calculated winter  $p\text{CO}_2$  in the KERFIX station was only available in 1993, with calculated values lower than all existing machine learning  $p\text{CO}_2$  products. In addition, there are a few other time series stations, but both of them lack winter measurements or lack  $p\text{CO}_2$  measurements. Therefore, we only used the SOFS time series station, as this station has many winter measurements with good continuity.

**2) My main question for the methods section concerns the following (l. 76-78):**

**"The surface ocean  $p\text{CO}_2$  converted from the Surface Ocean  $\text{CO}_2$  Atlas version 2023 (SOCAT v2023) dataset was used for  $p\text{CO}_2$  mapping by fitting the non-linear relationship between  $p\text{CO}_2$  and environmental variables"**

**To which environmental variables?**

**Response:** The conversion was carried out using in-situ sea surface temperature and atmospheric pressure. The description of conversion between  $p\text{CO}_2$  and  $f\text{CO}_2$  has been added in the method section as follows:

The gridded  $f\text{CO}_2$  was converted to  $p\text{CO}_2$  using in-situ sea surface temperature and atmospheric pressure (Landschützer et al., 2013), and then the converted  $p\text{CO}_2$  was used in training neural networks:

$$p\text{CO}_2 = f\text{CO}_2 \cdot \exp\left(P_{atm}^{surf} \frac{B+2\cdot\delta}{R\cdot T}\right)^{-1} \quad (1)$$

where  $P_{atm}^{surf}$  is the atmospheric pressure using ERA5 sea level pressure product (Hersbach et al., 2020),  $B$  and  $\delta$  are virial coefficients calculated from sea surface temperature (Weiss, 1974),  $R$  is the gas constant and  $T$  is the absolute temperature.

**3) Additionally, the list of predictors appears in the supplementary material only, and it is hard for the reader to understand why the winter predictors were chosen for each latitude area.**

*Response:* Thanks for the suggestion. A new section about the use of predictors has been added in the method section, and the context in supplementary material has been also moved to this new section. The predictors were chosen for each latitude area because of the latitude differences in  $p\text{CO}_2$  drivers. The surface ocean  $p\text{CO}_2$  is largely affected by the upwelling and biological drawdown in the high latitude Antarctic region, and is affected by meridional overturning circulation in the subantarctic region. While in the 35-50°S region, the variability of surface ocean  $p\text{CO}_2$  was mainly driven by the notable seasonal change in SST. The dividing of biogeochemical provinces using a self-organizing map method based on the similarity of environmental variables also presents a belt province south of 60°S and a belt province covering nearly 50-60°S in our previous work. Therefore, we chose  $p\text{CO}_2$  predictors for different latitude areas. The new section was as follows:

### *2.2 Selection and correction of $p\text{CO}_2$ predictors*

The  $p\text{CO}_2$  predictors input into the FFNN reflect the drivers of surface ocean  $p\text{CO}_2$  and its variability. When changing the input  $p\text{CO}_2$  predictors, both the FFNN predicted  $p\text{CO}_2$  value and the predicting error significantly change, and these changes can be even greater than those caused by altering the FFNN structure. However, the environmental factors driving  $p\text{CO}_2$  and its variability differ significantly among different regions. The surface ocean  $p\text{CO}_2$  is largely affected by the upwelling and biological drawdown in the Antarctic region, and is affected by meridional overturning circulation in the subantarctic region (DeVries et al., 2017; Gruber et al., 2019). This means that using different predictors in different latitude regions can better reflect the regional influencing factors of  $p\text{CO}_2$  and its variability. To find the best combination of  $p\text{CO}_2$  predictors in different regions, we have proposed a Stepwise FFNN algorithm in

previous work, where the changes in predicting error are fed back to the selection of input  $p\text{CO}_2$  predictors (Zhong et al., 2022). This algorithm allows for the objective selection of  $p\text{CO}_2$  predictors in different regions that result in the lowest  $p\text{CO}_2$  predicting error. The procedure of the Stepwise FFNN algorithm is determining  $p\text{CO}_2$  predictors one by one until no further reduction in predicting error is achieved by either adding or removing any predictors. Specifically, the first  $p\text{CO}_2$  predictor is selected by comparing predicting errors when individually using each collected environmental variable (listed in Table S1) as input of the FFNN. The variable with the lowest error is determined as the first  $p\text{CO}_2$  predictor, which is also the predictor that has the greatest impact on the distribution or variability of regional surface ocean  $p\text{CO}_2$ . Subsequently, leaving the first predictor unchanged, the predicting errors are compared when using each environmental variable as the second input of the FFNN. The environmental variable with the lowest error is determined as the second  $p\text{CO}_2$  predictor. In the same way, new predictors are continuously determined one after another, until the predicting error no longer continues to decrease regardless of which one variable is added as a  $p\text{CO}_2$  predictor. Meanwhile, whenever a new predictor is determined, the algorithm also tests if the predicting error will decrease when sequentially removing each determined predictor, in order to eliminate co-correlation and prevent overfitting. For example, when the fourth predictor is determined, the model tests the change in predicting error by individually removing each one from the previously determined three predictors. If the error decreases after removing a previously determined predictor, this predictor is highly correlated with other determined predictors. By adding and removing variables in the input of the FFNN one by one in this way, the algorithm ultimately identifies a set of  $p\text{CO}_2$  predictors that minimize the  $p\text{CO}_2$  predicting error. In this work, the single FFNN structure used in the previous Stepwise FFNN algorithm has been replaced with a structure of ensemble learning FFNNs with stronger fitting capabilities (see Figure 1), referred to as the Stepwise BEL algorithm.

However, the Stepwise BEL algorithm relies on predicting errors for determination of  $p\text{CO}_2$  predictors, and the number of SOCAT  $p\text{CO}_2$  measurements in the Southern Ocean during the winter season is much lower than in the summer, leading to a lower weighting on winter predicting errors compared to summer in the determination. As a result, the selected predictors are more reflective of factors influencing  $p\text{CO}_2$  distribution in the summer (such as biological drawdown) while neglecting those in the winter (such as enhanced vertical mixing). Therefore, we increased the weighting of winter data to be nearly equal to that of summer, to carry out a winter correction of

$p\text{CO}_2$  predictors in the Southern Ocean:

$$RMSE = \sqrt{\frac{3*\sum(\Delta p\text{CO}_2_{\text{May-S}})^2 + \sum(\Delta p\text{CO}_2_{\text{Oct-Apr}})^2}{3*N_{\text{May-S}} + N_{\text{Oct-Apr}}}} \quad (2)$$

where the  $\Delta p\text{CO}_2$  was the difference between predicted  $p\text{CO}_2$  and SOCAT  $p\text{CO}_2$  measurements, and  $N$  was the number of monthly SOCAT measurements ( $3*N_{\text{May-Sep}} \approx N_{\text{Oct-Apr}}$ ). Based on a self-organization map method, the Southern Ocean was divided into different regions according to the similarity of  $p\text{CO}_2$  drivers, including two belt regions and three sectors connecting to major basins (Zhong et al., 2022). Therefore, the selection of  $p\text{CO}_2$  predictors and reconstruction of  $p\text{CO}_2$  in this work was based on three latitude areas: 35-50°S, 50-60°S, and South of 60°S (Table 1). Since there were no observed effects of uneven seasonal distribution on the neural network training in the 35-50°S region connecting the major basins, the correction of  $p\text{CO}_2$  predictors is only conducted in the area south of 50°S.

