This file includes the responses to review1 and review 2.

Responses to review1:

Summary:

Xu and colleagues investigate the regional sea surface pCO_2 and air-sea flux in the Prydz Bay Antarctica using observations from the CHINARE cruise in February 2015. The authors divide the study regions into 3 sub-regions, based on the physical and biogeochemical controls of these subregions. Using a self-organizing map approach, the authors extrapolate the cruise data to the entire study region in order to estimate the carbon exchange of the Prydz Bay.

The Southern Ocean is still among the least observed and certainly least well understood ocean basins, hence I found this process study – investigating carbon variability and air-sea exchange in the Prydz Bay – to be very interesting and certainly relevant for the GB readership. More details on the strengths and weaknesses are listed below.

Strengths:

I found the manuscript and particularly the discussion of the processes comprehensive and logically built-up. The authors further make use of an appropriate and previously applied method based on machine learning (i.e. the SOM method) to extrapolate the cruise information to the full region of interest. They use independent validation data to test how well their approach reproduces observations from the SOCAT dataset and use this information to estimate the uncertainty of their integrated air-sea flux.

Weaknesses:

Up-front, I would like to note that there are several language issues – too many to be all named here (just one example: line 232: "In Pacific Ocean" should be "In the Pacific Ocean") – hence I do recommend English language editing.

During my review, I have encountered a few things that need clarification or some more information from the authors. They are listed from the most to least concerning. Additional comments (not of major concern) with line-numbers can be found at the end of this document:

1. Method section: At the moment, it is impossible for a reader who has not worked with the SOM approach to understand the methods section. Sentences like: "The SOM is trained using unsupervised learning to project the input space of training samples to a feature space (Kohonen, 1984), which is usually represented by grid points in tow-dimension space." Imagine a BG reader who is interested in the carbon exchange of the Prydz Bay but has never worked with a SOM. How is that person supposed to understand wording like"unsupervised, feature space, weight vector, training data, labeling data, etc." without reading several other papers first? As a SOM user I had no issues to follow this section but in my view, it has to be simplified for the more general BG audience. Furthermore, the authors miss to mention what distance function the SOM uses to detect the "winner neuron" (Euclidean distance maybe?). Furthermore, I don't think the phrase "resolve nonlinear relationships" (see abstract) is appropriate, since a SOM is a clustering algorithm that clusters based on similarities, but does not explicitly "resolve" a relationship.

<u>Response</u>: We have revised the introduction part about the SOM method to make it easy to understand what is SOM. And in the 2.2 section we have revised the sentences and adjusted the structure to make it easy for the reader to know how SOM works. In our SOM analysis we used Euclidean distance (the shortest distance) to select winner neurons and we have added this to the manuscript. We agree with the reviewer's suggestion and have changed the phrase 'resolve

nonlinear relationships' to be 'to overcome a complex relationship among the biogeochemical and physical conditions in the Prydz Bay region'.

2. Training data: This links a bit to my point above but goes a bit more in-depth: I am not sure how data have been handled. On line 177 the authors state that the data have been "the four proxy parameters were logarithmically normalized" but table 1 suggests otherwise. In table 1 all values are absolute values. Besides that, I am not convinced that it makes sense to logarithmically normalize all 4 proxies. It makes sense for the skewed MLD and CHL-a but not really for salinity and temperature. Besides, I wonder how the normalization effects the distance function (which is not mentioned). Euclidean distances depend on the data-value range of each proxy. Also, what I am missing is a discussion why exactly the 4 proxies have been chosen? Why not sea surface height, wind speed, sea level pressure? What makes the 4 proxies so unique? I know they have been used by other authors, but the reader of THIS study needs this information.

<u>Response</u>: In table 1 all values are absolute values of the four proxies to show the value range. For the skewness and the N coverage percentage, the normalized data are shown in parenthesis. According to the change of skewness and N coverage percentage we found out only MLD and Chla data needed to be normalized for both the training and labeling dataset. Since we used Euclidean distance function to select the winner neuron and it depends on the data-value range of each proxy. The normalization for MLD and Chla dataset is to avoid weighting issue raised from the different magnitude among the variables.

In section 2.1 we have discussed the four proxies which will affect the distribution of pCO_2 in the surface sea water. The dissolution of CO_2 into water is mainly affected by temperature and pressure of water. The variation of salinity has little effect on the dissolution of CO_2 . However the sea ice changed quickly in the study region and we chose salinity to be a proxy to simulate pCO_2 . Moreover, in the region where local biology activities are active, pCO_2 will be affect strongly by photosynthesis. The mixed layer depth will prevent the upward mixing of nutrients and limits the biological production therefore we chose MLD as another proxy to simulate pCO_2 . Sea surface height and sea level pressure are not major factors to the distribution of oceanic pCO_2 . Wind speed is vital for the sea-air gas exchange and it is included in the air-sea flux equation.

3. Uncertainty: line389 states: "increased from week-1 (2.13 TgC) to week-2 (2.24TgC) due to increased wind speed." I was a bit disappointed here. First there is the effort to calculate uncertainties, then it is neglected in the text. Given the final uncertainty estimate, it is very unlikely that this regional difference of 0.1 TgC is significant. In general I suggest to add uncertainties wherever possible to avoid such misinterpretations.

<u>Response</u>: We have added uncertainties to the carbon uptake in section 3.4 and we have changed 'increased' to be 'changed mildly'.

4. Validation, comparison: I appreciate that the authors do a comparison with SOCAT data and include this in the overall flux uncertainty. I think that there need to be a bit more info in the text what cruise from SOCAT you are comparing to (this information is available on socat.info), or what the average spatial and temporal distance (which should be possible

since a nearest grid method was used) between the cruises is. That certainly contributes to the mismatch as well. Otherwise, I was quite impressed by the relatively small (~22µatm) difference. It might not sound small at first but your are comparing small special scale and high frequency temporal scale data based on the extrapolation of a single cruise. Therefore, 22µatm is impressive in my view. Furthermore, the RMSE tells the reader about the spread, but it would be valuable to add the mean (or absolute mean) difference between the SOM derived CO₂ and the SOCAT cruise. This would give you an indication of the bias.

<u>Response</u>: We have added the information of the cruise we selected from SOCAT in section 2.3. We have calculated the absolute mean difference between the SOM derived CO_2 and the SOCAT cruise. According to the validation, the SOM derived pCO_2 is generally lower than the SOCAT. Since the dataset from SOCAT does not cover the low- pCO_2 area towards the south, the precision might be of great uncertainty.

Methods section: On many occasions the authors re-grid data to the desired 0.1*0.1 resolution, but a bit more information on all data that were regridded and the algorithm would be appreciated. Ideally in form of a table. Additionally, I am missing the motivation why 0.1*0.1 was chosen. Why not 0.5*0.5 or even 0.05*0.05. Just to be clear, I don't suggest changing the resolution, but the text needs some motivation/technical explanation on why the current resolution was chosen that justifies all the data handling (i.e. regridding of proxy data)

<u>Response</u>: The 0.1*0.1 resolution of our study was desired according to the study area. It is a small area from 63E to 83E and 64S to 70S and the 0.1 resolution is the optimal. In the paper of Telszewshi et al. (2009), it was a basin-wide area from 9.5E to 75.5E and 10.5N to 75.5N, so their resolution was a 1 latitude by 1 longitude resolution. For a global area, Takahashi et al.(2012) chose 4*5 resolution. For our study area, it would be too rough if the resolution of 0.5, and the matrices would be too big if the resolution of 0.05.

The other data including remote sensing data and modeled data of different resolution were regridded to be the same resolution of 0.1 * 0.1 by Kriging method. We have added some explanation in the text. We think it is clear in the text.

Recommendation:

I have found this study to be interesting and to be of value to the BG readership. While I have raised some (partly major) concerns above I think that they can be resolved by the authors. I therefore recommend major revisions of the manuscript.

Specific and minor comments to the text:

- 1. Abstract line 14: Please also add the temporal resolution to the spatial resolution **Response:** We have added 'weekly' to the spatial resolution in abstract.
- Abstract lines 27-29: This last sentence is out of context and is not something you can conclude from this study, hence it needs to be removed.
 Response: We have removed the last sentence.
- 3. Lines 32-33 reads "The role of the ocean south of 60S in the transport of CO₂ to or from the atmosphere is still uncertain despite of its importance of reducing anthropogenic CO₂

in the atmosphere" – that is a conflicting statement as it currently reads. If we know the importance of reducing atmospheric CO_2 how can its role be uncertain?

<u>Response</u>: It was a mistake. Here we mean 'the amount of carbon uptake in the ocean south of 60'. We have revised it.

- Lines 76-77: "Therefore, the direction of the sea-air CO₂ transfer is mainly regulated by the oceanic *p*CO₂" this statement needs a reference
 Response: We have added the references needed.
- Line 84:"The SOM analysis, based on neural network (NN), a type of artificial neural network" – the second part (based on neural network) can be removed <u>Response:</u> It has been removed.
- 6. Line 117: "Salinity records the physical processes" When I read this sentence I also think of larger scale circulation and mixing in the context of physical processes, whereas this statement links to the follow-up discussion about brine rejection. Maybe a different term would be more appropriate.

Response: It has been revised.

- Line 130: How was the interpolation done?
 <u>Response:</u> We gridded the chlorophyll-a data from Modis according the cruise track.
- 8. Lines 133-136: "The mixed layer links the atmosphere to the deep ocean and plays a critical role in climate variability. Very few studies have emphasized the importance of accounting for the vertical mixing through the mixed layer depth" Firstly, I disagree. Several studies have emphasized the importance of vertical mixing of carbon (but also nutrients, etc) through the mixed layer. Secondly, I caution the authors to mention the role in climate variability here. Their study does not resolve the necessary timescales to discuss either seasonal or interannual or decadal (whatever variability the authors refer to) variability.

<u>Response</u>: We have made the correction and have removed the mention about the role in climate variability since in our study it didn't relate to that.

9. Lines 154-155 'SOM based multiple non-linear regression' – This must have been a mistake or typo here, since the SOM (unlike e.g. a back propagation network) does not perform a regression (also not a non-linear one). Instead the SOM clusters data based on similar environmental conditions.

<u>Response</u>: Yes, we agree the reviewer's suggestion and have removed 'multiple non-linear regression'.

10. Lines 194-195: "until the neural network sufficiently represents the nonlinear interdependence of proxy parameters used in training." – how is this judged? When do you know that its sufficient? I suppose this is judged by the number of SOM iterations, but how is set?

Response: Because SOM analysis is a powerful technique to estimate pCO_2 from among the

non-linear relationships of the parameters (Telszewski et al., 2009;), actually, we presumed the nonlinear interdependence of proxy parameters are sufficiently represented after the training procedure. Also, we used the som_make() function in the SOM toolbox for training data. Thus, we updated the sentence accordingly.

11. Line 215: "I could not figure out where the factor 30.8*10-4 comes from? Please explain in the text

<u>Response</u>: The factor is induced according to the simplification of the equation. We have added the explanation in the text.

- 12. Line 264: "robustly divided" I caution the authors here: How can you be sure the division is "robust"? Have you done any test that would proof robustness?
 <u>Response:</u> Three regions are divided according to the distribution of oceanic *p*CO₂. From the distribution of *p*CO₂ as shown in Fig.2-a there are three ranges. One is from 291.98 µatm to 379.31 µatm, the second is from 200 to 310µatm and the third is below 200µatm. We roughly divided the study region according to the three ranges of *p*CO₂ and the range of the depth of water in the Prydz Bay region. It was a mistake to use the word 'robustly'.
- 13. Lines 281-282: "region atmospheric pCO₂ was stable from 374.6µatm to 387.8µatm" That is a difference of 13µatm I would not call this stable at all! I suppose this difference is largely the result of sea level pressure variability and relative humidity in the surface layer, hence it would be interesting to see the molar fractions (in ppm) for comparison if available.
 <u>Response:</u> We don't have sea level pressure data and relative humidity in the surface layer. We have revised this sentence and removed 'stable'.
- Line 285: "biological consume" should be "biological uptake" <u>Response:</u> It has been revised.
- 15. Line 318-319:"for a same period" This would be important information. Furthermore, have you considered ARGO biogeochemistry floats from the SOCCOM array? They are deployed since 2013 and may add some additional independent estimate. This might however be beyond this manuscript.

<u>Response</u>: Thanks for letting us know the SOCCOM. We have searched from SOCCOM but we can't find dataset useful for our study. However SOCCOM is a helpful website and we will turn to it when we other analyses in the Southern Ocean next time.

Figure 4b: It would be easier visible if x-axis and y
 Response: We have changed the x-axis and y to be the same range.

Responses to review2:

General comments

The manuscript 'variation of Summer Oceanic pCO_2 and Carbon Sink in the Prydz Bay Using SOM Analysis Approach' by Suqing Xu et al. presents their cruise data plus its analysis regarding oceanic and atmospheric pCO_2 and the related air-sea pCO_2 flux. The results can potentially be of interest to readers interested in the Southern Ocean carbon cycling, and its variability in time and space. It also provides an opportunity to the authors to show a practical example of the application of SOM in biogeochemistry. In order for the manuscript to be appreciated by the biogeochemical community, the authors should provide a better description of its relevance and importance for the greater Southern Ocean. S I am not an expert on SOM or neural networks, I cannot judge the methodology on that method in detail. I should however be able to understand what is presented in section 2.2. and I find this difficult at times. Several times mention is made of methods (like 'a linear method' or 'Linear regression extrapolation method') without further information on what is done: This makes reproducibility of the work without consulting the authors impossible. Besides that, I unfortunately often find the language to be confusing/imprecise, and therefore recommend professional English language checking before resubmitting. The language made it more difficult for me to judge the value of the manuscript, and I expect I can provide a more in-depth review after the language is improved. The manuscript would also improve if it were shortened as compared to the current version, as there is enough space to increase the information density in the manuscript in my opinion.

Specific comments

1. The introduction

The introduction thoroughly describes the geographic setting of the Prydy Bay. I appreciate this, but it makes the introduction unbalanced as the questions 'why is this study of relevance' and 'what is new' are only covered by a few sentences. The authors describe the issue that the manuscript wants to address, namely the sparse spatiotemporal coverage of the Southern Ocean (SO) carbon cycle. They also tell the reader that they address the issue using the SOM approach. However, to what extent does research on the Prydz Bay support our understanding of the SO carbon cycle? On page 2, line 38-39 it is mentioned that the Prydz Bay is the third largest embayment in the Antarctic continent. No other reasons are given for the study of in specific this bay: What makes this bay (potentially) important for the SO carbon cycle even though it is small as compared to the total surface area of the SO? To what extent is this Bay representative for the SO as a whole (or just other parts of the SO), i.e. do the authors think their approach or data are useful for and representative of other areas in the SO? Why was the month February chosen to do the cruise?

<u>Response:</u> The Prydz Bay region is the third largest embayment in the Antarctic continent and one of the source regions of Antarctic Bottom water (AABW) as well as the Weddell Sea and the Ross Sea (Jacobs and Georgi,1977; Yabuki et al., 2006). Studies have reported that Prydz Bay is a strong carbon sink in the austral summer (Gibsonab and Trullb, 1999; Gao et al., 2008; Roden et al., 2013). It is important to study the carbon cycle in the Prydz Bay. We have revised this part and added the information. The Prydz bay is part of the SO. SOM has been applied to simulate oceanic pCO_2 to overcome a complex relationship among the biogeochemical and physical conditions. We chose the beginning of February to early March because we had the in situ measurements during that time.

In the first sentence, it is mentioned that the SO is important for anthropogenic CO₂ uptake. The authors cannot distinguish between natural and anthropogenic carbon fluxes based on their measurements: Some sentences should be added to describe that the SO is a natural source of carbon to the atmosphere, but a sink for anthropogenic carbon – and that both are highly variable but creating a net sink for total carbon over the past decades. Here an argument could be made for their own study and cruise, which aims to reduce the spatiotemporal sparsity of the data and get a better understanding of the variability of the contemporary pCO_2 and its driving mechanisms. The authors call the Bay a sink at several instance (for example P3, L101 and P5, L125): Some numbers from previous studies should be given to support the statement that the Bay as a whole is a sink for carbon before presenting your own results.

<u>Response</u>: Sentences have been added to describe the SO on its role for carbon dioxide. About our study and cruise, we have added the argument. Recently studies have shown that there is a strong carbon sink in Prydz Bay especially in summer and we have added the references to support the statement.