**Table 1 Winter correction of  $p\text{CO}_2$  predictors.**

Area	$p\text{CO}_2$ predictors
35-50°S	Pacific sector SST, sin(Longitude), $x\text{CO}_2$ , Latitude, SSS, Photosynthetically Available Radiation, Chlorophyll, Mixed layer depth, cos(Longitude), Mixed layer depth <sub>anom</sub> , Remote sensing reflectance at 531nm and 555nm
Indian sector	SST, Total absorption at 645nm, Number of months since January 1992, Mixed layer depth, SSS, W velocity of ocean currents at 105m, Surface pressure, Total absorption at 678nm, W velocity of ocean currents at 195m, Total backscattering at 667nm, Nitrate, Total absorption at 555nm, Mixed layer depth <sub>anom</sub> , Particulate organic carbon, DIC, W velocity of ocean currents at 65m, Remote sensing reflectance at 488nm, Total backscattering at 443nm
Atlantic sector	Latitude, SSS, Dry air mixing ratio of atmospheric $\text{CO}_2$ , Particulate organic carbon, Total backscattering at 488nm, Mixed layer depth, Diffuse attenuation coefficient, Total backscattering at 412nm, Sea surface height, cos(Longitude), SST, Remote sensing reflectance at 460nm, Total backscattering at 547nm, Bathymetry, Total absorption at 678nm, Total backscattering at 469nm, Remote sensing reflectance at 678nm
50-60°S uncorrected	SSS <sub>anom</sub> , SST, Mixed layer depth, Dry air mixing ratio of atmospheric



	CO <sub>2</sub> <sub>anom</sub> , Bathymetry, Sea surface height <sub>anom</sub> , W velocity of ocean currents at 105m, DIC, Dissolved oxygen, Nitrate
50-60°S corrected	Dry air mixing ratio of atmospheric CO <sub>2</sub> , Mixed layer depth, SST, DIC, month, SSS, Bathymetry, Latitude, W velocity of ocean currents at 105m, Dissolved oxygen, W velocity of ocean currents at 5m, Dry air mixing ratio of atmospheric CO <sub>2</sub> <sub>anom</sub> , Mixed layer depth <sub>anom</sub>
S of 60°S uncorrected	DIC, Bathymetry, SSS, Alkalinity, cos(Longitude), SST, Sea surface height <sub>anom</sub> , W velocity of ocean currents at 195m, 5m, and 65m, SSS <sub>anom</sub>
S of 60°S corrected	Bathymetry, SSS, Alkalinity, SST, month, W velocity of ocean currents at 65m, 105m, and 195m, Dissolved oxygen, cos(Longitude), Sea surface height, Latitude, SSS <sub>anom</sub>

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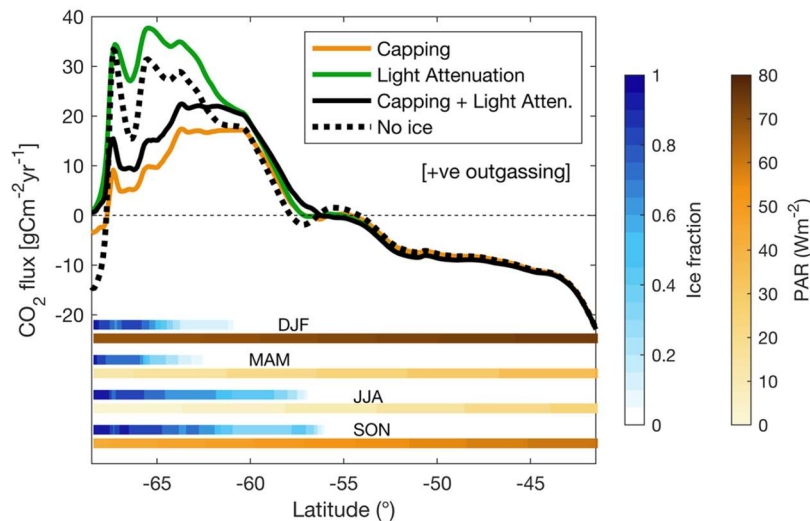
(Uncorrected predictors were selected by a Stepwise BEL algorithm updated from Zhong et al., 2022, corrected predictors were selected using the same algorithm but increasing the weighting of winter SOCAT measurements; The sort order of  $p\text{CO}_2$  predictors indicated a relative contribution on decreasing predicting errors. The predictors denoted by subscript "anom" represent the monthly anomaly obtained by subtracting the monthly climatology. Data sources of used products are listed in Supplementary Table 1.)

**4) In the conclusion section, my concern is about the statement on lines 502-506: Is there an estimate for this in the future? In figure 9 we see the decrease in the S. Ocean carbon sink in the scenarios where 50% or 100% of the sea ice melts - but within the period ~1992-2022 considered in this study. What are the modelled predictions (please cite the models, like in figure 7, for instance), despite the discrepancy in the ocean carbon sink?**

**Response:** We did not estimate the specific carbon sink intensity in the future. Predicting the future variability is not what machine learning  $p\text{CO}_2$  mapping is skilled in. But based on current estimate that the atmospheric  $p\text{CO}_2$  increases at an average rate of  $1.90 \mu\text{atm yr}^{-1}$  in the Southern Ocean areas with sea ice, compared to the  $1.53 \mu\text{atm yr}^{-1}$  of surface ocean  $p\text{CO}_2$ , we can suppose that the high latitude Antarctic seawaters would be still a carbon source but inhibited by sea ice in the future.