In Figure 1, an inset could be added to visualize the location of Fig. 1 on the Antarctic continent. **<u>Response</u>**: For Fig. 1, we have added an inset to show the location of the Prydz Bay in the Antarctic continent.

P3,L64-66: How does a marine ecosystem interact with the physical environment to make it complicated to study pCO_2 ? Clarify your statement, as it currently is imprecise.

<u>Response</u>: We have revised this sentence. Here we mean due to the special physical environment and complicated ecosystem, it is difficult to study the spatiotemporal variation of pCO_2 .

When describing the methods, clarify that in situ data from the cruise are combined with remotely sensed data to arrive at a gridded product.

<u>Response</u>: We have revised to clarify that in situ data from the cruise are combined with remotely sensed data.

2.1 In situ data

Here the authors present how they took their underway measurements and present them in Fig.2. The first time I read this section, I missed a good structure: The section starts with an explanation of the cruise and instruments used (until line 115). Then, the following paragraphs came to me as a bit of a surprise. One could help the reader find a better flow through the text by explaining that there are several processes/water characteristics that can influence the pCO_2 flux (which is the topic of this study). Then, the sea ice paragraph(lines 116-120), the information on the SSS and SST collection (lines 132-end of section) come more naturally. It is important to defend why specifically these proxies/data are used to do your study (create a gridded pCO_2 map). Don't forget to start the title with a capital letter i. It is unclear tome whether the results presented in Fig.2 are 4-week mean results or how they are calculated from the 4 cruise legs: Add more information to both the caption and the text.

Response: The results presented in Fig.2 are the data along the track cruise when R/V Xuelong

sailed from east to west from the beginning of February to early March. It has been added in the caption and the text. We have added the information to explain some processes that can influence the pCO_2 distribution in the text.

2.2 SOM method and input variables

This section is generally hard to follow, maybe partly because I am not familiar with SOM. It should be improved so that also people new to SOM are able to understand and appreciate what you have done. Which 'environmental parameters' and which 'observational dataset's (Fig.3) are used? Lines 205-220 (or even up to 228) could be moved up in order to introduce the reader earlier to the datasets. Then the authors can explain what they are used for and how.

<u>Response</u>: Thanks for the suggestion. We have reconstructed this section and make it more clear about the 'environmental parameters' and 'observational datasets ' in the text. We have also revised the sentence about SOM method to make it easier to be understood.

2.3 Validation of SOM derived oceanic pCO₂

This section raises a lot of questions from my side. To what extent is SOCAT comparable to your data? Are the data both summer data? Why do you talk about assimilating several years together, but then only take 2015 from SOCAT (line 239)? Could you maybe compare your data to a model estimate of pCO_2 for this region? Lines 232-235: How is the equilibrium between atmospheric and surface ocean pCO_2 , do you mean pCO_2 -disequilibrium? Why do you describe this if you did not apply this method after all?

<u>Response</u>: We use dataset from SOCAT for the same period, which is February 2015. The dataset from SOCAT for validation as shown in Fig4-a. We prefer in situ measurements to model output to validate our results. We have removed line 232-238. Line 232-238 was a discussion and we think it didn't relate to the text.

2.4 Carbon uptake in the Prydz Bay

This section is quite clear to me: You have combined wind speed data and your pCO_2 measurements to arrive at a flux using Eq 2. However, you should clarify 1) where you used a 'scaling factor' (P10, L247-248) (in Eq. 2?), and 2) that that used your SOM-based pCO_2 product to calculate pCO_2 in Eq.2 (did you?). In addition, you write that the transfer velocity is a function of wind speed and temperature (Line 245) and then you write about a gas transfer rate (Line 248) (=transfer velocity?) which you apply a scaling factor to. I am left with the question which gas transfer rate or velocity you have used / how you calculated it.

<u>Response</u>: The original Eq.2 was a simplified equation considering the unit conversion factor. Now we have added the original sea-air CO_2 flux equation in the text and we have revised this part and added some information.

3.1 the distribution of underway measurements

Here you present your underway measurements for three areas. On what basis did you divide the Prydz Bay in these subregions? You write the division is 'robust' (P11, L264): Did you test what effect the choice of your division has on your results? It would be helpful to the reader if you added a plot figure with the subdivision of the Prydz Bay into its three regions. Add units to all numbers (especially salinity lacks the psu unit throughout this section). I assume you are describing the

results that are visualized in Fig 2 in this section: you should make reference to it if this is the case. Throughout the text of this section, you should be more precise on whether the values are regional means, 4-week means, and how you calculated this (refer to the methods). When you say decrease or increase (like P12, L291), it is not always clear to me whether it decreases/increases in time or space or whether the mean is lower or higher than in the neighboring sub-region. This causes for example confusion when SST's 'vary sharply' (L293) but 'decreased slightly' just the sentence above (L291). The readability of this section may improve by summarizing your main results in a table. A sentence should be added either here on the methods where the relationship between chlorophyll-a (as remotely observed) and biological productivity is stated.

<u>Response</u>: Three regions are divided according to the distribution of oceanic pCO_2 and depth of water. From the distribution of pCO_2 as shown in Fig.2-a and Table.2 there are three ranges. One is from about 300µatm to 380µatm, the second is from 200µatm to 350µatm and the third is below 250µatm. We roughly divided the study region according to the three ranges of pCO_2 and the range of the depth of water in the Prydz Bay region. It was a mistake to use the word 'robustly'. We have made the change to the text.

We have added units to all numbers. We have added the subdivision lines on Figures. 5. We have added the reference to Fig 2 in this section.

Section 3.1 was about the in-situ measurements and the average values we discussed were regional mean. We have added the information in the text to avoid the confusion about the numbers. A table was added to the text summarizing our main results. A sentence has been added here about the relationship between chlorophyll-a and biological productivity.

3.2 Quality and maps of SOM-derived oceanic pCO_2

You compare your results to SOCAT and calculate the RMSE. Could you also provide the R2 of the best-fit line (red line in Fig. 4b)? You say your RMSE is consistent but not as good as most of the neuron methods. Do you mean it is on the high side of the accuracies previously reported, or why is it not as good? Could you calculate/estimate how many extra data points you would need to gain an improved precision of your SOM approach? You could probably comment on the limited amount of data that retrieving more data is not realistic with the resources and time available. SOCAT is not perfect either: A comment on its limited overlap with your study area would be appropriate here. It is surprising that the SOM estimate is generally higher than the SOCAT one, as SOCAT does not cover the low- pCO_2 area towards the south. Did you sample your SOM-derived pCO_2 dataset on the SOCAT locations, or did you compare all SOCAT in the area to all your data points in Fig. 4b? The first would probably be a fairer comparison and provide a better outcome as well. Fig.4a could be plotted in the same way as Fig.2 to make it easier for the reader to compare the spatial coverage. Response: Our RMSE is on the high side of the accuracies previously reported and the correlation coefficient has been added in the text. There are two reasons accounting for the precision. One is the limited spatial coverage of the in situ measurements to be labeled in SOM method. Increasing the spatial coverage of the labeling data will help to increase the precision of SOM derived oceanic pCO_2 . The other one is the dataset from SOCAT is not sufficient neither for space overlap nor for time overlap. The best way to get an improved precision of the SOM approach is to have a full coverage measurement in the study area. In our study, we selected the SOM derived oceanic pCO_2 according to the location of the datasets from SOCAT for validation. As mentioned in the text, SOM derived pCO_2 is generally lower than the SOCAT one. We have plotted Fig.4a as Fig.2.

3.3 Spatial and temporal distributions of SOM-derived pCO₂

Here I expect the presentation of your main result: the pCO_2 maps of Figure 6. However, the text mostly describes the sea ice situation of the region: Why is this done here? Maybe a different title would be more appropriate? If sea ice is a main driving factor for pCO_2 , this should be argued using the results. If the authors could add regional sub-division lines on the maps in Fig. 6, it might be easier to argue for the chosen sub-division (i.e. Shelf region, etc).

<u>Response</u>: We agreed with the reviewer and have revised this section. This section is mainly about the result of SOM derived pCO_2 . We have presented the spatial and temporal distribution of SOM derived pCO_2 . We have added regional sub-division lines on the maps.

3.4 Carbon uptake in Prydz Bay

This section is quite clear, although it would be good to clarify when mean values are reported, and whether they are regional means or temporal means, or both. From the figure on page 17 (which has no number?) it is hard to read the pCO_2 changes: one could either present it as a table, or adjust the y-axis range. Please make sure the figure is suitable for the color blind (and check this throughout the manuscript): Use for example different shapes for the three different lines in the upper graph, and add shapes in the lower one.

Response: We have changed the figure to be a table and we have made the revised in the text.

Supplementary information

The text at the start of the SI is already used in the main text, I do not see the need to provide it twice, and would recommend to remove it from the SI.

Technical corrections

I made an effort to pick out the most important language issues. However, as recommended in the general comments, I would strongly advise the authors to revise their language throughout the manuscript and to have it checked before resubmitting.

1. Try to prevent the use of the word 'it' throughout the manuscript: replace by the actual subject of the sentence.

Response: We have made the changes in the text.

- Caption of Fig.1: replace 'The circulations in the ' by 'The ocean circulation in the '. Replace sentence 'The weekly sea ice extents for our study periods were overlapped on the cruise.' By 'During the 4-week cruise, the sea ice extent varied as indicated by the contoured white areas:' and replace 'the white shadow' by a fourth contoured area.
 Response: It has been replaced.
- Check all figures on their suitability for color-blind people <u>Response</u>: We have checked all the figures.
- P2, L33: replace 'of reducing anthropogenic CO₂ in the atmosphere' with 'in regulating atmospheric carbon and acting as a net sink for anthropogenic carbon' or similar.
 <u>Response:</u> It has been replaced.

- P2, L35: replace 'this status derives' by 'This uncertainty comes' <u>Response:</u> It has been replaced.
- P2,L36: replace 'for' with 'because of' <u>Response:</u> It has been replaced.
- 7. P2, L38: move 'lying in the Indian Ocean section' to the next sentence and replace 'lying' by 'situated'

<u>Response</u>: It has been moved and replaced.

- P2, L39-40: move 'With Cape Darnley ... to the east' to the end of the sentence or rephrase whole sentence, try to use the main verb as early as possible in a sentence Response: It has been moved and rephrased.
- P2, L41: replace 'varies' by 'increases' (or does it go up and down?) <u>Response:</u> It has been replaced.
- P3, L51-52: Add 'the': 'The Fram Bank and the Four Ladies Bank' <u>Response:</u> It has been added.
- P3, L52: a spatial barrier for Response: It has been revised.
- 12. P3, L54: replace 'part of it' by 'partly' **Response:** It has been replaced.
- P3, L63-64: rephrase sentence to clarify the sequence of events <u>Response:</u> It has been rephrased.
- 14. P2,L67: the importance for what? Replace 'carbon cycle' by 'carbon cycling'. This relates to comment 1 as well: how does studying the Prydz Bay relate to the SO carbon cycle? <u>Response:</u>We have added the importance of study carbon cycling in the Prydz Bay and added the information about the Prydz Bay related to the SO carbon cycle in the introduction section.
- P3, L69: use present tense where possible: 'is' <u>Response:</u> It has been replaced.
- 16. P3, L72: remove first word 'the' **Response:** It has been removed.
- P3,L77: Add 'A' before 'linear'. Clarify that it was not you doing this by adding 'In earlier studies, ...' <u>Response:</u> It has been revised.
- P4, L78: What is a big scale? The entire Prydz Bay, the SO?
 <u>Response:</u> We have revised and made it clear to be 'that alinear regression extrapolation method has been applied to expand the cruise data to study the carbon cycle in the Southern

Ocean'.

- 19. P4, L79: Start a new sentence at 'however'. Simplicity can be a good thing: why is calculating pCO₂ based on SST and CHL insufficient? How do you know what controlling factors to select? <u>Response</u>: There are two opposing processes primarily govern CO₂ chemistry in seawater: sinking of biological products from the photic zone to deep-ocean regimes (i.e., the biological pump), and upward transport by upwelling deep waters of CO₂ and nutrients formed by the decomposition of biological debris (i.e., the physical pump). It is not sufficient to simulate oceanic *p*CO₂ based on SST and CHL in previous studies, of which the RMSE tended to be high. From our previous researches and other studies we chose SST, CHL, MLD and SSS to be the controlling factors and we have added the information in the text.
- 20. P4, L83: remove 'the' before 'February' <u>Response:</u> It has been removed.
- P4, L84: Is NN a type of neural network? The acronym NN is not used anywhere else in the manuscript so not need to define it. What makes it artificial?
 <u>Response:</u> NN is an abbreviation for neural network. Here artificial means artificial intelligence.
- 22. P4, L85: Remove 'been' <u>Response:</u> It has been removed.
- 23. P4, L88: Add 'and' before 'chlorophyll' <u>Response:</u> It has been added.
- 24. P4,L92: Remove 'been' and replace 'a' before spatial-temporal by 'the' **Response:** It has been removed.
- P4, L97: Add the word 'cruise' after 'CHINARE'. Do the same on P4, L108. <u>Response:</u> They have been revised.
- P4, L98: replace 'to the early of March' with 'to early March'. Check general fluency of lines 97-99.
 <u>Response:</u> It has been replaced.
- 27. P4, L99: replace 'is show' by 'are shown' **Response:** It has been replaced.
- 28. P4, L101: here the authors suddenly discuss carbon absorption: the readers have not learned before that this area is considered to be a sink for carbon, so it would be could to introduce the reader to that earlier in the introduction
 Begnenest It has been revised and we have added the information that the Brudz Bey is a

<u>Response</u>: It has been revised and we have added the information that the Prydz Bay is a carbon sink in the introduction.

- 29. P4,L102: Replace 'followed' by 'follows' <u>Response:</u> It has been replaced.
- P4, L104: Add ', and' and remove '.' <u>Response:</u> It has been revised.
- P4, L108: 'at the beginning of February 2015', did the cruise not extend into March? Why 'beginning'?
 <u>Response:</u> It has been revised. The cruise was from the beginning of February to early March.
- 32. P5, L115: replace ' pCO_2 in atmosphere' by 'atmospheric pCO_2 '. Check also that each time you use the word pCO_2 , that you use an italicized letter p (also in captions, and axes titles) **Response:** It has been revised.
- P5, L116/117: Replace 'in polar region' by 'in polar regions' <u>Response:</u> It has been replaced.
- P5, L117: Move sentence 'Salinity records the physical processes' to later in the paragraph, because you first need to explain what salinity has to do with sea ice. It would also fit to explain to the reader why this is all relevant for a study of *p*CO₂.
 <u>Response:</u> It has been revised.
- P5, L117-118: Replace 'During freezing, salt is excluded ... [] ... brine rejection' with 'During freezing, brine is rejected from ice, thereby increasing sea surface salinity'.
 <u>Response:</u> It has been revised.
- P5, L119: replace 'to dilute' with 'thereby diluting' <u>Response:</u> It has been replaced.
- P5, L125: Remove 'clearly' <u>Response:</u> It has been removed.
- P5, L127-128: 'the active biological process': Do you mean photosynthesis?
 <u>Response:</u>Yes and we have added information about the relationship between chlorophyll-a and biological productivity in the text.
- 39. P5, L128-129: Explain the relationship between chlorophyll-a and biological productivity before you directly connect them and the consecutive effect on pCO₂ in this sentence. Response:
- P5, L129: Clarify that you used remote sensing data, and provide the reader with uncertainties associated with this method. Be consistent writing Modis either as Modis or MODIS.
 <u>Response</u>: We have clarified that we used remote sensing data from MODIS. The uncertainty

associated was mentioned in the last paragraph in section 2.2.