The modeled predictions similarly suggested a winter CO<sub>2</sub> release inhibited by sea ice in the Southern Ocean. The recent research based on a 2-D channel model and an

analytical model indicated that sea ice coverage affects the air-sea CO<sub>2</sub> flux by physical barrier and limiting biological photosynthesis, and CO<sub>2</sub> emissions to the atmosphere will increase significantly in the area around 65°S if the sea ice completely melts (Gupta et al., 2020). Also, research based on mooring observations in the West Antarctic Peninsula continental shelf suggested that a reduction in sea ice may be expected to weaken the Southern Ocean oceanic CO<sub>2</sub> sink, by allowing additional outgassing in autumn and winter (Shadwick et al., 2021).



The figure cited from Gupta et al., 2020. They compared CO<sub>2</sub> flux that the seasonal ice cover affects physical CO<sub>2</sub> exchange only (Capping in orange), biological photosynthesis only (light attenuation in green), both together (solid black), and no ice cover (dotted black). If there is no ice cover, the no-ice carbon source (dotted black) around 65°S would be stronger than the result with the current ice cover fraction (solid black), which is consistent with our results.

Gupta, M., Follows, M. J., & Lauderdale, J. M. (2020). The effect of Antarctic sea ice on Southern Ocean carbon outgassing: Capping versus light attenuation. *Global Biogeochemical Cycles*, 34(8), e2019GB006489.

Shadwick, E. H., De Meo, O. A., Schroeter, S., Arroyo, M. C., Martinson, D. G., & Ducklow, H. (2021). Sea ice suppression of CO<sub>2</sub> outgassing in the West Antarctic Peninsula: Implications for the evolving Southern Ocean carbon sink. *Geophysical Research Letters*, 48, e2020GL091835.

**5) How does the calculated uncertainty in sea-air CO<sub>2</sub> fluxes (section "uncertainty") affect the estimates of the decreasing C sink from this manuscript?**

Response: The uncertainty did not affect the result that the seawater under sea ice coverage acts as a carbon source and the additional CO<sub>2</sub> release caused by sea ice melting will decrease the Southern Ocean carbon sink intensity. The uncertainty represents the potential difference between estimated carbon sinks and the true values caused by the bias in  $p\text{CO}_2$  mapping and gas transfer velocity. This difference only affects the intensity of carbon sources covered by sea ice and is not big enough to turn carbon sources into carbon sinks. Therefore, the uncertainty may make the estimated additional CO<sub>2</sub> release (or decrease in the total Southern Ocean carbon sink) caused by sea ice melting differ from the real situation to some extent.

## **Annotation:**

### **1) Line 45: gas transfer?**

Response: The word has been corrected into “gas transfer velocity”.

### **2) Line 56: Is this relative to the last 3 decades, as in the paragraph above?**

Response: The 40% was estimated for the historical period since the Industrial Revolution. Specifically, the contribution of the Southern Ocean on global ocean anthropogenic CO<sub>2</sub> uptakes was estimated to be 43% from 1870 to 1995 by Frölicher et al., 2015. The original text has been modified as:

The Southern Ocean south of 35°S was a strong carbon sink and has contributed to about 40% of global ocean anthropogenic CO<sub>2</sub> uptakes from 1870 to 1995 (Sabine et al., 2004; Fletcher, S. E. M. et al., 2006; Frölicher et al., 2015; Landschützer et al., 2015).

### **3) Line 70: overestimation in comparison to the in situ observations? Or to model outputs?**

Response: The overestimation refers to the stronger carbon sink of machine learning methods compared to the in-situ observations. The original text has been modified as:

The strongly seasonally uneven surface ocean *p*CO<sub>2</sub> measurements with missing winter observations may result in an overestimation of the Southern Ocean carbon sink from *p*CO<sub>2</sub> products compared to the in-situ observations (Bushinsky et al., 2019; Hauck et al., 2020; Gloege et al., 2021; Friedlingstein et al., 2022). Besides supplying more measurements from sailboats or floats (Landschützer et al., 2023), whether the overestimation in *p*CO<sub>2</sub>-based machine learning methods compared to the in-situ observations can be solved by improving algorithms is worth investigating.

### **4) Line 78: which ones?**

Response: A new section about the selection of *p*CO<sub>2</sub> predictors has been added in the method section, and the used *p*CO<sub>2</sub> predictors are listed in Table 1 now.

### **5) Line 90: which drivers were more relevant in winter and summer?**

Response: In the areas between 50-60°S, the *p*CO<sub>2</sub> distribution was more relevant to the enhanced vertical mixing in summer and to the biological drawdown in winter. The original text has been modified as follows:

However, the Stepwise BEL algorithm relies on predicting errors for determination of  $p\text{CO}_2$  predictors, and the number of SOCAT  $p\text{CO}_2$  measurements in the Southern Ocean during the winter season is much lower than in the summer, leading to a lower weighting on winter predicting errors compared to summer in the determination. As a result, the selected predictors are more reflective of factors influencing  $p\text{CO}_2$  distribution in the summer (such as biological drawdown) while neglecting those in the winter (such as enhanced vertical mixing).

**6) Line 129: please check the format o "k" along the text - you stated using it in italic font**

**Response:** Thanks for the suggestion. The velocity  $k$  has been all corrected to the italic font.

**7) Line 154: how this affects the numbers for the correction of the size of the Southern Ocean carbon sink at section 3 in this manuscript?**

**Response:** The uncertainty did not affect the difference between uncorrected and corrected carbon sinks. As it was calculated from the  $p\text{CO}_2$  RMSE of corrected neural networks, the uncertainty only affects the size of the corrected Southern Ocean carbon sink. The numbers for the correction of the size of the Southern Ocean carbon sink were mainly related to the decrease in mean  $p\text{CO}_2$  bias from  $-3.13\sim-5.77\ \mu\text{atm}$  to  $-0.25\sim-0.74\ \mu\text{atm}$  after the winter correction. The RMSE decrease after correction also makes the carbon sink uncertainty smaller than the uncorrected result, but the corrected uncertainty and the correction size of carbon sinks are not directly related.

**8) Strikeout in Line 166**

**Response:** The sentence has been modified as follows:

**Original:** The SOCAT measurements in the Southern Ocean are concentrated in summer with low surface ocean  $p\text{CO}_2$  (Figure 2a). While in winter, the number of measurements with high surface ocean  $p\text{CO}_2$  was only about one-fifth of that in summer.

**Modified:** The SOCAT measurements in the Southern Ocean are concentrated in summer with low surface ocean  $p\text{CO}_2$  (Figure 2a), with the number of high- $p\text{CO}_2$  winter measurements only about one-fifth of that in summer.