- P5, L130: Replace link by appropriate reference.
 <u>Response</u>: We prefer the link to show where the data comes from.
- P5, L138-139: This sentence seems to repeat lines 121-122 on this page.
 <u>Response</u>: It has been deleted.
- P5/6, L139-141: Rephrase sentence to make clear to the reader that there are two main methods in use, and what the advantages are of the 'difference criterion' method in the SO.
 <u>Response</u>: It has been rephrased.
- 44. P6, L141: Add 'therefore' between 'we' and 'calculated' <u>Response</u>: It has been added.
- 45. P6, L142: Replace 'the' with 'on' <u>Response</u>: It has been replaced.
- 46. P6, L142-143: 'of with ...' Do you mean 'of which'? I do not understand this sentence, sorry. **Response**: Yes, we mean 'of which'.
- 47. P6, L143-144: Why where the data gridded? They were point data from the CTD taken along the track, so why where they not already on the right spatial and temporal 'resolution' (do you mean interval?)?
 <u>Response</u>: Yes, we gridded the point data from the CTD taken along the track in interval and we have revised the sentence.
- P6, L150-151: Start with a capital letter t. Some words have disappeared from the caption.
 <u>Response</u>: It has been revised.
- P7, L161: Replace 'dimension' by 'dimensional' <u>Response</u>: It has been replaced.
- 50. P7, L 163: 'Input variables', how do these relate to the boxes in Fig.3?'as a vector' is more fluent than 'in a vector form'
 <u>Response</u>: The input variables related to the environmental parameters in Fig.3. We have made it clear the input variables and the environmental parameters. We have also changed to be 'as a vector'.
- 51. P8, L173: did not all your underway measurements include measurement of pCO_2 ? <u>**Response**</u>: The underway measurements included measurement of pCO_2 . Here we mean: for the training process, the input environmental parameters are those from satellite and model data of 0.1 resolution. However, the measurement of pCO_2 was along the cruise track and it has a spatiotemporal limitation compared to satellite data.

- 52. P8, L178: Why did you quantify skewness and what did you do with the results? Is taking the logarithm an accepted method to improve the N coverage? Why does the coverage increase when taking the log?
- 53. P8, L186: Why is this not done for SST and SSS?

<u>Response to No.52&53</u>: In table 1 all values are absolute values of the four proxies to show the value range. For the skewness and the N coverage percentage, the normalized data are shown in parenthesis. According to the change of skewness and N coverage percentage we found out only MLD and Chla data needed to be normalized for both the training and labeling dataset. Since we used Euclidean distance function to select the winner neuron and it depends on the data-value range of each proxy. The normalization for MLD and Chla dataset is to avoid weighting issue raised from the different magnitude among the variables.

In section 2.1 we have discussed the four proxies which will affect the distribution of pCO_2 in the surface sea water. The dissolution of CO_2 into water is mainly affected by temperature and pressure of water. The variation of salinity has little effect on the dissolution of CO_2 . However the sea ice changed quickly in the study region and we chose salinity to be a proxy to simulate pCO_2 . Moreover, in the region where local biology activities are active, pCO_2 will be affect strongly by photosynthesis. The mixed layer depth will prevent the upward mixing of nutrients and limits the biological production therefore we chose MLD as another proxy to simulate pCO_2 . Sea surface height and sea level pressure are not major factors to the distribution of oceanic pCO_2 . Wind speed is vital for the sea-air gas exchange and it is included in the air-sea flux equation.

- 54. P9, L198: Add 'part of the' between 'second' and 'process'. Also, it is either each neuron or all neurons (i.e. is it plural or singular here?)
 <u>Response</u>: It has been added and corrected to be 'neuron'.
- 55. P9,L213: What is meant with '8-d'? 8 dimensions, 8 days? If 8 days, why not 7 if used as weekly data?

<u>Response</u>: '8-d' meant 8 days here. Our study period was from the beginning of February to March 4. When we used 8 days as weekly it was proper to cover the study period.

- 56. P10, L243: Replace 'by two items' with 'using pCO₂ and the transfer velocity across the airsea interface' or something similar.
 <u>Response</u>: It has been replaced.
- 57. P10, L246: Replace 'delta' with ' \triangle ' **Response**: It has been replaced.
- 58. P10, L247: What scaling factor are you talking about here? Is it in Wq.2? <u>Response</u>: The scaling factor for the gas transfer rate is 0.251. It was not shown in Eq.2 because Eq.2 is a simplified equation taking into account the unit conversion factor. We have revised this part to make it clear.

- P10, L251: Check that equation has one format/font and denote units in []-brackets. <u>Response</u>: It has been revised.
- 60. P10, L252: Check superscripts of pCO₂-air and pCO₂_sea, also add 'and' before pCO₂_sea and end the sentence with 'respectively'
 <u>Response</u>: It has been checked.
- 61. P10, L256: I am again confused by the use of the word regridding, your are working with sample data- why do you regrid? You mean you gridded the data from the point measurements you had of atmospheric *p*CO₂? What linear method did you use?
 <u>Response</u>: The atmospheric *p*CO₂ was of the cruise track. When we got the SOM derived oceanic pCO2 it was of 0.1*0.1 resolution. In order to calculate the air-sea flux we need to extrapolate the atmospheric *p*CO₂ to be the same 0.1*0.1 resolution. We used linear method.
- P10, L258-259: Do you mean you integrated the gridded flux over the area of Prydz Bay, taking into account the ice-free area only? How did you take ice into account?
 <u>Response</u>: We have added the information to the text. The sea-air flux was calculated according to the proportion of ice-free area.
- P11, L267: No need to use the acronym AD if you only use it once <u>Response</u>: It has been revised.
- 64. P12, L300: What is formed here? The subject of the sentence is the Shelf region, but a regions cannot be formed by modification of water.
 <u>Response</u>: It was a mistake and we have changed the subject to be 'water inside the Shelf region'.
- 65. P12, L305-306: If the region was ice-free, Fig.5 cannot be correct?
 <u>Response</u>: Fig.5 is correct and the ice shown in Fig.5 is permanent ice. We have revised the sentenced to be 'the most least ice-covered'.
- 66. P12, L314-315: When and where does the biological pump become the dominant factor setting the distribution of pCO_2 ? How do you know this is the main contributor to the pCO_2 variations? **Response**: The low oceanic pCO_2 was consistent with the high chlorophyll value in the Shelf region. For four weeks biological pump was the dominant factor setting the distribution of pCO_2 . In the Shelf region other factors didn't show such pattern with oceanic pCO_2 .
- 67. P16, L371: What indicators did you use to conclude that the stability of the water was weak? **Response**: The original sentence is not proper here. We have removed this sentence.
- P16, L377: flew? Please rewrite this sentence.
 <u>Response</u>: It was a mistake. It should be 'flowing' and we have corrected it.
- 69. P18, L395: 10¹²gram=Tg

<u>Response</u>: It has been revised.

- P18, L400: Please provide references to this statement and mention it earlier in the manuscript.
 <u>Response</u>: The references have been added and we have added the information in the introduction.
- P18, L408-410: So does the region take up more carbon than on average in the ocean? I.e., is it a relatively large sink as compared to its area?
 <u>Response</u>: Yes, this region takes up more carbon than on average in the ocean. Though small area, it is a relatively large sink. Taking into account the Prydz Bay is one of the resources of AABW (Antarctic Bottom Water), large amount uptake of atmospheric CO₂ may have an effect on the ocean acidification in the long run.

1	Variation of Summer Oceanic <i>p</i> CO ₂ and Carbon Sink in the Prydz Bay Using SOM Analysis
2	Approach
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11	Abstract
12	This study applies a neural network technique to produce maps of oceanic surface p CO ₂ in the
13	Prydz Bay in the Southern Ocean on a weekly 0.1° longitude · 0.1° latitude0.1 longitude · 0.1
14	latitude grid based on in-situ measurements obtained during the 31thst CHINARE cruise from
15	February to early March of 2015 for February 2015. The study area was divided into three
16	regions, namely, the Open-ocean region, Sea-ice region and Shelf region. The distribution of
17	oceanic pCO_2 was mainly affected by physical processes in the Open-ocean region, where
18	mixing and upwelling became-were the main controls. While in the Sea-ice region, oceanic
19	pCO ₂ changed sharply due to the strong change inof seasonal ice. For In the Shelf region,
20	biological factors wasere the main control. The weekly oceanic pCO_2 was estimated using a self-
21	organizing map (SOM) by with four proxy parameters (Sea Surface Temperature, Chlorophyll a
22	concentration, Mixed Layer Depth, and Sea Surface Salinity) to overcome the complex
23	relationship betweenthe biogeochemical and physical conditions in the Prydz Bay region.resolve
24	the nonlinear relationships under complicated biogeochemical conditions in Prydz Bay region.
25	The reconstructed oceanic pCO_2 <u>data</u> coincides well with the in-situ investigated pCO_2 from
26	SOCAT, in the with a root-mean-square error of 22.14 µatm. The Prydz Bay was mainly a strong
27	CO ₂ sink in February 2015, with a monthly averaged uptake of $\frac{23.57\pm6.3618.7\pm4.93}{23.57\pm6.3618.7\pm4.93}$ TgC. The
28	oceanic CO ₂ sink is pronounced in the Shelf region due to its lowest oceanic p CO ₂ and with peak
29	biological production. Strong potential anthropogenic CO ₂ untake in the Shelf region will

20	enhance the s	acidification in t	he deen water	of Prydz Bay and	affect the deep ocer	n acidification
50	ennance the a		ne deep water	or right Day and	and the deep beer	in actumenton

- 31 in the long run since it contributes to the formation of Antarctic bottom water.
- 32

33 1 Introduction

The amount of carbon uptake occurring in the ocean south of 60°S duringthe transport of 34 35 CO_2 to or from the atmosphere is still uncertain despite its importance in regulating atmospheric carbon and acting as a net sink for anthropogenic carbon The role of the ocean south of 60°S in 36 the transport of CO2 to or from the atmosphere is still uncertain despite of its importance of 37 reducing anthropogenic CO2 in the atmosphere (Sweeney et al., 2000, 2002; Morrison et al., 38 2001; Sabine et al., 2004; Metzl et al., 2006; Takahashi et al., 2012). This uncertainty arisesfrom 39 both the strong seasonal and spatial variations that occur around Antarctica and the difficulty of 40 obtaining field measurements in the region because of its hostile weather and remoteness. This 41 status derives from both the strong seasonal and spatial variations that occur around Antarctica, 42 and the difficulty of field measurements in the region for its hostile weather and remoteness. 43 44 Following the Weddell and Ross seas, the Prydz Bay is the third-largest embayment in the 45 Antarctic continent. Situated in the Indian Ocean section, the Prydz Bay is located close to the 46 Amery Ice Shelf to the southwest and the West Ice Shelf to the northeast, with Cape Darnley to the west and the Zhongshan and Davis stations to the east, lying in the Indian Ocean section, is 47 the third largest embayment in the Antarctic continent. With Cape Darnley to the west and the 48 49 Zhongshan Station and Davis Station to the east, Prydz Bay is close to the Amery Ice Shelf to the southwest and the West Ice Shelf to the northeast (Fig. 1). In this region, Wwater depth varies 50 51 increases sharply northward from 200 m to 3000 m.







- 55 Fig. 1 Ocean circulations in the Prydz Bay derived from Roden et al. (2013), Sun et al. (2013), Wu et al.
- 56 (2017). ASC: Antarctic Slope Current; CoC: Antarctic Coastal Current; ACC: Antarctic Circumpolar Current.
- 57 During the 4-week cruise, the sea ice extent varied as indicated by the contoured white areas: the pink line is
- 58 for week-1(20150202-20150209), the black line is for week-2 (20150210-20150217), the red line is for the

week-3 (20150218-20150225) and a fourth contoured area is for week-4 (20150226-20150305). The
circulations in the Prydz Bay derived from Roden et al. (2013), Sun et al. (2013), Wu et al. (2017). ASC:
Antaretic Slope Current; CoC: Antaretic Coastal Current; ACC: Antaretic Circumpolar Current. The weekly
sea ice extents for our study periods were overlapped on the cruise. the pink line is for week-1(2015020220150209), the black line is for week-2 (20150210-20150217), the red line is for the week-3 (2015021820150225) and the white shadow is for week-4 (20150226-20150305).

65

The inner continental shelf is dominated by the Amery Depression, which mostly ranges in 66 depth from 600 to 700 mis mostly 600 to 700 m deep. The depression is bordered by two shallow 67 banks (<200 m): the Fram Bank and the Four Ladies Bank, which form a spatial barrier for water 68 exchange with the outer oceanic waterforming a spatial barrier to water exchange with the outer 69 oceanic water (Smith and Trégure, 1994). The Antarctic Coastal Current (CoC) flows westward, 70 bringing in cold waters from the east. When the CoCit reaches the shallow Fram Bank, it turns 71 72 north and then partly of it flows westward, while part some of it turns eastward, back to the inner shelf, resulting in the clockwise-rotating Prydz Gyre (see Fig.1). The circulation to the north of 73 the bay is characterized by a large cyclonic gyre, extending from within the bay to the Antarctic 74 Divergence at about approximately 63°S (Nunes Vaz and Lennon, 1996; Middleton and 75 Humphries, 1989; Smith et al., 1984; Roden et al., 2013; Wu et al., 2017Nunes Vaz and Lennon, 76 1996; Middleton and Humphries, 1989; Smith et al., 1984; Roden et al., 2013; Wu et al., 2017). 77 The inflow of this large gyre hugs the eastern rim of the bay, and favours the onshore intrusions 78 of warmer modified Circumpolar Deep Water (mCDW) across the continental shelf break (Heil 79 et al., 1996). A wWestward flow along the shelf, that which is part of the wind-driven Antarctic 80 Slope Current (ASC), supplies water to the Prydz Bay. In the austral summer, with longer 81 daylight and increased solar radiation, sea surface temperature increases, ice shelf breaks and sea 82 ice melts, resulting in stratification of the water column. Prydz Bay region is host to a marine 83 ecosystem that interacts with the physical environment which makes it complicated to study the 84 spatiotemporal variability and mechanism of oceanic pCO2-85 86 It has been reported that the Prydz Bay is a strong carbon sink, especially in the austral summerDespite the importance of earbon cycle in the Southern Ocean, the observations are 87 rather limited to analyze the spatiotemporal variation in the Prydz Bay. The analysis of temporal 88 89 variability and the spatial distribution mechanism of oceanic pCO₂ in Prydz Bay was limited to

90 eruises or stations (Gibsonab et al., and Trullb, 1999; Gao et al., 2008; Roden et al., 2013).

91 Moreover, studies have shown that the Prydz Bay region is one of the source regions of Antarctic 92 Bottom Water as well as the Weddell and Ross seas(Jacobs and Georgi, 1977; Yabukiet al., 2006). It is thus important to study the carbon cycle in the PrydzBay. However, the analysis of 93 94 the temporal variability and spatial distribution mechanism of oceanic pCO₂ in the Prydz Bay is limited to cruises or stations due to its uniquephysical environment and complicated marine 95 96 ecosystem (Smith et al., 1984; Nunes Vaz et al., 1996; Liu et al., 2003). To estimate regional sea-97 air CO₂ fluxes, it is necessary to interpolate between in-situ measurements to obtain the maps of oceanic pCO2. Such an interpolation approach, however, is still a difficult task because, as 98 99 observations are too sparse in over both time and space to capture the high pCO2-variability in 100 <u>pCO₂</u>. Satellites do not measure pCO_2 , but they do provide give access to the parameters related to the processes that control its variability. The seasonal and geographical variability of surface 101 102 water pCO_2 is indeed much greater than that of atmospheric pCO_2 . Therefore, the direction of the sea-air CO₂ transfer is mainly regulated by-the oceanic pCO₂₋₃ and the method of spatially and 103 104 temporarily interpolating in situ measurements of oceanic pCO₂ has long been used(Takahashi et al., 2002 and 2009; Olsen et al., 2004; Jamet et al., 2007; Chierici et al., 2009). In earlier studies, 105 a linear regression extrapolation method was applied to expand cruise data to study the carbon 106 cycle in the Southern Ocean (Rangama et al., 2005; Chen et al., 2011; Xu et al., 2016). Linear 107 regression extrapolation method has been applied to expand the cruise data to a big scale area to 108 study the carbon cycle in the Southern Ocean (Rangama et al., 2005; Chen et al., 2011; Xu et al., 109 110 2016), <u>Hhowever</u>, thise linear regression relied simply either on either chlorophyll-a (CHL) or on 111 sea surface temperature (SST) parameters. Thus, this method can not sufficiently is insufficient to 112 represent all the controlling factors. In this study, we applied self-organizing map (SOM) 113 analysis to expand our observed data sets and estimated the oceanic pCO_2 in the Prydz Bay from 114 February to early March of 2015.during the February 2015. 115 The SOM analysis, which is a type of artificial neural network, has been proven to be a 116 useful method for extracting and classifying features in the geosciences, such as trends in (and between) input variables(Gibson et al., 2017; Huang et al., 2017b). The SOM analysis, based on 117 neural network (NN), a type of artificial neural network, has been proved to be a useful method 118 119 for extracting and classifying features in geoscience (Gibson et al., 2017; Huang et al., 2017b). The SOM uses an unsupervised learning algorithm (i.e., with no need for a priori, empirical or 120 theoretical descriptions of input-output relationships), thus enabling us to identify the 121