**9) Strikeout in Line 166**

**Response:** The unnecessary title "the" has been removed.

**10) Table 1: what is the meaning of the bold numbers?**

Response: The bold numbers are the lowest RMSE, which is also the adopted training period in the final  $p\text{CO}_2$  product construction. The description has been added in the table annotation.

**11) Line 221: add “between”**

Response: the sentence has been modified as follows:

In contrast, there is no significant underestimation of winter surface ocean  $p\text{CO}_2$  in the Southern Ocean between 35-50°S.

**12) Line 240: would be good to have a list of the predictors, in a table or in the main text, not only in the supplementary file. In the discussion, you should also name the predictors.**

Response: A new section about predictors has been added in the method section, and the predictor list has been moved to Table 1 of this section now. The predictors have been listed in the full name, and the data source of used products has been listed in the supplementary Table S1.

**13) Line 267: Where is the SOFS station located (latitude area - between 35-50S, or between 50-60S, or further south of 60S?) I have found it, but the reader may not be familiar to it.**

Response: The location of the SOFS station (142.0°E, 46.8°S) has been added in the method section where the SOFS station is first referred.

**14) Line 376: driven?**

Response: The text has been corrected as follows:

Research based on an idealized upper ocean box model also suggested that the slowed growth rate of atmospheric  $p\text{CO}_2$  and the global sea surface temperature response to the 1991 eruption of Mt Pinatubo volcanic were two external forces to explain the global-scale reduction in the ocean carbon sink, and the reinvigoration of carbon sink was driven by the acceleration of atmospheric  $p\text{CO}_2$  growth after 2001 (McKinley et al., 2020).

**15) Line 398: how many models? where is the data available? directly from**

**Friedlingstein et al. 2022?**

Response: The GOBMs are an average of 10 global ocean biogeochemical models. The data is available at <https://doi.org/10.18160/GCP-2022>, this link can be found in Friedlingstein et al. 2022. The description in Figure 7 annotation has been modified as follows:

Figure 7. Global ocean carbon sink over the past three decades after the Southern Ocean correction. GOBMs: average results of 10 global ocean biogeochemical models (<https://doi.org/10.18160/GCP-2022>, Friedlingstein et al., 2022);

**16) Line 442: One should avoid writing that "figure X shows" - it is better if you describe and discuss your result, then direct the reader to the figure.**

Response: Thanks for the suggestion. The sentence has been modified as follows:

If sea ice melted completely, the changes in simulated carbon sink intensity without considering indirect factors based on the recent sea-air  $p\text{CO}_2$  difference were different between summer and winter periods in the Southern Ocean (Figure 9).

**17) Line 503: Is there an estimate for this in the future? In figure 9 we see the decrease in the sink in the scenarios where 50% or 100% of the sea ice melts - but within the period ~1992-2022.**

Response: We did not perform a quantitative future estimate, but only speculated the theoretical future change based on current data. Predicting future changes is not what the used machine learning is good at. In addition, the released  $\text{CO}_2$  from areas with melting sea ice may further affect the sea ice melting speed, and predicting the sea ice melting speed is not in our expertise area. The quantitative prediction may be carried out in future works through model simulations.

Decision letter and referee reports: second round

15th May 24

Dear Professor Li,

Your manuscript titled "Melting sea ice will weaken carbon sinks in the Southern Ocean" has now been seen by 2 reviewers, and we include their comments at the end of this message. They find your work of interest, but some important points are still raised. We are interested in the possibility of publishing your study in *Communications Earth & Environment*, but would like to consider your responses to these concerns and assess a revised manuscript before we make a final decision on publication.

We therefore invite you to revise and resubmit your manuscript, addressing the remaining concerns of both reviewers, along with a point-by-point response that takes into account the points raised. Please highlight all changes in the manuscript text file.

We are committed to providing a fair and constructive peer-review process. Please don't hesitate to contact us if you wish to discuss the revision in more detail.

Please use the following link to submit your revised manuscript, point-by-point response to the referees' comments (which should be in a separate document to any cover letter), a tracked-changes version of the manuscript (as a PDF file) and the completed checklist:

[redacted]

\*\* This url links to your confidential home page and associated information about manuscripts you may have submitted or be reviewing for us. If you wish to forward this email to co-authors, please delete the link to your homepage first \*\*

We hope to receive your revised paper within six weeks; please let us know if you aren't able to submit it within this time so that we can discuss how best to proceed. If we don't hear from you, and the revision process takes significantly longer, we may close your file. In this event, we will still be happy to reconsider your paper at a later date, as long as nothing similar has been accepted for publication at *Communications Earth & Environment* or published elsewhere in the meantime.

Please do not hesitate to contact us if you have any questions or would like to discuss these revisions further. We look forward to seeing the revised manuscript and thank you for the opportunity to review your work.

Best regards,

Jose Luis Iriarte Machuca, PhD  
Editorial Board Member  
*Communications Earth & Environment*

Alireza Bahadori, PhD  
Associate Editor  
*Communications Earth & Environment*

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Please refer to our data policies at <http://www.nature.com/authors/policies/availability.html>.

REVIEWER COMMENTS:

Reviewer #3 (Remarks to the Author):

Dear Drs. Li and Song,

Thank you for addressing the comments in your comprehensive rebuttal letter, to both reviewers. The revised manuscript is much clearer now, especially now listing the chosen pCO<sub>2</sub> predictors.

The abstract could be a little clearer, as the following:

"This overestimation can be mitigated by a winter correction in algorithms, with the average Southern Ocean carbon sink during 1992-2021 corrected to -0.87 PgC yr<sup>-1</sup> from the original -1.01 PgC yr<sup>-1</sup>. Furthermore, the most notable underestimation of surface ocean pCO<sub>2</sub> mainly occurred in regions south of 60°S and was hiding under ice cover. If sea ice melts completely, there could be a further reduction of about 0.14 PgC yr<sup>-1</sup> in the Southern Ocean carbon sink due to exposure of high pCO<sub>2</sub> seawater to the atmosphere in winter."

I understand that the authors have improved/corrected the prediction of the S. Ocean C sink for 1992-2021 to -0.87 PgC/yr but the assumption of total melting of sea ice isn't something of a future scenario? Maybe you should add a sentence from the text (page 20) in the abstract (suggestion):

"This overestimation can be mitigated by a winter correction in algorithms, with the average Southern Ocean carbon sink during 1992-2021 corrected to -0.87 PgC yr<sup>-1</sup> from the original -1.01 PgC yr<sup>-1</sup>. Furthermore, the most notable underestimation of surface ocean pCO<sub>2</sub> mainly occurred in regions south of 60°S and was hiding under ice cover. As the surface ocean pCO<sub>2</sub> under sea ice coverage in the winter is much higher than the atmosphere, if sea ice melts completely, there could be a further reduction of about 0.14 PgC yr<sup>-1</sup> in the Southern Ocean carbon sink."