122 relationships between the state variables of the phenomena being analysed, where our 123 understanding of these cannot be fully described using mathematical equations and thus where applications of knowledge-based models are limited (Telszewski et al., 2009). In the field of 124 125 oceanography, SOM has been applied for the analysis of various properties of the seawater, such as sea surface temperature (Iskandar, 2010; Liu et al., 2006), and chlorophyll concentration 126 (Huang et al., 2017a; Silulwane et al., 2001). In the past decade, SOM has also been applied to 127 128 produce basin-scale pCO2 maps, mainly in the North Atlantic and Pacific Ocean, by using different proxy parameters (Lafevre et al., 2005; Friedrich & Oschlies, 2009a, 2009b; Nakaoka et 129 130 al., 2013; Telszewski et al., 2009; Hales et al., 2012; Zeng et al., 2015; Laruelle et al., 2017). 131 SOM has been provend to be useful tofor expanding the-a spatial-temporal coverage of direct measurements or to for estimateing properties whose satellite observations are technically 132 133 limited. One of the main benefits of the neural network method over the more traditional techniques is that it provides more accurate representations of highly variable systems of 134 135 interconnected water properties there is more accurate representation of the highly variable system of interconnected water properties (Nakaoka et al., 2013). 136 We conducted a survey during the 31st CHINARE cruise in the Prydz Bay (Fig. 2). During 137 the 31th CHINARE in Prydz Bay, we have conducted a survey on partial pressure of CO2 in 138 oceanic water and atmosphere from the beginning of February to the early of March (data of the 139 eruise track is shown in Fig. 2). This study is aimed to apply the SOM method, combined with 140 141 remotely sensed data, to reduce the spatiotemporal scarcity of contemporary $\triangle p CO_2 data$ and 142 toobtain a better understanding of the capability of carbon absorption in the Prydz Bay from 143 63°E to 83°E and 64°S to 70°S from February to early March of 2015. to reconstruct the temporal and spatial variability of oceanic pCO2 distribution in Prydz Bay from 63°E to 83°E, 144 145 64°S to 70°S and discuss the capability of carbon absorption in February 2015. The paper is organized as followsed. Section 2 provides the descriptions of the in_-situ 146 147 measurements and-the SOM methods. Section 3 presents the analysis and discussion of the results-, and Ssection 4 presents the a summary of this research. 148 149 2 Data and methods

150 2.1 in situ data

151 The in situ underway pCO_2 values of marine water and the atmosphere wereas collected 152 during the 31^{thst} CHINARE cruise, when the R/V Xuelong sailed from east to west from the

153 beginning of February to early March, 2015 (see Fig.2a, b).at the beginning of February 2015 154 (see Fig.2-a, b). Sea water at a depth of 5 meters underneath beneath the sea surface was pumped 155 continuously to the GO system (GO Flowing pCO_2 system, General Oceanics Inc., Miami FL, 156 USA), and the partial pressure of the sea surface water wais measured by an infrared analyzer (LICOR, USA, Model 7000). The analyzer was calibrated every 2.5-3 h using four standard 157 158 gases supplied by NOAA's Global Monitoring Division at pressures of 88.82 ppm, 188.36 ppm, 399.47 ppm, 528.92 ppm-supplied by NOAA's Global Monitoring Division. The 159 160 accuracy of the measured pCO_2 data is within 2 µatm (Pierrot et al., 2009). The uUnderway 161 atmospheric pCO_2 in atmosphere was were simultaneously collected by the GO system. Due to the biological and physical pumps of carbon cycling in the ocean (Hardman-Mountford et al., 162 2009; Bates et al., 1998a, 1998b; Barbini et al., 2003; Sweeney, 2002), the key factor controlling 163 its gradient in sea-air levels is the solubility of CO₂. The solubility of CO₂ is affected by 164 165 temperature and salinity in the water as well as biological activities, such as phytoplankton taking up CO₂ through photosynthesis and organisms releasing CO₂ through respiration (Chen et 166 al., 2011). There are several processes that can influence the distribution of oceanic pCO2. 167 Sea ice melt has a significant impact on the local stratification and circulation in polar 168 169 regions. During freezing, brine is rejected from ice, thereby increasing the sea surface salinity. When ice begins to melt, fresher water is added into the ocean, thereby diluting the ocean water, 170 171 i.e., reducing its salinity. Changes in salinity thus record physical processes. Salinity records the 172 physical processes. During freezing, salt is excluded from ice, and thus increase the ocean surface salinity. This is so called brine rejection. When ice begins to melt, fresher water is added 173 174 into the ocean to dilute the ocean water, i.e., reducing the salinity. In this study, we treat salinity as an index for the changes of in sea ice. The underway sea surface temperature SST and 175 conductivity data wasere recorded by a Conductivity-Temperature-Depth sensor (CTD, Seabird 176 177 SBE 21) along the cruise track. Later, sea surface salinity was calculated according tobased on the recorded conductivity and temperature data. The distributions of underway SST and SSS 178 arewere shown in Fig.2 c and d. 179 180 In austral summer, when sea ice started to melt, ice algae were released into the seawater, 181 and the amount of living biological species and primary productivity increased; thus, high

- 182 <u>chlorophyll-a values were observed (Liu et al., 2000; Liu et al., 2003). In pPrevious studies it</u>
- 183 hashave been reported that the summer sink in the Prydz Bay is clearly biologically driven and

184	<u>that</u> the <u>change in</u> pCO_2 change is often well-correlated with surface chlorophyll-a concentration
185	(Rubin et al., 1998; Gibsonab et al., 1999; Chen et al., 2011; Xu et al., 2016). When sea ice starts
186	to melt, the active biological process affects oceanic pCO2-significantly (Chen et al., 2011; Xu et
187	al., 2016). The chlorophyll-a value is regarded as an important controlling factor of pCO_2 .
188	Remote sensing data of chlorophyll-a obtained from MODIS with a resolution of 4 km
189	(http://oceancolor.gsfc.nasa.gov) were interpolated according to the cruise track (Fig.2e).Daily
190	Modis chlorophyll-a data of 4 km resolution (<u>http://oceancolor.gsfc.nasa.gov</u>) are interpolated to
191	the observation section and time. The interpolated result along the cruise track is shown in
192	Fig.2e.
193	The ocean mixed layer is characterized as having nearly uniform physical properties
194	throughout the layer, with a gradient in its properties occurring at the bottom of the layer. The
195	mixed layer links the atmosphere to the deep ocean. and plays a critical role in climate
196	variability. Very few Previous studies have emphasized the importance of accounting for the
197	vertical mixing through the mixed layer depth (MLD, Dandonneau, 1995; Lüger et al., 2004).
198	The stability and stratification of this layer prevent the upward mixing of nutrients and limits the
199	biological production, and thus affecting the sea-air CO ₂ exchange. There are two main methods
200	used to calculate the MLD: one is based on the difference criterion, and one is based on the
201	gradient criterion. Early studies suggested that the MLD values determined in the Southern
202	Ocean using the difference criterion are more stable (Brainerd and Gregg, 1995; Thomson and
203	Fine, 2003). The vertical profile of sea water including potential density was measured by a
204	Seabird SBE 11. Comparison of MLD based on the difference and gradient criteria (Brainerd
205	and Gregg, 1995; Thomson and Fine, 2003) suggested that MLD determined using a difference
206	eriterion is more stable in the Southern Ocean. Thus, Ffollowing Dong et al. (2008), we
207	calculated the mixed layer depth (see Fig.2-f) based on the difference criteria, of within which
208	sigma theta changed by 0.03 kg/m ³ . The MLD values at the stations along the cruise were later
209	gridded linearly to match the spatial and temporal-resolution of the-underway measurements. in
210	situ data along the cruise track.





222 2.2 SOM method and input variables

223	We hypothesize that oceanic pCO_2 can be reconstructed through using the SOM based
224	multiple non-linear regressionmethod with four proxy parameters (Eq. 1): sea surface
225	temperature (SST), chlorophyll-a concentration (CHL), the abundance of photo-synthesizing
226	organisms in the surface ocean represented by the chlorophyll-a concentration (CHL), mixed
227	layer depth (MLD), and sea surface salinity (SSS).

228 pCO_2^{sea} =SOM (SST, CHL, MLD, SSS) (1)

229 The SOM is trained using unsupervised learning to project the input space of 230 training samples to a feature space (Kohonen, 1984), which is usually represented by grid points 231 in two-dimension space. Each grid point, which is also called a neuron cell, is associated with a weight vector having the same number of components as the vector of input data (Zeng et al., 232 233 2017). During the SOM analysis, three steps are taken to estimate oceanic pCO_2 fields (see Fig. 234 3). Input variables to estimate pCO2 are prepared in a vector form. The input environmental parameters(in this study, SST, CHL, MLD, and SSS)used to estimate pCO2 are prepared as a 235 236 vector. Here, Tthe SOM analysis was carried out by using the MATLAB SOM tool box 2.0 (Vesanto, 2002). It has been developed by the Laboratory of Computer and Information Science 237 in the Helsinki University of Technology and is available from the following web page: 238

239 http://www.cis.hut.fi/projects/somtoolbox.



121 in obtain weekly CQC maps for Echangy to carly March O (2015 Selematic scheme of the main-three-step 123 involved in the SOM neural network calculations leading to weekly pCQ: maps for February 2015. 124 During the training process, each neuron's weight vectors are represented by theing 125 presented with the input environmental parameters in the SOM training function. Because SOM 126 malysis is known to be a powerful technique with which to estimate pCQ-based on the non- 127 linear relationships of the parameters are sufficiently represented after the training proceedure. 128 relationships of the proxy parameters are sufficiently represented after the training proceedure. 129 observed occanic pCQ: data are not needed in the first step. 120 During the second part of the process, each preconditioned SOM neuron is labelled with an 129 observed pCQ: and nomalized SST. CHL, MLD and SSS data, is presented to the neural 129 network. We used Fueldean distances (i.e., the shortest distances) to select the winner neurons. 129 Refore the training process, the labelled SOM neuron screated by the face on in 120 process and the trained SOM neuron screated by the far process are used to produce the occanic 120 process and the trained SOM neuron screated by the far proxy parameters week 121 process and	241	Fig. 3. Schematic diagram of the main three steps involved in the SOM neural network calculations used	
 involved in the SOM neural network advalations leading to weekly pCO, maps for Fobuary 2015. During the training process, each neuron's weight vectors are repeatedly trained by being presented with the input environmental parameters in the SOM training function. Because SOM analysis is known to be a powerful technique with which to estimate pCO-based on the non: linear relationships of the parameters are sufficiently represented after the training procedure. This process results in the clustering of similar neurons and the self-organization of the map. The observed occanic pCO; data are not needed in the first step. observed pCO; and normalized ST, CHL, MLD and SSS data, is presented to the neural network. We used Fueldean distances (i.e., the shortest distances) to select the winner neurons. After the labelling process, the neurons are represented as five-dimensional vectors. Finally, during the mapping process, the labeled SOM neuron screted by the second process and the trained SOM neurons created by the first process are used to produce the oceanic pCO2value of each winner neuron based on its geographical grid point in the study area. Before the training process, the input training dataset and labelling dataset are nalysed and prospectively normalized, the skwness values of CHL and MLD changed, especially for the training dataset. The N everage represents the percentage of the training data that are labelled. He data N coverage values of the training data sets of the four proxy parameters were logarithmically normalized, the skewness values of CHL and MLD and SSS are 82.1%, SS's and st.1%, respectively, which maybe due to their insufficient spatiotemporal coverage and/or bias between the labelling and training data sets. The Ne overage of the training data sets to resolve the data coverage values of for both the training	242	to obtain weekly pCO2 maps for February to early March of 2015. Schematic scheme of the main three step	
214 During the training process, each neuron's weight vectors are repeatedly trained by being 215 presented with the input environmental parameters in the SOM training function. Because SOM 216 analysis is known to be a powerful technique with which to estimate <i>p</i> (C)-based on the non- 217 linear relationships of the proxy parameters are sufficiently represented after the training procedure. 218 relationships of the proxy parameters are sufficiently represented after the training procedure. 219 This process results in the clustering of similar neurons and the self-organization of the map. The 219 observed oceanic <i>p</i> (C)-data are not needed in the first step. 210 observed <i>p</i> (C)-and normalized SST. CHL, MLD and SSS data, is presented to the neural 216 retwork. We used Euclidean distances (i.e., the shortest distances) to select the winner neurons. 217 process and the training process, the labelled SOM neurons created by the second 218 process is process, the input training dataset and labelling dataset are analysed and 219 Before the training process, the input training dataset and labelling dataset are analysed and 219 prospectively nonnalized to create an even distribution. The statistics and ranges of the values of 220 prospectively nonnalized to create an even distribution. The statistics and ranges of the ralues 1. <t< td=""><td>243</td><td>involved in the SOM neural network calculations leading to weekly pCO2 maps for February 2015.</td><td></td></t<>	243	involved in the SOM neural network calculations leading to weekly pCO2 maps for February 2015.	
245 presented with the input environmental parameters in the SOM training function. Because SOM 266 analysis is known to be a powerful technique with which to estimate pCO-based on the non- 277 linear relationships of the proxy parameters are sufficiently represented after the training procedure. 278 This precess results in the clustering of similar neurons and the self-organization of the map. The 279 observed oceanic pCO-ydata are not needed in the first step. 281 During the second part of the process, each preconditioned SOM neuron is labelled with an 276 observed pCO ₂ and normalized SST. CHL. MLD and SSS data, is presented to the neural 276 beserved pCO ₂ and normalized SST. CHL. MLD and SSS data, is presented to the neural 276 relationships of the propess, the labelled SOM neurons created by the second 277 process and the training process, the labelled SOM neurons created by the second 278 process and the input of propess, the input training dataset and labelling dataset analysed and 279 Before the training process, the input training datasets of the four proxy parameters were 281 logarithmically normalized to create an even distribution. The statisfies and ranges of the values of 274 The data X coverage values of the training data sets of CHL and MLD changed, especially for the 275 t	244	During the training process, each neuron's weight vectors are repeatedly trained by being	
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247 linear relationships of the parameters (Telszewski et al., 2009), we assumed that the non-linear 248 relationships of the proxy parameters are sufficiently represented affer the training procedure, 249 This process results in the clustering of similar neurons and the self-organization of the map. The 250 observed oceanic pCO: data are not needed in the first step. 251 During the second part of the process, each proceeditioned SOM neuron is labelled with an 252 observed pCO: and normalized SST, CHL, MLD and SSS data, is presented to the neural 254 network. We used Euclidean distances (i.e., the shortest distances) to select the winner neurons. 255 After the labelling process, the neurons are represented as five-dimensional vectors, 256 Finally, during the mapping process, the labelled SOM neurons created by the second 257 prospectively normalized to create an even distribution. The statistics and ranges of the values of 261 parsheiter greened in Table I. When the datasets of the four proxy parameters were 252 logarithmically normalized, the skewness values of CHL and MLD changed, especially for the 253 Before the training data sets of CHL, MLD and SSS are 82,1%, 85% and 254 thatase. The N coverage represents the percentage of the training data sets changed 255 bestween the labelling and tr	246	analysis is known to be a powerful technique with which to estimate pCO ₂ based on the non-	
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250 observed oceanic pCO; data are not needed in the first step. 251 During the second part of the process, each preconditioned SOM neuron is labelled with an 252 observation dataset of in situ oceanic pCO; values. The labelling dataset, which consists of the 253 observed pCO; and normalized SST, CHL, MLD and SSS data, is presented to the neural 254 network. We used Euclidean distances (i.e., the shortest distances) to select the winner neurons. 255 After the labelling process, the labelled SOM neurons created by the second 256 Finally, during the mapping process, the labelled SOM neurons created by the second 257 process and the trained SOM neurons created by the first process are used to produce the oceanic 260 prospectively normalized to create an even distribution. The statistics and ranges of the values of 261 all variables are presented in Table 1. When the datasets of the four proxy parameters were 262 logarithmically normalized, the skewness values of CHL, and MLD changed, especially for the 263 between the labelling and training data sets of CHL, MLD and SSS are 82.1%, 85% and 264 The data N coverage values of the training data sets of CHL, MLD and SSS are 82.1%, 85% and 265 between the labelling and training data sets. The N coverage of the logarithmic datasets horesolve the data 266 <t< td=""><td>249</td><td>This process results in the clustering of similar neurons and the self-organization of the map. The</td><td></td></t<>	249	This process results in the clustering of similar neurons and the self-organization of the map. The	
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 267 <u>to 93.6% and to 98.7% for CHL and MLD, respectively. Thus, the common logarithms of the</u> 268 <u>CHL and MLD values are used for both the training and labelling datasets to resolve the data</u> 269 <u>coverage issue arising from significantly increasing the data coverage as well as to overcome the</u> 270 <u>weighting issue arising from the different magnitudes between variables (Ultsch and Röske,</u> 271 <u>2002).</u> <u>##axin: #ja(#ja)</u> 	266	between the labelling and training data sets. The N coverage of the logarithmic datasets changed	
268 CHL and MLD values are used for both the training and labelling datasets to resolve the data 269 coverage issue arising from significantly increasing the data coverage as well as to overcome the 270 weighting issue arising from the different magnitudes between variables (Ultsch and Röske, 271 2002). 272 *###式的: 英语(英国)	267	to 93.6% and to 98.7% for CHL and MLD, respectively. Thus, the common logarithms of the	
269 coverage issue arising from significantly increasing the data coverage as well as to overcome the 270 weighting issue arising from the different magnitudes between variables (Ultsch and Röske, 271 2002). 272 *###式的: 英语(英国)	268	CHL and MLD values are used for both the training and labelling datasets to resolve the data	
 270 weighting issue arising from the different magnitudes between variables (Ultsch and Röske, 271 2002). 272 本格式的: 英语(英国) 	269	coverage issue arising from significantly increasing the data coverage as well as to overcome the	
271 2002). 272 #格式的: 英语(英国)	270	weighting issue arising from the different magnitudes between variables (Ultsch and Röske,	
272 带格式的: 英语(英国)	271	2002).	
	272	带格式的: 英语(英国)	

273 More realistic pCO2 estimates were expected from the SOM analysis when the distribution 274 and variation range of the labeling variables closely reflect the training data sets (Nakaoka et al., 275 2013) while our underway measurements with pCO2 value have a spatiotemporal limitation to cover the range of the variation of training data sets. Before the training process, the input 276 277 training dataset and labeling dataset are analyzed and prospectively normalized to make an even distribution. The statistics and range of the values of each variable are presented in Table1. 278 279 When the dataset of four proxy parameters were logarithmically normalized the skewness of CHL and MLD changed obviously especially for the training dataset. The N coverage represents 280 281 the percentage of the training data that are labeled. The data N coverage of training data set of 282 CHL, MLD and SSS are 82.1%, 85% and 81.1% respectively, which might be due to the insufficient spatiotemporal coverage and or bias between the labeling and training data sets. The 283 284 N coverage of the logarithmically datasets changed to 93.6% and to 98.7% respectively for CHL 285 and MLD. Thus the common logarithm of CHL and MLD values are used for both the training 286 and labeling datasets in order to resolve the data coverage issue from significantly increasing the 287 data coverage as well as to overcome the weighting issue raised from the different magnitude

288 among the variables (Ultsch and Röske, 2002).

Table 1. Statistics of labeling and training data sets showing the distribution and coverage of

290 each variable.

Coverage o	f each variable	SST(C)	CHL(mg/m ³)	MLD(m)	SSS(psu)
Labeling	Max	0.81	11.13	40.69	33.81
	Min	-1.44	0.17	7.84	32.43
	Mean	-0.27	3.80	14.41	33.27
	Skewness	0.4(-0.2)#	0.8(-0.3)	0.9(0.4)	0.6(0.6)
Training	Max	2.48	40.17	48.95	34.17
	Min	-1.8	0.06	10.46	28.64
	Mean	-0.53	1.36	14.79	33.16
	Skewness	0.5(-0.6)	4.3(0.5)	2.6(0.8)	-0.9(-1.0)
	N coverage* (%)	91.3(92.5)+	82.1(93.6)	85.0(98.7)	81.1(80.4)

291 # the skewness of common logarithm of each variable is shown in the parenthesis.

292 * [number of training data within the labeling data range]/[total number of training data]

+ the percent labeling data coverage of normalized variables is shown in the parenthesis

294

295	During the training process, a neuron's weight vectors are repeatedly trained by being
296	presented with the input vectors, until the neural network sufficiently represents the nonlinear
297	interdependence of proxy parameters used in training. This process results in clustering of
298	similar neurons and self-organization of the map. The observed oceanic pCO2 is not needed at
299	the first step.
300	During the second process, each preconditioned SOM neurons is labeled with an observed
301	oceanic pCO2 value. The labeling dataset consisting of the observed pCO2 and the normalized
302	SST, CHL, MLD and SSS is presented to the neural network and then a winner neuron is found.
303	After the labeling process, neurons are represented by five-dimensional vectors.
304	Finally, during the mapping process, the labeled SOM neurons created by the second process
305	and trained SOM neurons created by the first process are used to produce oceanic pCO2 of the
306	winner neuron according to the geographical grid points of the study area.
307	In this study, we construct weekly oceanic pCO_2 maps from February to early March of
308	2015 using four datasets, i.e., SST, CHL, MLD, and SSS.We used four datasets including SST,
309	CHL, MLD, and SSS (SCMS) to train the SOM. Considering the size of our study region, we
310	chose a spatial resolution of 0.1° latitude by 0.1° longitude. For SST, we used daily data from
311	AVHRR ONLY (https://www.ncdc.noaa.gov/oisst) with a of 1/4° spatial resolution (see Fig.S1).
312	CHL data represent are the 8-D composite chlorophyll-a data from MODIS-Aqua
313	(http://oceancolor.gsfc.nasa.gov) at with a space resolution of 4km (see Fig.S2). We also used
314	the daily SSS and MLD data (see Fig.S3-4) from the 1/12° global analysis and forecast product
315	from the Copernicus Marine Environment Monitoring Service (CMEMS,
316	http://marine.copernicus.eu/). Sea ice concentration data areis from the daily 3.125-km AMSR2
317	dataset (Spreen et al., 2008, available on https://seaice.uni-bremen.de, see Fig.S5).
318	All the daily datasets were first averaged to be 8-d fields, which are -regarded as weekly
319	forin this study. The period from the beginning of February to early March comprises From the
320	beginning of February to the early of March we have four independent week series, which are
321	week-1 (from 02/02/2015 to 02/09/2015), week-2 (from 02/10/2015 to 02/17/2015), week-3
322	(from 02/18/2015 to 02/25/2015), and week-4 (from 02/26/2015 to 03/05/2015). The weekly
323	proxy parameters (SCMS) were further re-gridded with to a horizontal resolution of $0.1^{\circ} \cdot 0.1^{\circ}$
324	using the Kriging method. In the SOM analyses, input vectors with missing elements are
1	

325 excluded. Consequently, oceanic pCO2 created in this study has weekly frequency and 0.1 longitude - 0.1 latitude resolution from 63°E to 83°E and 64°S to 70°S. 326 327 We compared the assimilated datasets of SST from AVHRR with the in situ measurements obtained by CTD along the cruise. Their relationship is 0.97, and their root-mean-square error 328 (RMSE) is 0.2°C. Comparing tThe SSS and MLD fields from the Global Forecast system 329 330 eompare reasonably well with the in situ measurements, with relationshipsyields correlations of 0.76 and 0.74, respectively and the RMSEs of 0.41 and 5.15m, respectively. The uncertainty of 331 332 the MODISodis CHL data in the Southern Ocean is approximatelyabout 35% (Xu et al., 2016). 333 For the labelling procedure, the observed oceanic pCO_2 together with the corresponding in situ SST, SSS, MLD, and Modis-MODIS CHL products in vector form are used as the input dataset. 334 335 2.3 Validation of SOM derived SOM-derived oceanic pCO2 336 More realistic pCO₂ estimates are expected from SOM analyses when the distribution and 337 variation ranges of the labelling variables closely reflect those of the training data sets (Nakaoka et al., 2013). However, our underway measurements ofpCO2values have spatiotemporal 338 339 limitations preventing them from covering the range of variation of the training data sets. To validate the oceanic pCO_2 values reconstructed by the SOM analysis, we used the fugacity of 340 oceanic CO2 datasets from the Surface Ocean CO2 Atlas (hereafter referred to as "SOCAT" 341 data,http://www.socat.info) version 5 database (Bakker et al., 2016).We selected the dataset from 342 343 SOCAT (the EXPOCODE is 09AR20150128, see cruise in Fig. 4a) that coincided with the same 344 period as our study. The cruise lasted from Feb. 6 to Feb. 27, 2015, and fCO₂ measurements were made every 1 min at a resolution of 0.01°. We recalculated pCO2 values based on the obtained 345 346 fCO2values provided by the SOCAT data using the fugacity correction (Pfeil et al., 2013). To 347 validate the oceanic pCO₂-reconstructed by the SOM analysis, we used the fugacity of oceanic CO2-datasets (referred as "SOCAT" data hereinafter) from the Surface Ocean CO2 Atlas 348 349 (SOCAT: http://www.socat.info) version 5 database (Bakker et al., 2016). In Pacific Ocean, the 350 Atlantic Ocean or regions away from coast, datasets from different years can be assimilated to a 351 reference year to have a good spatial coverage according to the equilibrium between sea surface 352 and atmosphere (Takahashi et al., 2006; Wong et al., 2010; Nakaoka et al., 2013). However, the 353 same approach should be applied carefully because the sea ice condition varies from year to year 354 in the Southern Ocean. The sea ice cover has a great impact on the oceanic pCO2. SOCAT data in February from different years do have a good spatial coverage in Prydz Bay. However we 355

356	could only select dataset for our study period in 2015 (see Fig. 4-a) although it covers limited
357	area in study region. We recalculated pCO2-values from the obtained fCO2 offered in SOCAT
358	data according to the fugacity correction (Pfeil et al., 2013).
359	-2.4 Carbon uptake in the Prydz Bay
360	—The flux of CO ₂ between the atmosphere and the ocean was determined <u>using ΔpCO₂ and</u>
361	the transfer velocity across the sea-air interface, as shown in Eq. 2, where K is the gas transfer
362	velocity (in cm h ⁻¹), and the quadratic relationship betweenwind speed (in units of m s ⁻¹) and the
363	Schmidt number is expressed as $(Sc/660)^{-0.5}$, by two items. L is the solubility of CO ₂ in seawater
364	(in mol litre ⁻¹ atm ⁻¹) (Weiss, 1974). For the weekly estimation in this study, the scaling factor for
365	the gas transfer rate is changed to 0.251 for shorter time scales and intermediate wind speed
366	ranges (Wanninkhof, 2014). Considering the unit conversion factor (Takahashi et al., 2009), the
367	weekly sea-air carbon flux in the Prydz Bay can be estimated using Eq. (3): One is the difference
368	in CO2-concentration across the sea-air interface and the other is the transfer velocity which is a
369	function primarily of wind speed and temperature. The equation to calculate the sea air carbon
370	flux was simplified as a function of wind speed and delta pCO2 (from sea to air) in eq. 2, Xu et
371	al. (2016). For the weekly estimation in this study, the scaling factor for the gas transfer rate is
372	changed to 0.251 for a shorter time scale and at intermediate wind speed ranges (Wanninkhof,
373	2014). For each grid, weekly sea air carbon flux in the Prydz Bay can be estimated by Eq. (2):
374	$\underline{Flux_{sea-air}} = K \times L \times \Delta pCO_2 (2)$
375	$\underline{Flux}_{\text{sea-air}}[g \text{ C/(m^2 \cdot \text{week})}] = 30.8 \times 10^{-4} \times \text{U}^2 \times (\rho \text{CO}_2^{\text{sea}} - \rho \text{CO}_2^{\text{air}}) $ (3)
376	where U represents the wind speed 10 m above sea level, and pCO_2^{sea} and pCO_2^{air} are the partial
377	pressures of CO_2 in sea water and the atmosphere, respectively.
378	$Fhux_{\text{sea-air}}(g \text{ C/(m^2-week))}=30.8\times10^{-4}\times \text{U}^2\times(\rho \text{CO}_2^{\text{sea}}-\rho \text{CO}_2^{\text{air}})$ (2)
379	where U represents wind speed 10 m above sea level, pCO2_sea and pCO2_air are partial
380	pressure of CO ₂ in sea water and atmosphere.
381	We downloaded weekly ASCAT wind speed data (http://www.remss.com/, see Fig. S6)
382	with a of $1/4^{\circ}_{\circ}$ degree and then regridded the dataset to fit the 0.1° longitude \cdot 0.1° latitude spatial
383	resolution of <u>the SOM</u> -derived oceanic pCO_2 . We regridded the atmospheric pCO_2 collected
384	along the cruise track to fit the spatial resolution of the SOM-derived oceanic pCO_2 data using a
385	by linear method. The total carbon uptake was then obtained by accumulating the flux of each
386	grid by-in each area according to Jiang et al. (2008) and using the proportion of ice-free areas

387	(Takahashi et al., 2012). When the ice concentration is less than 10% in a grid, we regard the
388	grid box ascomprising all water. When the ice concentration fallsbetween 10% and 90%, the flux
389	is computed as being proportional to the water area. In the cases of leads or polynyas due to the
390	dynamic motion of sea ice (Worby et al., 2008), we assume the grid box to be 10% open water
391	when the satellite sea ice cover is greater than 90%. with the proportion of ice-free area (Xu et al.,
392	2016).
393	

394 **3 Results and discussion**

395 3.1 the distributions of underway measurements

396 During austral summer, daylight lasts longer and solar radiation increases. With increasing sea surface temperature, ice shelves break and sea ice melts, resulting in the stratification of the 397 398 water column.From Starting in the beginning of February, R/V Xuelong sailed from east to west along the sea ice edge, and its underway measurements are shown in Fig.2. Based on the water 399 400 depth and especially the different ranges of oceanic pCO₂ (see Fig.2a and Table2), Based on the water depth and the sea ice condition, the study area can be roughly divided into three regions, 401 namely, the Open-ocean region, Sea-ice region and Shelf region (see Table2).the study area is 402 robustly divided into three regions, the Open ocean region, Sea ice region and the Shelf region. 403 The Open-ocean region ranges northward from 66°S to 64°S, where was from 66°S 404 northward to 64°S where locates the Antarctic Divergence Zone is located and with water depths 405 406 are greater than 3000 m. In the Open-ocean region, the oceanic pCO₂was the highest, varying 407 from 291.98 µatm to 379.31 µatm, with a regional mean value of 341.48 µatm. The Antarctic Divergence Zone AD zone was characterized by high nutrients and low chlorophyll (HNLC) 408 concentrations, with high pCO_2 attributed to the upwelling of deep waters, thus suggesting the 409 importance of physical processes in this area (Burkill et al., 1995; Edwards et al., 2004). UThe 410 underway sea surface temperature in this region are relatively high, with an average value of -411 412 0.23°C0.36°C due to the upwelling Circumpolar Deep Water (CDW), while inat the sea ice edge (73°E, 65.5°S to 72°E, 65.8°S), the SST decreased below-to less than -1°C. From 67.5°E 413 westward, affected by the large gyre, cold water from the high latitude lowered down the SST to 414 415 below-less than 0°C. Near the sea ice edge, SSS decreased quickly to 31.7 psu due to the diluted water-: while along the 65°S cruise, it reached to 33.3 psu; and then, moving westwardern from 416 67.5°E_a affected by the fresher and colder water brought by the large gyre_a it decreased to 32.5 417

418 psu. The satellite chlorophyll-a image showed that the regional mean was as low asit was of low 419 value of 0.45 mg/m³, except when the vessel near the sea ice edge recorded CHL values that 420 increased to be 2.26 mg/m³. The lowest pCO₂value was found near the sea ice edge due to 421 biological uptake. The distribution of MLD varied along the cruise. Near the sea ice edge, 422 because of the melting of ice and direct solar warming, it constituted a low-density cap existed over the water column, and the MLD was as shallow as 10.21 m. The maximum value of MLD 423 424 in the Open-ocean region wasis 31.67 m. In the Open-ocean region, atmospheric pCO_2 was varied 425 stable from 374.6 µatm to 387.8 µatm. Oceanic pCO2 varied from 291.98 µatm to 379.31 µatm 426 with an average value of 341.48 µatm. Along the 65°E cruise in the east part of the Open-ocean 427 region, the oceanic pCO_2 was relatively high, reaching an equilibrium with atmospheric pCO_2 . The lowest value was found near the sea ice edge due to biological consume. For In the western 428 429 part of this region, the oceanic pCO2 decreased a littleslightly due to the mixture of low pCO2 430 from higher latitudes brought by the large gyre. Mixing and upwelling were the dominant factors 431 for <u>affecting the</u> oceanic pCO_2 in this region. 432 The seasonal Sea-ice region (from 66°S to 67.25°S) is located between the Open-ocean 433 region and the Shelf region. In this sector, sea ice changed strongly, and the water depth varied 434 sharply from 700 m to 2000 m. The oceanic pCO2values ranged from 190.46 µatm to 364.43 435 µatm, with a regional mean value of 276.48 µatm. Sea ice continued to change and reform from late February to the beginning of March (Fig. 6). Sea ice kept changing and reforming from the 436 437 late of February to the beginning of March. The regional mean seaSea surface temperature 438 decreased slightly compared to that in the Open-ocean region, and the average value was -0.72°C. With the rapid changes in sea ice-changing, the sea surface temperature and salinity 439

varied sharply from -1.3°C to 0.5°C and from 31.8 <u>psu</u> to 33.3 <u>psu</u>, respectively. When sea ice melted, <u>the</u> water temperature increased, biological <u>activity increased</u>, <u>activities became active</u> and chlorophyll-a value increased <u>slightly to reach a regionalby a small amount to an</u> average of 0.549 mg/m³. Due to the rapid change <u>inof</u> sea ice cover, the value of MLD varied from 12.8 m to 30.9 m. The average value of oceanic pCO_2 was 276.48 µatm ranging from 190.46 µatm to 364.43 µatm.