In page 21 there is still a sentence beginning with "Figure 9 shows the simulated carbon sink intensity in the Southern Ocean under different sea ice coverage without considering indirect factors based on the recent sea-air pCO<sub>2</sub> difference..." - I suggest rewriting and starting with the main information first and then cite the figure (fig. 9).

I have noticed that there were a change in the authors' list, is there a reason why Dr. Fan Wang no longer is a co-author?

Reviewer #4 (Remarks to the Author):

Thanks for your answer, the article has shown good improvements.

This article offers a promising approach for dealing with PCO<sub>2</sub> bias measurements, it is definitely worth publishing. However, I notice some issues that needs to be resolved:

-The label format is not consistent across the article (fig. 9 as label in bold format while fig.8 has not for example). I would recommend the authors put a title to all figures (one for each subfigure) and use the same format for all of them.

-Fig.5 has a) and b) label figure in bold and c) and d) labels not in bold. Be consistent.

-The references need to be in a different color compared to the rest of the text.

-Also to make the result more robust I would encourage to try the same methodology with another data set so to compare with SOCCAT results. The authors can add this second dataset results in supplemental material.

Once this is done I will endorse the publication of it.

**Reviewer #3:**

Thank you for addressing the comments in your comprehensive rebuttal letter, to both reviewers. The revised manuscript is much clearer now, especially now listing the chosen  $p\text{CO}_2$  predictors.

1) The abstract could be a little clearer, as the following:

"This overestimation can be mitigated by a winter correction in algorithms, with the average Southern Ocean carbon sink during 1992-2021 corrected to  $-0.87 \text{ PgC yr}^{-1}$  from the original  $-1.01 \text{ PgC yr}^{-1}$ . Furthermore, the most notable underestimation of surface ocean  $p\text{CO}_2$  mainly occurred in regions south of  $60^\circ\text{S}$  and was hiding under ice cover. If sea ice melts completely, there could be a further reduction of about  $0.14 \text{ PgC yr}^{-1}$  in the Southern Ocean carbon sink due to exposure of high  $p\text{CO}_2$  seawater to the atmosphere in winter."

I understand that the authors have improved/corrected the prediction of the S. Ocean C sink for 1992-2021 to  $-0.87 \text{ PgC/yr}$  but the assumption of total melting of sea ice isn't something of a future scenario? Maybe you should add a sentence from the text (page 20) in the abstract (suggestion):

"This overestimation can be mitigated by a winter correction in algorithms, with the average Southern Ocean carbon sink during 1992-2021 corrected to  $-0.87 \text{ PgC yr}^{-1}$  from the original  $-1.01 \text{ PgC yr}^{-1}$ . Furthermore, the most notable underestimation of surface ocean  $p\text{CO}_2$  mainly occurred in regions south of  $60^\circ\text{S}$  and was hiding under ice cover. As the surface ocean  $p\text{CO}_2$  under sea ice coverage in the winter is much higher than the atmosphere, if sea ice melts completely, there could be a further reduction of about  $0.14 \text{ PgC yr}^{-1}$  in the Southern Ocean carbon sink."

**Response: Thanks for the suggestion. The abstract has been modified as the suggestion.**

2) In page 21 there is still a sentence beginning with "Figure 9 shows the simulated carbon sink intensity in the Southern Ocean under different sea ice coverage without considering indirect factors based on the recent sea-air  $p\text{CO}_2$  difference..." - I suggest rewriting and starting with the main information first and then cite the figure (fig. 9).

**Response: Thanks for the suggestion. The beginning of the paragraph has been modified as the following:**

**"Assuming complete sea ice melt and neglecting indirect factors based on the recent sea-air  $p\text{CO}_2$  difference, the changes in simulated carbon sink intensity vary between summer and winter periods in the Southern Ocean (Figure 9)."**

3) I have noticed that there were a change in the authors' list, is there a reason why Dr. Fan Wang no longer is a co-author?

Response: Thanks for the notification. Wang Fan made an important contribution to this article, but we mistakenly deleted in the re-submission when we wanted to put Wang Fan in a more forward position. The mistake has been corrected and the co-author Fan Wang has been put in fourth place now.

#### Reviewer #4:

Thanks for your answer, the article has shown good improvements.

This article offers a promising approach for dealing with  $PCO_2$  bias measurements, it is definitely worth publishing. However, I notice some issues that needs to be resolved:

1) The label format is not consistent across the article (fig. 9 as label in bold format while fig.8 has not for example). I would recommend the authors put a title to all figures (one for each subfigure) and use the same format for all of them.

Response: Thanks for the suggestion. We have corrected all labels to in bold format as the following:

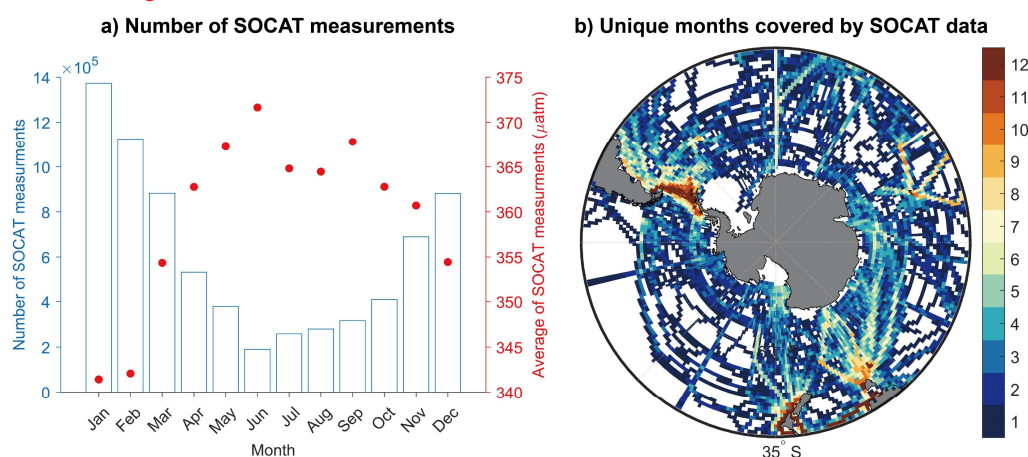


Figure 2. The number of a) SOCAT  $fCO_2$  measurements in each month and b) unique months covered by SOCAT measurements in the Southern Ocean south of 35°S from 1992 to 2021.