The Shelf region (from 67.25°S southward) is characterized by shallow depths of less thanof
low depth below 700m, and it is surroundedsurrounding by the Amery Ice Shelf, and the West
Ice Shelf. Water inside the Shelf region is formed by the , and the stretching permanent sea ice

from the West Ice Shelf, formed by modification of low-low-temperature and high-salinity shelf
water (Smith et al., 1984). Two shallow banks (<200m): Fram Bank to the north-west and Four
Ladies Bank to the north east, forming a spatial barrier for the inner shelf to water exchange with
the outer oceanic water (Smith and Tréguer, 1994) The Prydz Bay coastal current flowsed from
east to west in the semi-close bay. The oceanic pCO ₂ values in this region were the lowest of
those in all three sectors; these values ranged from 151.70 µatm to 277.78 µatm, with a regional
<u>average of 198.72 µatm. There is always aA</u> fresher, warmer surface layer is always present over
the bay, which is known as the Antarctic Surface Water (ASW). During our study period, the
Shelf region was the least ice-covered region completely ice free, aA large volume of freshwater
was released into the bay, resulting in low sea surface temperature (an average of -0.61°C) and
salinity (an average is 32.4 psu). As shown in Fig.2-f, the mixed layer depth in most of the inner
shelf is low-in most of the inner shelf. Due to the vast shrink of sea ice and strong stratification
in the upper water, algal blooming occurreded and chlorophyll values wereas high, with an
average of 1.93 mg/m ³ . The oceanic pCO_2 in this region turned out to be the lowest in three
sectors. The average of oceanic <i>p</i> CO ₂ is 198.72 µatm with a range from 151.70 µatm to 277.78
µatm. The chlorophyll-a value was remarkably high, reaching11.04 mg/m ³ when sea ice retreated
eastwardly from 72.3°E, 67.3°S to 72.7°E, 68°S. Chlorophyll-a value shows remarkably as high
as 11.04 mg/m ³ from 72.3°E, 67.3°S to 72.7°E, 68°S when sea ice retreated eastwardly. The
biological pump became the dominant factor controlling the distribution of oceanic p CO ₂ . In the
bay mouth close to the Fram Bank, due to local upwelling, the water salinity increased
remarkably toapproximately33.2 psu.In the bay mouth close to the Fram Bank, due to the local
upwelling water salinity increased remarkably to around 33.2. Biological pump becomes the
dominant factor of the distribution of oceanic pCO2-
Table 2 The regional mean values of underway measurements in three sub-regions

	<u><i>p</i>CO₂ [µatm]</u>	<u>SST [°]</u>	CHL [mg/m ³]	MLD [m]	SSS [psu]
<u>Open-ocean region</u> (66°S - 64°S)	<u>341.48</u>	<u>-0.23</u>	0.45	<u>20.13</u>	<u>32.61</u>
<u>Sea-ice region</u> (66°S - 67.25°S)	276.48	<u>-0.72</u>	0.59	<u>19.44</u>	<u>32.42</u>
<u>Shelf region</u> (67.25°S - 70°S)	<u>198.72</u>	<u>-0.61</u>	<u>1.95</u>	<u>16.84</u>	<u>32.46</u>

475	
476	3.2 Quality and maps of SOM derived SOM-derived oceanic <i>p</i> CO ₂
477	We selected SOM derived SOM-derived oceanic pCO_2 values to fit the cruise track of
478	SOCAT for athe same period in February 2015 using a nearest grid method. The slope of the
479	seatter plot showed that SOM derived oceanic pCO2 is lower than the SOCAT data (see Fig. 4-
480	b). The RMSE between the SOCAT data and the SOM derived SOM-derived result wais
481	calculated as follows:
482	$RMSE = \sqrt{\frac{\sum \left(pco_2^{sea}(SOM) - pco_2^{sea}(SOCAT)\right)^2}{n}} $ (43)
483	where n is the number of the validation datasets. The RMSE $canould$ be used-interpreted as an
484	estimation of the uncertainty in <u>the SOM derived SOM-derived</u> oceanic pCO_2 in <u>the</u> Prydz Bay. In
485	this study, the RMSE of the SOM-derived oceanic pCO_2 and SOCAT datasets is 22.14 μ atm, and
486	the correlation coefficient R ² is 0.82. The absolute mean difference is 23.58 µatm. The RMSE
487	obtained in our study This is consistent with the accuraciesy (6.9 µatm to 24.9 µatm) obtained
488	achieved in previous studies that used neuron methods to reconstruct oceanic pCO ₂ using neuron
489	methods to reconstruct oceanic <i>p</i> CO ₂ (Nakaoka et al., 2013, Zeng et al., 2002; Sarma et al., 2006;
490	Jo Y H et al., 2012; Hales et al., 2012; Telszewshi M., et al., 2009). However, this The precision
491	of this study is on the high side of those that have been previously reported not as good as most of
492	the neuron methods. The slope of the scatter plot indicates that the SOM-derived oceanic
493	pCO2data are lower than the SOCAT data (see Fig. 4b). Thus, the precision of these data may
494	have greater uncertainty because the SOCAT dataset does not cover the low-pCO2 area towards
495	the south. Thus, Increasing the spatial coverage of the labelling data will help to increase the
496	precision of SOM derived the SOM-derived oceanic <i>p</i> CO ₂ .





500	Fig. 4 a) the cruise lines from SOCAT used to validate the SOM-derived oceanic pCO_2 for the study period in
501	2015; b) comparison between the SOM-derived and observed SOCAT oceanic pCO2dataa)The cruise lines
502	from SOCAT to validate the SOM derived oceanic pCO2 for the study period in 2015; b) Comparison between
503	the SOM derived and observed SOCAT oceanic pCO2,
504	
505	3.3 Spatial and temporal distributions of SOM derivedSOM-derived oceanic pCO2
506	The weekly mean maps of SOM-derived oceanic pCO2 in the Prydz Bay are shown in Fig. 5.
507	In the Open-ocean region, the oceanic pCO_2 values were higher than those in the other two
508	regions due to the upwelling of the CDW. During all four weeks, this region was nearly ice-free,
509	while the average sea ice coverage was 18.14% due to the presence of permanent sea ice (see
510	Fig.6). The oceanicpCO ₂ distribution decreased from east to west in the Open-ocean region, with
511	lower values observed at the edge of sea ice. In the western part of the Open-ocean region,
512	oceanic pCO ₂ decreased due to mixing with low oceanic pCO ₂ flowing from high-latitude
513	regions caused by the large gyre. From week-1 to week-4, the maximum oceanic pCO2 increased
514	slightly and reached 381.42 μ atm, which was equivalent to the pCO ₂ value of the atmosphere.
515	In the Sea-ice region, sea ice continued to rapidly melt and reform. The weekly mean sea ice
516	coverage percentage was 29.54%, occupying nearly one-third of the Sea-ice region. As shown in
517	Fig.5, the gradient of the oceanic pCO_2 distribution increased from south to north affected by the
518	flow coming from the Shelf region by the large gyre. In the eastern part of this region, adjacent
519	to the sea ice edge, the oceanic pCO_2 values were lower. The oceanic pCO_2 changed sharply from
520	155.86 µatm (near the sea ice edge) to 365.11 µatm (close to the Open-ocean region).
521	In austral winter, the entire Prydz Bay basin is fully covered by sea ice, except in a few
522	areas, i.e., the polynyas, which remain open due to katabatic winds (Liu et al., 2017). When the
523	austral summer starts, due to coincident high wind speeds, monthly peak tides, and/or the effect
524	of penetrating ocean swells, the sea ice in the Shelf region starts to melt first in early summer
525	(Lei et al., 2010), forming the Prydz Bay Polynya. The semi-closed polynya functions as a
526	barrier for water exchange in the Shelf region and causes a lack of significant bottom water
527	production, hindering the outflow of continental shelf water and the inflow of Antarctic circle
528	deep water, resulting in the longer residence time of vast melting water and enhanced
529	stratification (Sun et al., 2013).Due to vast melting of the sea ice, the sea surface salinity
530	decreased and algae bloomed; biological productivity promptly increased, and the chlorophyll-a

531	concentration reached itspeak value. As shown in Fig. 5, the distribution of oceanic pCO_2 in the
532	Shelf region was characterized by its lowest values. The obvious drawdown of oceanic
533	pCO20ccurred in the Shelf region due to phytoplankton photosynthesis during this summer
534	bloom. The lowest oceanic pCO_2 in the Shelf region was 153.83 µatm, except at the edge of the
535	West Ice Shelf, where the Shelf oceanic pCO_2 exceeded 300 µatm. The oceanic pCO_2 was the
536	lowest in week-1, which coincided with a peak in chlorophyll-a, as evidenced by satellite
537	images. The regional oceanic pCO ₂ increased slightly in week-4 compared to the other three
538	weeks
539	In austral winter, the entire Prydz Bay basin is fully covered by sea ice except for a few
540	areas, the polynyas, remaining open due to katabatic winds (Liu et al., 2017). As the austral
541	summer starts, with the increasing sunlight, sea surface temperature increased, ice shelf broke
542	and drifted out. Due to coincident high wind speeds, monthly peak tides, and/or the effect of
543	penetrating ocean swell, sea ice in the Shelf region started to melt in early summer (Lei et al.,
544	2010), forming Prydz Bay Polynya. The AMSR2 sea ice extent and mean ice concentration in
545	each region are shown in Fig. 5, respectively. The Shelf region has the least sea ice extent
546	(1.38x10 ⁴ km ²) and concentration (13.54%), without significant temporal variation. The semi-
547	close polynya functions as a barrier for water exchange in the Shelf region and lack of significant
548	bottom-water production, hindering outflow of continental shelf water and inflow of Antarctica
549	eirele deep water, resulting in a longer residence time for the vast melting water and enhanced
550	stratification (Sun et al., 2013). Due to vast sea ice melting, sea surface salinity decreased, algae
551	bloomed, the biological productivity increase promptly, the value of chlorophyll-a concentration
552	reached the peak, the Shelf region became a strong CO2 sink. As shown in Fig. 6, an obvious
553	drawdown of oceanic pCO2 in Shelf region due to phytoplankton photosynthesis during the
554	summer bloom. The lowest oceanic pCO_2 in the Shelf region was 153.83 µatm except in the edge
555	of West Ice Shelf oceanic pCO2 reached over 300 µatm. The oceanic pCO2-was the lowest in
556	week-1 (from 02/02/2015 to 02/09/2015) which is coincident with a peak/bloom in the

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chlorophyll a evidenced by the satellite images.

Fig.5 Distribution of weekly mean SOM-derived oceanic pCO2 in the Prydz Bay (unit: µatm) from Feb. 2, 2015 to Mar. 5, 2015. The black contour represents a sea ice concentration of 15%.



Fig. 6 Percentage ofsea ice coverage in three sub-regions from Feb. 2, 2015 to Mar. 5, 2015 (blue: Open-

ocean region; red: Sea-ice region; green: Shelf region).





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570 As shown in Fig.5-a, Sea ice in Open-ocean region and Sea-ice region started to melt from 571 Jan 13, 2015, during February it decreased to the lowest and then it began to reform from Mar.3, 2015. The average sea ice extent in Open-ocean region and Sea-ice region were 3.85-104 km² 572 and 3.56-104 km². During our study period, in the Sea-ice region, sea ice kept melting and 573 reforming rapidly and the average value of sea ice coverage percent is 29.54%. Oceanic pCO2 574 changed sharply from 155.86 µatm to 365.11 µatm. 575 576 In the Open-ocean region, sea ice started to melt in the beginning of February. In most area of the Open-ocean region it was sea ice free while the average sea ice coverage is only 18.14%. 577

Fig. 5 a) Sea ice extent (unit: 10⁴ km²) in study area (gray line) and three sub-regions (blue: Open ocean region; red: Sea-ice region; green: Shelf region); b) Averaged ice concentration in three sub regions
 from Feb. 2, 2015 to Mar. 5, 2015.

578	The ice cover is mainly associated with the outstretching permanent sea ice. Affected by the
579	upwelling CDW, the stability of water was weak and not suitable for the growth of
580	phytoplankton. It is also evidence by, the observed biological productivity, which was below 0.5
581	mg/m ³ . From the distribution of SOM derived oceanic pCO ₂ as shown in Fig. 6, oceanic pCO ₂
582	value was the highest compared to the Sea-ice region and the Shelf region. From week-1 to
583	week-4, oceanic pCO2 increased a little and reached 381.42 µatm which was equivalent to that of
584	atmosphere. In the western part of Open-ocean region, oceanic pCO2-decreased due to mixing
585	with low oceanic <i>p</i> CO ₂ flew from the high latitude by the large gyre.
586	
587	Fig. 6 Weekly SOM derived SOM derived Prydz Bay pCO ₂ (unit: µatm) distribution in February 2015,
588	the black contour representing sea ice concentration of 15%.
589	3.4 Carbon uptake in <u>the</u> Prydz Bay
590	During our Over the whole study period, the entire region was undersaturated, with CO2
591	being absorbed by the ocean. The regional the averaged ocean-air pCO_2 difference ($\triangle pCO_2$)
592	wais highlargest in the Shelf region, then follows followed by the Sea-ice region and Open-ocean
593	region (see Table3). The regional and weekly mean $\triangle pCO_2$ from in the Shelf region changed
594	from -184.31µatm in week-1 to -141.00 µatm in week-2to -141.00 µatm as the chlorophyll
595	decreased. <u>The ΔpCO_2 The sea-air difference of pCO_2</u> in the Sea-ice region and Open-ocean
596	region showed the same patterns-, It-increasinged from week-1 to week-3 then decreasinged in
597	week_4. Based on the $\triangle pCO_2$ and wind speed <u>data</u> , the uptake of CO_2 in these three regions is
598	presented in Table3.(eq. 2) in three regions is presented in Fig. 7. The uncertainty of the carbon
599	uptake depends on the errors associated with the wind speed, the scaling factor and the accuracy
600	of the SOM-derived pCO ₂ according to Eq.3. The scaling factor will yield a 20% uncertainty in
601	the regional flux estimation. The errors in the wind speeds of the ASCAT dataset ar eassumed to
602	be 6% (Xu et al., 2016); the error in the quadratic wind speed is 12%. The RMSE of the SOM-
603	derived pCO ₂ is 22.14 µatm. Considering the errors described above and the uncertainty
604	occurring when the sea-air computation expression is simplified (1.39%, Xu et al., 2016), the
605	total uncertainty of the final uptake is 27%. In the Shelf region, the low oceanic pCO_2 levels
606	drove relatively intensive CO ₂ uptake from the atmosphere. <u>The C</u> arbon uptake in <u>the Shelf</u>
607	region changed mildly from week-1 (2.51±0.68 TgC, 10 ¹² gram=Tg) to week-2

608 (2.77±0.75 TgC).increased from week-1 (2.13 TgC) to week-2 (2.24 TgC) due to increased wind

- 609 speed. In contrast, in week-3 While in week-3, wind speed slowed down, resulting in the uptake
- 610 of CO₂ in Shelf region decreasinged to 2.10 ± 0.57 TgC1.70 TgC. In week-4, even though the
- 611 $\triangle pCO_2$ was the lowest of all four weeks, the total absorption still increased to be
- 612 <u>2.63±0.7152.03</u> TgC due to the high wind speed (averaged value of 7.9 m/s). The total carbon
- 613 uptake in the three regions of the Prydz Bay, integrated from February to early March of2015,
- 614 was 23.57 TgC, with an uncertainty of ± 6.36 TgC.
- 615 Table3 Regional and weekly mean ΔpCO_2 , wind speed and uptake of CO_2 in three sub-
- 616 regions (negative values represent directions moving from air to sea).



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Fig. 7 Timeseries of weekly averaged $\triangle p CO_2$, wind speed and uptake of atmospheric CO₂ in Open-ocean region (blue line, the negative value means the direction from sea to air), Sea-ice region (red line) and Shelf region (yellow line).

Studies have reported that Prydz Bay is a strong carbon sink in the austral summer. Roden et 625 626 al. (2013) estimated the coastal Prydz Bay to be an annual net sink for CO₂ of 0.54±0.11 mol/(m²·year), i.e., 1.48±0.3 g/(m²·week). Gibsonab et al. (1999) estimated the averaged sea-air 627 flux in the summer ice-free period sea-air flux-to be more than 30 mmol/(m²·day), i.e., 9.2 628 g/(m²·week). Our study suggests that the sea-air flux during the strongest period in of athe year, 629 i.e., February, could be much larger. The average flux obtained here, 18.84 g/(m²·week), is twice 630 of the averaged as large as the average value over a longer period (November to February) 631 632 reported/estimated by Gibsonab et al. (1999). 633 As the region recording the strongest surface unsaturation of these three regions in summerAs the strongest surface unsaturation in summer, the Shelf region has a potential carbon 634 uptake of 10.01±2.7 Tg C from February to early March, which accounts for approximately 635 5.0‰-6.7‰ 8.10 Tg C for February, which accounts for approximately 4.05‰-5.4‰ of the net 636 637 global ocean CO2 uptake according to Takahashi et al. (2009), even though its total area is only 78*103 km² while its total area is only 78*103 km². Due to the sill constraint of sill, there is 638 639 limited exchange between water masses in and outside the Prydz Bay. During winter, the dense 640 water formed by the ejection of brine brine ejection in the Bay, can potentially uptakes more 641 anthropogenic CO2 from the atmosphere, and that can_descends to greater depth, thus enhancing 642 the acidification in-the deep water. According to Shadwick et al. (2013), the winter values of pH 643 and Ω decreased more remarkably than those in summer values. As the bottom water in the

644 Prydz Bay is a possible source of Antarctic Bottom Water (Yabuki et al., 2006), the Shelf region 645 may act as to transfer anthropogenic CO_2 at the surface to the deep water, and then may thus influence the deep ocean acidification of the deep ocean over long timescales.in the long run. 646 The total carbon uptake in Prydz Bay of three regions integrated over the whole February 647 648 2015 was 18.7 TgC. The uncertainty depended on the errors for the wind speed, the scaling factor and the accuracy of SOM derived pCO2 according to Eq.2. The scaling factor will yield a 649 650 20% uncertainty to regional flux estimation. The errors in wind speeds of Ascat dataset is 651 assumed to be 6% (Xu et al., 2016) and will be 12% in quadratic wind speed. For the SOM 652 derived pCO2 the RMSE is 22.14 µatm. Considering the errors above and an uncertainty 653 occurred when the sea-air computation expression was simplified (1.39%, Xu et al., 2016), the total uncertainty of the final uptake is ± 4.93 TgC. 654 655 4 Summary Based on the different observed ranges of the distribution of ocean pCO2, According to 656 different controls factors of ocean pCO2, the Prydz Bay region was divided into three sectors 657 from February to early March of 2015. for February 2015. In the Shelf region, biological factors 658 659 <u>exerted</u>was the main control for on oceanic pCO_{2} while in the Open-ocean region, mixing and upwelling became were the main controls. In the Sea-ice region, due to the rapid changes in sea 660 ice-changing, oceanic pCO_2 was controlled by both-the biological and physical processes. SOM 661 662 is an important tool to dofor the quantitative assessment of oceanic pCO_2 and succedent its subsequent sea-air carbon flux, especially in dynamic, high-high-latitude, and seasonally ice-663 covered regions. The estimated results revealed that the SOM technique could be used to 664 665 reconstruct the variations of in oceanic pCO2 associated with bio-geochemical processes expressed by the variabilityies in four proxy parameters: SST, CHL, MLD and SSS. The RMSE 666 of the SOM derived SOM-derived oceanic pCO_2 is 22.14 µatm for the SOCAT dataset. From 667 February to early March of 2015, Over February 2015, the Prydz Bay region was a strong carbon 668 sink, with a carbon uptake of 23.57±6.36 TgC18.7±4.93 TgC. The Sstrong potential uptake of 669 anthropogenic CO₂ in the Shelf region will enhance the acidification in the deep water region of 670 671 the Prydz bay and then may thus influence the acidification of the deep ocean acidification in the 672 long run becausesince it contributes to the formation of Antarctic bottom waterWater. 673

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674 Acknowledgments

	675	This work is supported by National Natural Science Foundation of China (NSFC41506209,
	676	41630969, 41476172, 41230529), Qingdao National Laboratory for marine science and
	677	technology (QNLM2016ORP0109), Chinese Projects for Investigations and Assessments of the
	678	Arctic and Antarctic (CHINARE2012-2020 for 01-04, 02-01, and 03-04). This work is also
	679	supported by Korea Polar Research Institute grants PE18060 and PE18070. We would like to
	680	thank China Scholarship Council (201704180019) and State Administration of Foreign Experts
	681	Affairs P. R. China for their support in this research. We would like to thank the carbon group
	682	led by Zhongyong Gao and Heng Sun in We would like to thank the carbon group in GCMAC
	683	and the crew on R/V Xuelong for their support on the cruise. We are thankful to contributors of
	684	the SOCAT database and Mercator Ocean for providing the Global Forecast model output. We
	685	deeply appreciate Dr. Xianmin Hu in Bedford Institute of Oceanography, who provided us with
	686	useful technical instructions.
	687	References
	688 689	1. Bakker, D. C. E., Pfeil, B. Landa, C. S., Metzl, N., O'Brien, K. M., Olsen, A., Smith, K., Cosca,
	690	C., Harasawa, S., Jones, S. D., Nakaoka, S., Nojiri, Y., Schuster, U., Steinhoff, T., Sweeney,
	691	C., Takahashi, T., Tilbrook, B., Wada, C., Wanninkhof, R., Alin, S. R., Balestrini, C. F.,
	692	Barbero, L., Bates, N. R., Bianchi, A. A., Bonou, F., Boutin, J., Bozec, Y., Burger, E. F., Caj,
	693	WJ., Castle, R. D., Chen, L., Chierici, M., Currie, K., Evans, W., Featherstone, C., Feely, R.
	694	A., Fransson, A., Goyet, C., Greenwood, N., Gregor, L., Hankin, S., Hardman-Mountford, N.
	695	J., Harlay, J., Hauck, J., Hoppema, M., Humphreys, M. P., Hunt, C. W., Huss, B., Ibánhez, J.
	696	S. P., Johannessen, T., Keeling, R., Kitidis, V., Körtzinger, A., Kozyr, A., Krasakopoulou, E.,
	697	Kuwata, A., Landschützer, 3P., Lauvset, S. K., Lefèvre, N., Lo Monaco, C., Manke, A.,
	698	Mathis, J. T., Merlivat, L., Millero, F. J., Monteiro, P. M. S., Munro, D. R., Murata, A.,
	699	Newberger, T., Omar, A. M., Ono, T., Paterson, K., Pearce, D., Pierrot, D., Robbins, L. L.,
	700	Saito, S., Salisbury, J., Schlitzer, R., Schneider, B., Schweitzer, R., Sieger, R., Skjelvan, I.,
	701	Sullivan, K. F., Sutherland, S. C., Sutton, A. J., Tadokoro, K., Telszewski, M., Tuma, M., Van
	702	Heuven, S. M. A. C., Vandemark, D., Ward, B., Watson, A. J., and Xu, S.: A multi-decade
	703	record of high quality fCO2 data in version 3 of the Surface Ocean CO2 Atlas (SOCAT). Earth
	704	System Science Data 8: 383-413.doi:10.5194/essd-8-383-2016, 2016.
- 1		

705	<u>2.</u>	Barbini, R., Fantoni, R., Palucci, A., Colao, F., Sandrini, S., Ceradini, S., Tositti, L.,
706		Tubertini, O., and Ferrari, G. M.: Simultaneous measurements of remote lidar chlorophyll
707		and surface CO2 distributions in the Ross Sea. International Journal of Remote Sensing, 24,
708		<u>3807-3819, 2003.</u>
709	<u>3.</u>	Bates, N. R., Hansell, D. A., Carlson, C. A., and Gordon, L. I.: Distribution of CO2 species,
710		estimates of net community production, and air-sea CO2 exchange in the Ross Sea polynya,
711		Journal of Geophysical Research, 103, 2883-2896, 1998a.
712	<u>4.</u>	Bates, N. R., Takahashi, T., Chipman, D. W., and Knapp, A. H.: Variability of pCO ₂ on diel
713		to seasonal time scales in the Sargasso Sea, Journal of Geophysical Research, 103, 15567-
714		<u>15585, 1998b.</u>
715	<u>5.</u>	Brainerd, K. E., and Gregg, M. C.: Surface mixed and mixing layer depth, Deep Sea Res., part
716		<u>A, 42, 1521-1543, 1995.</u>
717	<u>6.</u>	Burkill, P. H., Edwards, E. S., and Sleight, M. A.: Microzooplankton and their role in
718		controlling phytoplankton growth in the marginal ice zone of the Bellingshausen Sea, Deep
719		Sea Research Part II: Topical Studies in Oceanography, 42(4), 1277-1290, 1995.
720	<u>7.</u>	Chen, L., Xu, S., Gao, Z., Chen, H., Zhang, Y., Zhan, J., and Li, W.: Estimation of monthly
721		air-sea CO ₂ flux in the southern Atlantic and Indian Ocean using in-situ and remotely sensed
722		data, Remote Sensing of Environment, 115(8), 1935-1941, 2011.
723	<u>8.</u>	Chierici, M., Olsen, A., Johannessen, T., Trinanes, J., and Wanninkhof, R.: Algorithms to
724		estimate the carbon dioxide uptake in the northern North Atlantic using ship-observations,
725		satellite and ocean analysis data, Deep-Sea Res. Pt. II, 56(8-10), 630-639, 2009.
726	<u>9.</u>	Dandonneau, Y.: Sea-surface partial pressure of carbon dioxide in the eastern equatorial
727		Pacific (August 1991 to October 1992): A multivariate analysis of physical and biological
728		factors, Deep Sea Research II, 42(2-3), 349-364, 1995.
729	<u>10</u> .	Dong, S., Sprintall, J., Gille, S. T., and Talley, L.: Southern Ocean mixed-layer depth from
730		Argo float profiles, Journal of Geophysical Research, 113, C06013, doi:
731		<u>10.1029/2006JC004051, 2008.</u>
732	<u>11</u> .	Edwards, A. M., Platt, T., and Sathyendranath, S.: The high-nutrient, low-chlorophyll regime
733		of the ocean: limits on biomass and nitrate before and after iron enrichment, Ecological
734		Modelling, 171, 103-125, 2004.

- 735 <u>12. Friedrich, T., and Oschlies, A.: Basin-scale *p*CO₂ maps estimated from ARGO float data: A</u>
 - 31

736		model study, J. Geophys. Res., 114, C10012, doi:10.1029/2009JC005322, 2009b.
737	<u>13.</u>	Friedrich, T., and Oschlies, A.: Neural network-based estimates of North Atlantic surface
738		pCO2 from satellite data: A methodological study, J. Geophys. Res., 114, C03020,
739		<u>doi:10.1029/2007JC004646, 2009a.</u>
740	<u>14.</u>	Gao, Z., Chen, L., and Gao, Y.: Air-sea carbon fluxes and there controlling factors in the
741		PrydzBay in the Antarctic, Acta OceanologicaSinica, 3(27), 136-146, 2008.
742	<u>15.</u>	Gibson, P. B., Perkins-Kirkpatrick, S. E., Uotila, P., Pepler, A. S., and Alexander, L. V.: On
743		the use of self-organizing maps for studying climate extremes, Journal of Geophysical
744		Research: Atmospheres, 122, 3891-3903, 2017.
745	<u>16.</u>	Gibsonab, J. A.E., and Trullb, T. W.: Annual cycle of fCO2 under sea-ice and in open water
746		in Prydz Bay, east Antarctica, Marine Chemistry, Volume 66, Issues 3-4, 187-200, 1999.
747	<u>17.</u>	Hales, B., Strutton, P., Saraceno, M., Letelier, R., Takahashi, T., Feely, R., Sabine, C., and
748		Chavez, F.: Satellite-based prediction of pCO2 in coastal waters of the eastern North Pacific,
749		Progress in Oceanography, 103, 1-15, 2012.
750	<u>18.</u>	Hardman-Mountford, N., Litt, E., Mangi, S., Dye, S., Schuster, U., Bakker, D., and Watson,
751		A.: Ocean uptake of carbon dioxide (CO2), MCCIP BriefingNoteswww.mccip.org.uk, 9pp,
752		<u>2009.</u>
753	<u>19.</u>	Heil, P., Allison, I. and Lytle, V. I.: Seasonal and interannual variations of the oceanic heat
754		flux under a landfast Antarctic sea ice cover, J. Geophys. Res., 101(C11), 25,741-25,752, doi:
755		<u>10.1029/96JC01921, 1996.</u>
756	<u>20.</u>	Huang, J., Xu, F., Zhou, K., Xiu, P., and Lin, Y.: Temporal evolution of near-surface
757		chlorophyll over cyclonic eddy lifecycles in the southeastern Pacific, Journal of Geophysical
758		Research: Oceans 122, 6165-6179, 2017a.
759	<u>21.</u>	Huang, W., Chen, R., Yang, Z., Wang, B., and Ma, W.: Exploring the combined effects of the
760		Arctic Oscillation and ENSO on the wintertime climate over East Asia using self-organizing
761		maps, Journal of Geophysical Research: Atmospheres, 122, 9107-9129, 2017b.
762	<u>22.</u>	Iskandar, I.: Seasonal and interannual patterns of sea surface temperature in Banda Sea as
763		revealed by self-organizing map, Continental Shelf Research, 30, 1136-1148, 2010.
764	<u>23.</u>	Jacobs, S. S. and Georgi, D. T.: Observations on the south-west Indian/Antarctic Ocean, In A

765 Voyage of Discovery, ed. by M. Angel, Deep-Sea Res., 24(suppl.), 43-84, 1977.

767	from VOS lines in situ measurements: Parameters needed to generate seasonally mean maps,
768	Ann. Geophys., 25, 2247-2257, 2007, http://www.ann-geophys.net/25/2247/2007/.
769	25. Jiang, L. Q., Cai, W. J., Wanninkhof, R., Wang, Y., and Lüger, H.: Air-sea CO2 fluxes on the
770	U.S. South Atlantic Bight: Spatial and seasonal variability, Journal of Geophysical Research,
771	113 (2008), C07019, doi:10.1029/2007JC004366, 2008.
772	26. Jo, Y. H., Dai, M. H., Zhai, W. D., Yan, X. H., and Shang, S. L.: On the variations of sea
773	surface pCO ₂ in the northern South China sea: A remote sensing based neural network
774	approach, Journal of Geophysical Research, 117, C08022, doi:10.1029/2011JC007745, 2012.
775	27. Kohonen, T.: Self-Organization and Associative Memory, Springer, Berlin, 1984.
776	28. Lafevre, N., Watson, A. J., and Watson, A. R.: A comparison of multiple regression and neural
777	network techniques for mapping in situ pCO ₂ data, Tellus B, 57(5), 375-384, 2005.
778	29. Laruelle, G. G., Landschützer, P., Gruber, N., Tison, J. L., Delille, B., and Regnier, P.: Global
779	high resolution monthly pCO2 climatology for the coastal ocean derived from neural network
780	interpolation, Biogeosciences, 14, 4545-4561, 2017.
781	30. Lei, R., Li, Z., Cheng, B., Zhang, Z., and Heil, P.: Annual cycle of landfastsea ice in Prydz
782	Bay, East Antarctica, Journal of Geophysical Research Atmospheres, 115(C2), C02006,
783	doi:10.1029/2008JC005223, 2010.
784	31. Liu C., Wang Z., Cheng C., Xia R., Li B., and Xie Z.: Modeling modified circumpolar deep
785	water intrusions onto the Prydz Bay continental shelf, East Antarctica, Journal of Geophysical
786	Research, Vol. 122, Issue 7, 5198-5217. DOI: 10.1002/2016JC012336, 2017.
787	32. Liu, Y., Weisberg, R. H., and He, R.: Sea Surface Temperature Patterns on the West Florida
788	Shelf Using Growing Hierarchical Self-Organizing Maps, Journal of Atmospheric and
789	Oceanic Technology, 23, 325-338, 2006.
790	33. Liu, Z. L., Ning, X. R., Cai, Y. M., Liu, C. G., andZhu, G. H.: Primary productivity