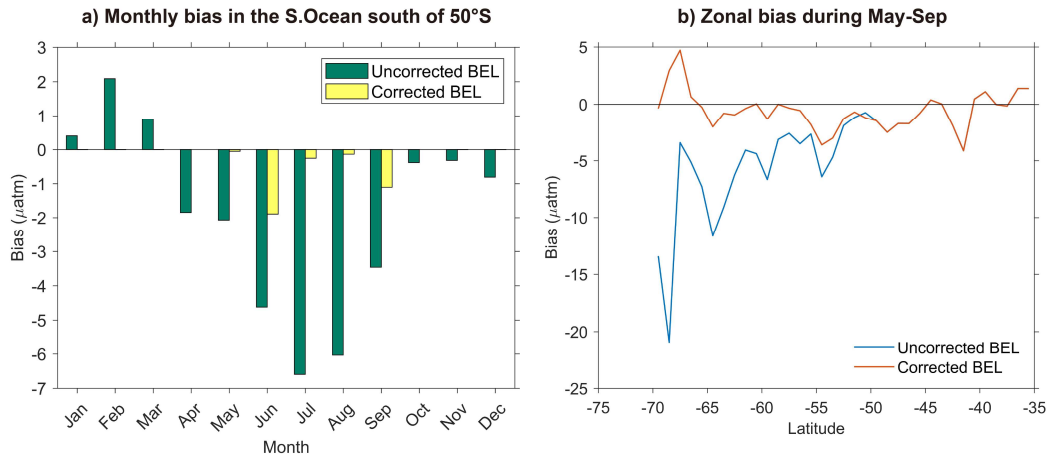


Figure 3. Distribution of bias between predicted  $p\text{CO}_2$  and SOCAT measurements in the Southern Ocean south of 35°S.

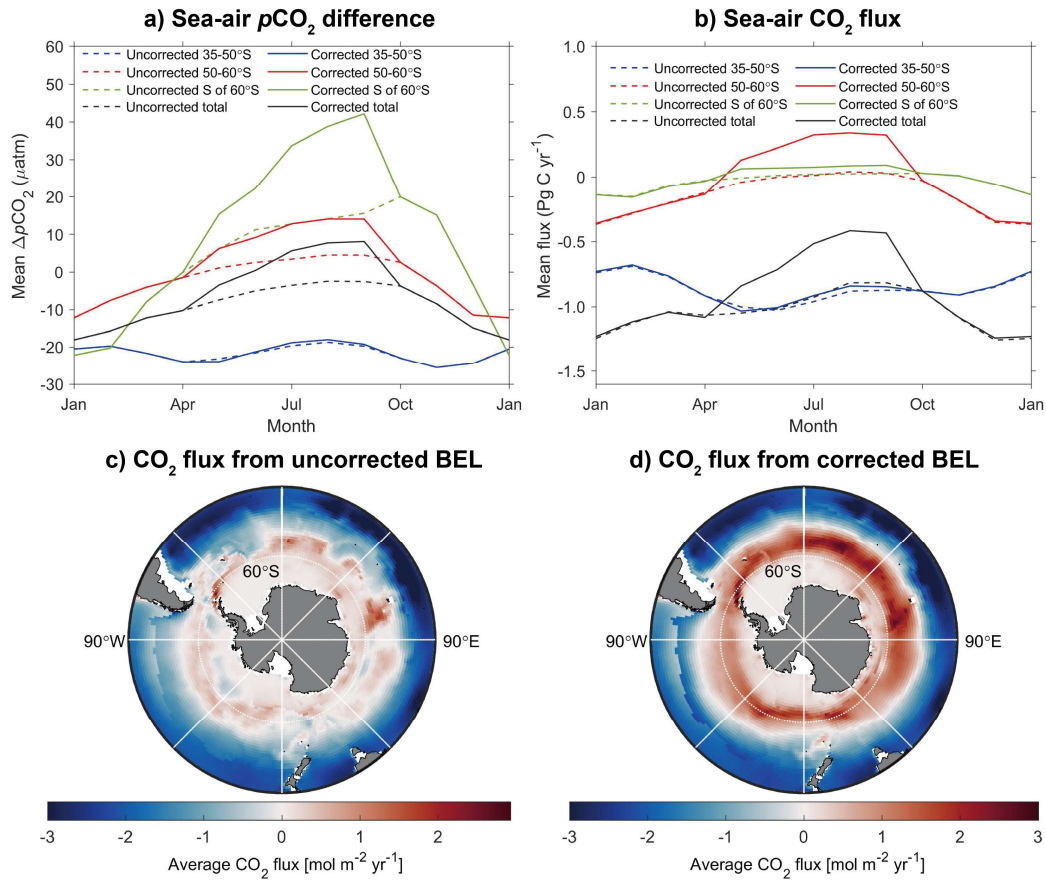


Figure 5. Distribution of average sea-air  $p\text{CO}_2$  difference and  $\text{CO}_2$  flux from May to September during 1992-2021.

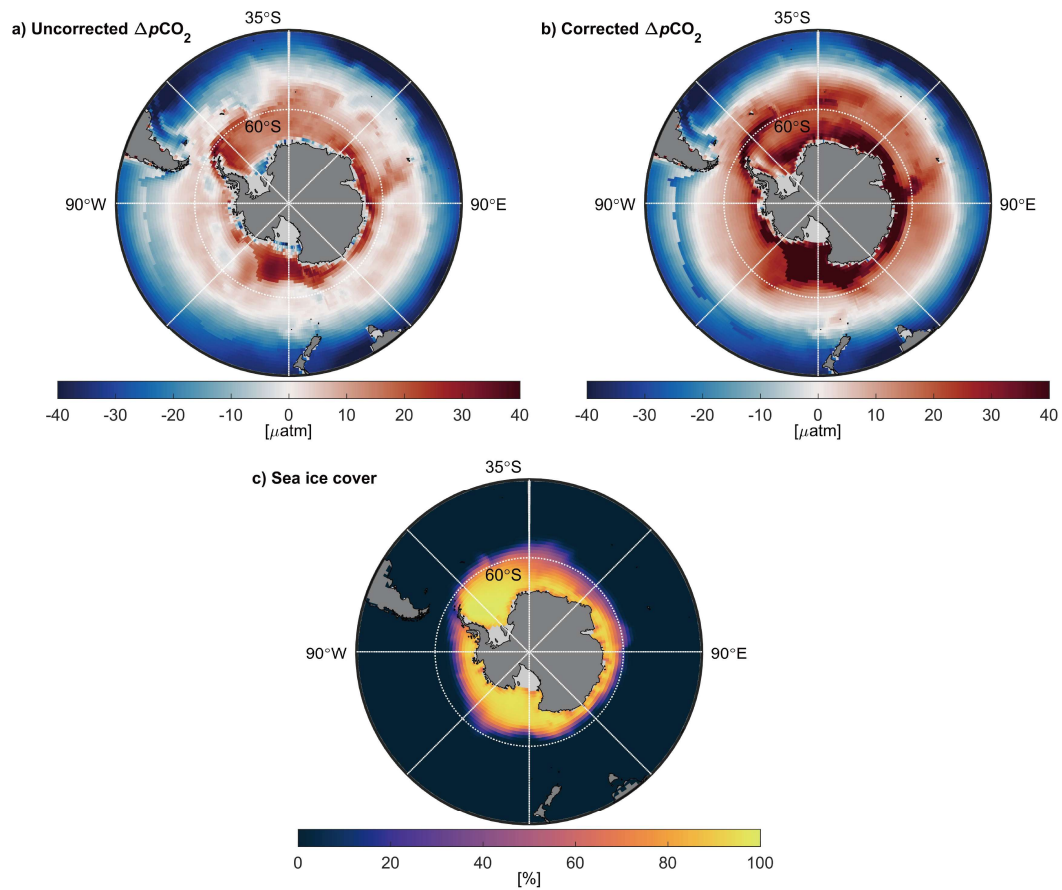


Figure 8. Distribution of average sea-air  $\Delta p\text{CO}_2$  and sea ice cover during May-Sep in the Southern Ocean.

2) Fig.5 has a) and b) label figure in bold and c) and d) labels not in bold. Be consistent.

Response: The label of Figure 5 has been corrected in bold.

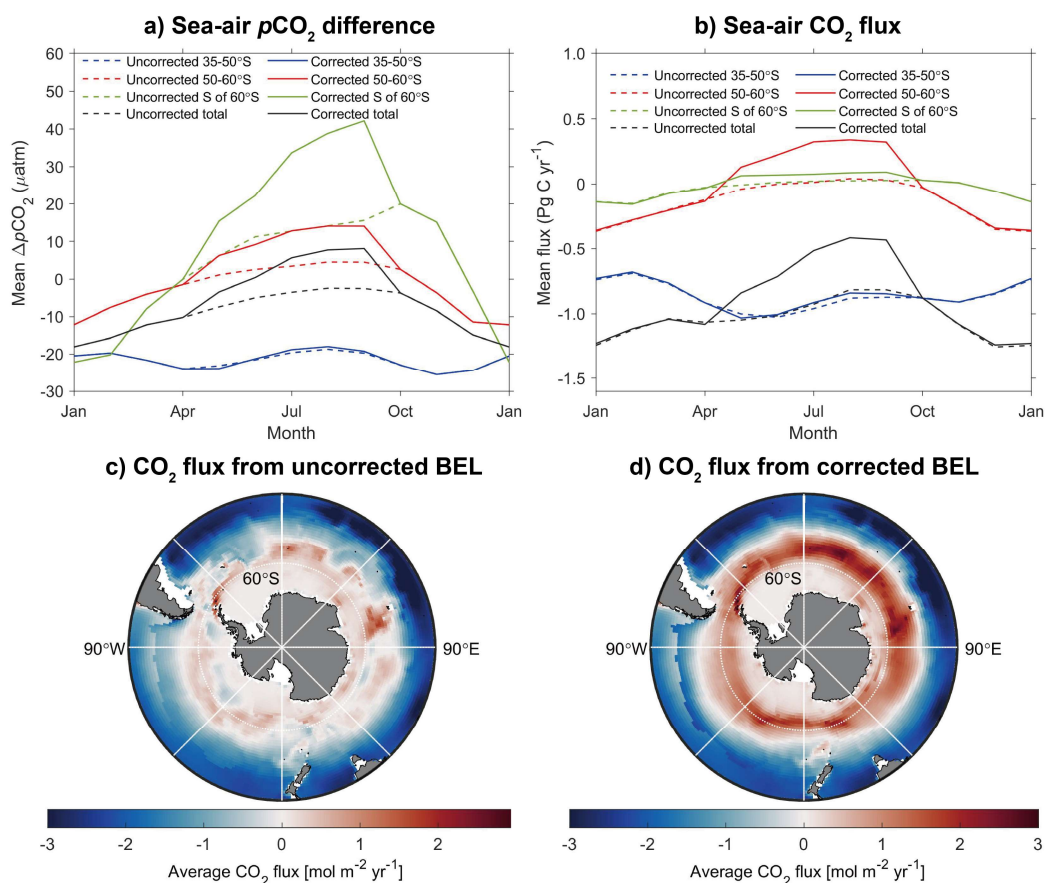


Figure 5. Distribution of average sea-air  $p\text{CO}_2$  difference and  $\text{CO}_2$  flux from May to September during 1992-2021.

3) The references need to be in a different color compared to the rest of the text.

Response: Thanks for the suggestion. The references have been changed to blue color.

4) Also to make the result more robust I would encourage to try the same methodology with another data set so to compare with SOCAT results. The authors can add this second dataset results in supplemental material.

Response: Thanks for the suggestion. The Southern Ocean Carbon and Climate Observations and Modeling (SOCCOM) float  $p\text{CO}_2$  data have been added for further evaluation (Figure S1). The description of the SOCCOM dataset and the results has been placed in supplemental material.

The SOCCOM dataset contains observations from biogeochemical profiling floats, processed with delayed-mode quality control method at the Monterey Bay Aquarium Research Institute (MBARI). The SOCCOM  $p\text{CO}_2$  data were derived from estimated total alkalinity and pH sampled every two meters in the upper 1000 meters using LIAR or CANYON algorithms (Johnson et al., 2017).



By averaging the SOCCOM data at depths of 2.77-5.00 m in each month and 1° grid into 230 samples, we estimated the bias between the float  $p\text{CO}_2$  data and our BEL FFNNs  $p\text{CO}_2$  product during June-September from 2014 to 2019. Although a great discrepancy exists between the BEL FFNNs mapped  $p\text{CO}_2$  and SOCCOM float  $p\text{CO}_2$ , the winter correction in the BEL algorithm still mitigated the underestimation of  $p\text{CO}_2$  by FFNNs. The uncorrected BEL FFNNs  $p\text{CO}_2$  is about 30  $\mu\text{atm}$  lower than float data along the 60°S areas during the winter period, while the corrected  $p\text{CO}_2$  show biases less than -20  $\mu\text{atm}$  in the Indian sector and Pacific sector (Figures S1a and S1b). In the Atlantic sector and the Drake Passage, after the winter correction, the BEL FFNNs  $p\text{CO}_2$  underestimated 10-20  $\mu\text{atm}$  compared to float data changed to be less biased. These changes in biases suggested that the regional average  $p\text{CO}_2$  of BEL FFNNs product will be closer to the float data. The average bias reduced from -16.8  $\mu\text{atm}$  to -6.5  $\mu\text{atm}$  and was better distributed along the  $y=x$  line after the winter correction (Figure S1c). However, a great discrepancy exists between BEL FFNNs  $p\text{CO}_2$  and the SOCCOM float data when float  $p\text{CO}_2$  is lower than 350  $\mu\text{atm}$  or higher than 450  $\mu\text{atm}$ . Notably, this discrepancy was not a shame in bad machine learning performance, but a difference exists between the SOCAT dataset and the SOCCOM dataset. Previous research also suggested a much weaker Southern Ocean carbon sink derived from the SOCCOM dataset than that from the SOCAT dataset (Bushinsky et al., 2019). Therefore, the evaluation based on SOCCOM float data can also prove the benefits of the winter correction in the estimate of the Southern Ocean carbon sink.

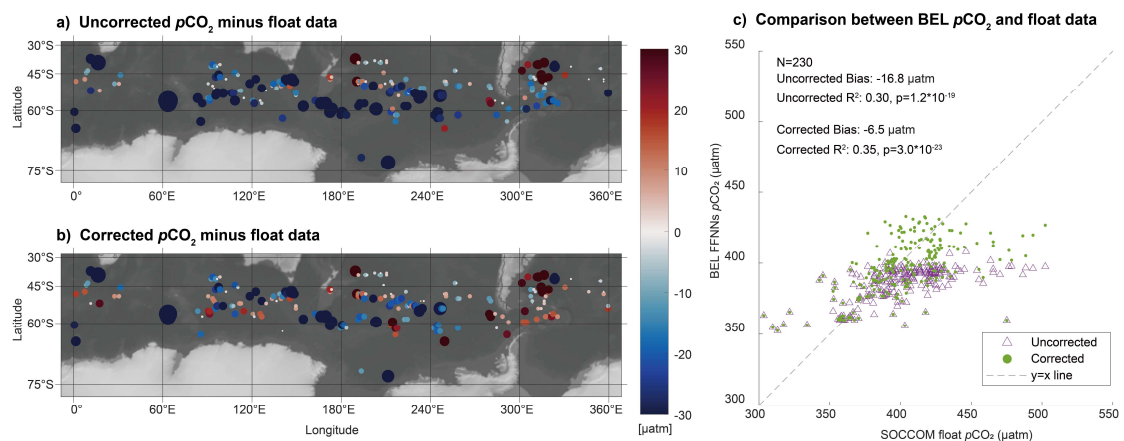


Figure S1. Comparison between BEL FFNNs  $p\text{CO}_2$  trained on SOCAT data and the independent SOCCOM float  $p\text{CO}_2$  observation during June-September since 2014. a): bias between uncorrected BEL FFNNs  $p\text{CO}_2$  and SOCCOM float data; b): bias between corrected BEL FFNNs  $p\text{CO}_2$  and SOCCOM float data; larger bubbles represent that the BEL FFNNs  $p\text{CO}_2$  is more biased, and blue bubbles represent lower BEL  $p\text{CO}_2$  than the float data; c) statical comparison between BEL FFNNs  $p\text{CO}_2$  and SOCCOM float



$p\text{CO}_2$ . Uncorrected BEL  $p\text{CO}_2$ : trained on SOCAT dataset using boosting ensemble learning FFNNs; Corrected BEL  $p\text{CO}_2$ : result after applying a winter correction by training BEL FFNNs on only winter SOCAT samples. SOCCOM float  $p\text{CO}_2$ : monthly and  $1^\circ$  averaged results from SOCCOM data at depths of 2.77-5.00 m from 2014 to 2019 (Johnson et al., 2017).

Bushinsky, S. M., Landschützer, P., Rödenbeck, C., Gray, A. R., Baker, D., Mazloff, M. R., ... & Sarmiento, J. L. (2019). Reassessing Southern Ocean air-sea  $\text{CO}_2$  flux estimates with the addition of biogeochemical float observations. *Global Biogeochemical Cycles*, 33(11), 1370-1388.

Johnson, Kenneth S.; Riser, Stephen C.; Boss, Emmanuel S.; Talley, Lynne D.; Sarmiento, Jorge L.; Swift, Dana D.; Plant, Josh N.; Maurer, Tanya L.; Key, Robert M.; Williams, Nancy L.; Wanninkhof, Richard H.; Dickson, Andrew G.; Feely, Richard A.; Russell, Joellen L. (2017). Southern Ocean Carbon and Climate Observations and Modeling (SOCCOM) Float Data Archive. UC San Diego Library Digital Collections. <https://doi.org/10.6075/J0TX3C9X>.

Decision letter and referee reports: third round

15th May 24

Dear Professor Li,

Your manuscript titled "Melting sea ice will weaken carbon sinks in the Southern Ocean" has now been seen by our reviewers, whose comments appear below. In light of their advice we are delighted to say that we are happy, in principle, to publish a suitably revised version in Communications Earth & Environment under the open access CC BY license (Creative Commons Attribution v4.0 International License).

We therefore invite you to revise your paper one last time to address the remaining concerns of our reviewers. At the same time we ask that you edit your manuscript to comply with our format requirements and to maximise the accessibility and therefore the impact of your work.

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We hope to hear from you within two weeks; please let us know if you need more time.

Best regards,

Dr Alireza Bahadori  
Associate Editor  
Communications Earth & Environment

REVIEWERS' COMMENTS:

Reviewer #4 (Remarks to the Author):

Dear Authors,

The revised manuscript looks much better for me, I endorse the publication of it with some additional changes to be added:

- all the equations have to be rewritten using latex form.
- the line number needs to be added in the articles
- Also the references need to be numbered as well.

Author responses: third round

Reviewer #4:

Dear Authors,

The revised manuscript looks much better for me, I endorse the publication of it with some additional changes to be added:

-all the equations have to be rewritten using latex form.

**Response: All equations in the manuscript have been rewritten using latex form.**

-the line number needs to be added in the articles

**Response: Thanks for the suggestion, we have added the line number.**

-Also the references need to be numbered as well.

**Response: The reference have been numbered in the order of appearance.**