24. Jamet, C., Moulin, C., and Lefèvre, N.: Estimation of the oceanic *p*CO₂ in the North Atlantic

766

- andchlorophyll a in the surface water on the route encircling the Antarctica duringaustral
 summer of 1999/2000, Polar Research, 112(4), 235-244, 2000.
- 34. Liu, Z., and Cheng Z.: The distribution feature of size-fractionated chlorophyll a and primary
 productivity in Prydz Bay and its north sea area during the austral summer, Chinese Journal
 of Polar Science, 14(2): 81-89, 2003.
- 796 35. Lüger, H., Wallace, D. W. R., Körtzinger, A., and Nojiri, Y.: The pCO₂ variability in the

797		midlatitude North Atlantic Ocean during a full annual cycle, Global Biogeochem. Cycles, 18,
798		<u>GB3023, doi:10.1029/2003GB002200, 2004.</u>
799	<u>36.</u>	Metzl, N., Brunet, C., Jabaud-Jan, A., Poisson, A., and Schauer, B.: Sumer and winter air-sea
800		CO2 fluxes in the Southern Ocean, Deep-Sea Research, 153: 1548-1563, 2006.
801	<u>37.</u>	Middleton, J. H., and Humphries, S. E.: Thermohaline structure and mixing in the region of
802		Prydz Bay, Antarctica, Deep Sea Research Part A, Oceanographic Research Papers, 36(8),
803		<u>1255-1266, 1989.</u>
804	<u>38.</u>	Morrison, J. M., Gaurin, S., Codispoti, L. A., Takahashi, T., Millero, F. J., Gardner, W. D.,
805		and Richardson, M. J.: Seasonal evolution of hydrographic properties in the Antarctic
806		circumpolar current at 170W during 1997-1998, Deep-Sea Research, I48: 3943-3972, 2001.
807	<u>39.</u>	Nakaoka, S., Telszewski, M., Nojiri, Y., Yasunaka, S., Miyazaki, C., Mukai, H., and Usui, N.:
808		Estimating temporal and spatial variation of ocean surface pCO_2 in the North Pacific using a
809		self-organizing map neural network technique, Biogeosciences, 10, 6093-6106, 2013.
810	<u>40.</u>	Nunes Vaz, R. A., and Lennon, G. W.: Physical oceanography of the Prydz Bay region of
811		Antarctic waters, Deep Sea Research Part I: Oceanography Research Papers, 43(5), 603-641,
812		<u>1996.</u>
813	<u>41.</u>	Olsen, A., Trinanes, J. A., and Wanninkhof, R.: Sea-air flux of CO2 in the Caribbean Sea
814		estimated using in situ and remote sensing data, Remote Sens. Environ., 89, 309-325, 2004.
815	<u>42.</u>	Pfeil, B., Olsen, A., Bakker, D. C. E., Hankin, S., Koyuk, H., Kozyr, A., Malczyk, J., Manke,
816		A., Metzl, N., Sabine, C. L., Akl, J., Alin, S. R., Bellerby, R. G. J., Borges, A., Boutin, J.,
817		Brown, P. J., Cai, WJ., Chavez, F. P., Chen, A., Cosca, C., Fassbender, A. J., Feely, R. A.,
818		González-Dávila, M., Goyet, C., Hardman- Mountford, N., Heinze, C., Hood, M., Hoppema,
819		M., Hunt, C. W., Hydes, D., Ishii, M., Johannessen, T., Jones, S. D., Key, R. M., Körtzinger,
820		A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lenton, A., Lourantou, A., Merlivat, L.,
821		idorikawa, T., Mintrop, L., Miyazaki, C., Murata , A., Nakadate, A., Nakano, Y., Nakaoka, Y.
822		Nojiri, A. M. Omar, X. A. Padin, GH. Park, K. Paterson, F. F. Perez, S., Pierrot, D., Poisson,
823		A., Ríos, A. F., Salisbury, J., Santana-Casiano, J. M., Sarma, V. V. S. S., Schlitzer, R.,
824		Schneider, B., Schuster, U., Sieger, R., Skjelvan, I., Steinhoff, T., Suzuki, T., Takahashi, T.,
825		Tedesco, K., Telszewski, M., Thomas, H., Tilbrook, B., Tjiputra, J., Vandemark, D., Veness,
826		T., Wanninkhof, R., Watson, A. J., Weiss, R., Wong, C. S., and Yoshikawa-Inoue, H.: A
827		uniform, quality controlled Surface Ocean CO2 Atlas (SOCAT), Earth Syst. Sci. Data, 5, 125-
•		

828		143, doi:10.5194/essd-5-125-2013, 2013.
829	<u>43.</u>	Pierrot, D., Neill, C., Sullivan, L., Castle, R., Wanninkhof, R., Lüger, H., Johannessen, T.,
830		Olsen, A., Feely, R. A., and Cosca, C. E.: Recommendations for autonomous underway pCO2
831		measuring systems and data-reduction routines, Deep-Sea Research Part II, 56, 512-522, 2009.
832	<u>44.</u>	Rangama, Y., Boutin, J., Etcheto, J., Merlivat, L., Takahashi, T., Delille, B., Frankignoulle,
833		M., and Bakker, D. C. E.: Variability of the net air-sea CO ₂ flux inferred from shipboard and
834		satellite measurements in the Southern Ocean south of Tasmania and New Zealand, Journal
835		of Geophysical Research: Oceans (1978-2012), 110(C9), doi: 10.1029/2004JC002619, 2005.
836	<u>45.</u>	Roden, N. P., Shadwick, E. H., Tilbrook, B., and Trull, T. W.: Annual cycle of carbonate
837		chemistry and decadal change in coastal Prydz Bay, East Antarctica, Marine Chemistry,
838		<u>155(4), 135-147, 2013.</u>
839	<u>46.</u>	Rubin, S.I., Takahashi, T., and Goddard, J.G.: Primary productivity and nutrient utilization
840		ratios in the Pacific sector of the Southern Ocean based on seasonal changes in seawater
841		chemistry, Deep-Sea Research I 45, 1211-1234, 1998.
842	<u>47.</u>	Sabine, L., Feely, R. A., Gruber, N., Key, R. M., Lee, K., Bullister, J. L., Wanninkhof, R.,
843		Wong, S., Wallace, D. W. R., Tilbrook, B., Millero, F. J., Peng, TH., Kozyr, A., Ono, T.,
844		and Rios, A. F.: The oceanic sink for anthropogenic CO2, Science, 305, 367-371,
845		doi:10.1126/science.1097403, 2004.
846	<u>48.</u>	Sarma, V. V. S. S., Saino, T., Sasaoka, K., Nojiri, Y., Ono, T., Ishii, M., Inoue, H. Y., and
847		Matsumoto, K.: Basin-scale pCO ₂ distribution using satellite sea surface temperature, Chl a,
848		and climatological salinity in the North Pacific in spring and summer, Global Biogeochemical
849		Cycles, 20, GB3005, doi:10.1029/2005GB002594, 2006.
850	<u>49.</u>	Shadwick, E. H., Trull, T. W., Thomas, H., and Gibson, J. A. E.: Vulnerability of polar oceans
851		to anthropogenic acidification: comparison of Arctic and Antarctic seasonal cycles, Scientific
852		Reports, 3: 2339, doi: 10.1038/srep02339, 2013.
853	<u>50.</u>	Silulwane, N. F., Richardson, A. J., Shillington, F. A., and Mitchell-Innes, B. A.: Identification
854		and classification of vertical chlorophyll patterns in the Benguela upwelling system and
855		Angola-Benguela front using an artificial neural network, South African Journal of Marine
856		Science, 23, 37-51, 2001.
857	<u>51.</u>	Smith, N. R., Zhaoqian, D., Kerry, K. R., and Wright, S.: Water masses and circulation in the

858 region of Prydz Bay Antarctica, Deep-sea-research, 31, 1121-1147, 1984.

859	<u>52.</u>	Smith, N., and Tréguer, P.: Physical and chemical oceanography in the vicinity of Prydz Bay,
860		Antarctica, Cambridge University Press, Cambridge, 1994.
861	<u>53.</u>	Spreen, G., Kaleschke, L., and Heygster, G.: Sea ice remote sensing using AMSR-E 89 GHz
862		channels, J. Geophys. Res., 113, C02S03, doi:10.1029/2005JC003384, 2008.
863	<u>54.</u>	Sun, W. P., Han, Z. B., Hu, C. Y., and Pan, J. M.: Particulate barium flux and its relationship
864		with export production on the continental shelf of Prydz Bay, east Antarctica, Marine
865		<u>Chemistry</u> , 157, 86-92, 2013.
866	<u>55.</u>	Sweeney, C., Hansell, D. A., Carlson, C. A., Codispoti, L. A., Gordon, L. I., Marra, J., Millero,
867		F. J., Smith, W. O., and Takahashi, T.: Biogeochemical regimes, net community production
868		and carbon export in the Ross Sea, Antarctica, Deep Sea Research II, 47(15-16), 3369-3394,
869		<u>2000.</u>
870	<u>56.</u>	Sweeney, C.: The annual cycle of surface water CO ₂ and O ₂ in the Ross Sea: a model for gas
871		exchange on the continental shelves of Antarctic, Biogeochemistry of the Ross Sea, Antarctic
872		<u>Research Series, 78, 295-312, 2002.</u>
873	<u>57.</u>	Sweeney, C.: The annual cycle of surface water CO ₂ and O ₂ in the Ross Sea: A model for gas
874		exchange on the continental shelves of Antarctic, Biogeochemistry of the Ross Sea, Antarctic
875		Research Series, 78, 295-312, 2002.
876	<u>58.</u>	Takahashi, T. Feely, R. A., Weiss, R. F., Wanninkhof, R. H., Chipman, D. W., Sutherland,
877		S. C., and Takahashi, T. T.: Global seaair CO2 flux based on climatological surface ocean
878		pCO ₂ , and seasonal biological and temperature effects, Deep-Sea Res. Pt. II, 49(9-10), 1601-
879		<u>1622, 2002.</u>
880	<u>59.</u>	Takahashi, T., Sutherland, S. C., Wanninkhof, R., Sweeney, C., Feely, R. A., Chipman, D.
881		W., Hales, B., Friederich, G., Chavez, F., Sabine, C., Watson, A. J., Bakker, D. C., Schuster,
882		U., Metzl, N., Yoshikawa-Inoue, H., Ishii, M., Midorikawa, T., Nojiri, Y., Körtzinger, A.,
883		Steinhoff, T., Hoppema, M., Olafsson, J., Arnarson, T. S., Tilbrook, B., Johannessen, T.,
884		Olsen, A., Bellerby, R., Wong, C. S., Delille, B., Bates, N. R., and de Baar, H. J. W .:
885		Climatological mean and decadal change in surface ocean pCO ₂ , and net sea-air CO ₂ flux
886		over the global oceans, Deep-Sea Res. Pt. II, 56(8-10), 554-577, 2009.
887	<u>60.</u>	Takahashi, T., Sweeney, C., Hales, B., Chipman, D. W., Newberger, T., Goddard, J. G.,
888		Iannuzzi, R. A., and Sutherland, S. C.: The changing carbon cycle in the Southern Ocean,
889		Oceanography, 25, 26-37, 2012.

890	61. Telszewski, M., Chazottes, A., Schuster, U., Watson, A. J., Moulin, C., Bakker, D. C. E.,
891	González-Dávila, M., Johannessen, T., Körtzinger, A., Lüger, H., Olsen, A., Omar, A., Padin,
892	X. A., Ríos, A. F., Steinhoff, T., Santana-Casiano, M., Wallace, D. W. R., and Wanninkhof,
893	R.: Estimating the monthly pCO ₂ distribution in the North Atlantic using a self-organizing
894	neural network, Biogeoscience, 6, 1405-1421, 2009.
895	62. Thomson, R. E., and Fine, I. V.: Estimating mixed layer depth from oceanic profile data, J.
896	Atmos. Oceanic Technol., 20, 319-329, 2003.
897	63. Ultsch, A., and Röske, F.: Self-organizing feature maps predicting sea levels, Information
898	<u>Sciences, 144, 91-125, 2002.</u>
899	64. Vesanto, J.: Data Exploration Process Based on the Self-Organizing Map: the Finnish
900	Academies of Technology, 2002.
901	65. Wanninkhof, R.: Relationship between wind speed and gas exchange over the ocean revisited,
902	Limnology and Oceanography: Methods, 12, 351-362, 2014.
903	66. Weiss, R. F.: Carbon dioxide in water and seawater: The solubility of a nonideal gas, Marine
904	<u>Chemistry</u> , 2, 201-215, 1974.
905	67. Worby, A. P., Geiger, C. A., Paget, M. J., Van Woert, M. L., Ackley, S. F., and DeLiberty, T.
906	L.: Thickness distribution of Antarctic sea ice, Journal of Geophysical Research 113, C05S92,
907	http://dx.doi.org/10.1029/2007JC004254, 2008.
908	68. Wu, L., Wang, R., Xiao, W., Ge, S., Chen, Z., and Krijgsman, W.: Productivity-climate
909	coupling recorded in Pleistocene sediments off Prydz Bay (East Antarctica), Palaegeography,
910	Palaeoclimatology, Palaeoecology, 485, 260-270, 2017.
911	69. Xu, S., Chen, L., Chen, H., Li, J., Lin, W., and Qi, D.: Sea-air CO2 fluxes in the Southern
912	Ocean for the late spring and early summer in 2009, Remote Sensing of Environment, 175,
913	<u>158-166, 2016.</u>
914	70. Yabuki, T., Suga, T., Hanawa, K., Matsuoka, K., Kiwada, H., and Watanabe, T.: Possible
915	source of the Antarctic Bottom Water in Prydz Bay region, J. Oceanogr., 62, 649-655, doi:
916	<u>10.1007/s10872-006-0083-1, 2006.</u>
917	71. Zeng, J. Nojiri, Y., Nakaoka, S., Nakajima, H., and Shirai, T.: Surface ocean CO2 in 1990-
918	2011 modelled using a feed-forward neural network, Geoscience Data Jounal, 2, 47-51, doi:
919	<u>10.1002/gdj3.26, 2015.</u>
920	72. Zeng, J., Mtsunaga, T., Saigusa, N., Shirai, T., Nakaoka, S., and Tan, Z.: Technical note:

921	Evaluation of three machine learning models for surface ocean CO ₂ mapping, Ocean Sci., 13,
922	303-313, http://doi.org/10.5194/os-13-303-2017, 2017.
923	<u>73.</u> Zeng, J., Nojiri, Y., Murphy, P. P., Wong, C. S., and Fujinuma, Y.: A comparison of $\triangle pCO_2$
924	distributions in the northern North Pacific using results from a commercial vessel in 1995-
925	1999, Deep Sea Res., Part II, 49, 5303-5315, 2002.
926	
927	1. Bakker, D. C. E., Pfeil, B. Landa, C. S., Metzl, N., O'Brien, K. M., Olsen, A., Smith, K., Cosca,
928	C., Harasawa, S., Jones, S. D., Nakaoka, S., Nojiri, Y., Schuster, U., Steinhoff, T., Sweeney,
929	C., Takahashi, T., Tilbrook, B., Wada, C., Wanninkhof, R., Alin, S. R., Balestrini, C. F.,
930	Barbero, L., Bates, N. R., Bianchi, A. A., Bonou, F., Boutin, J., Bozec, Y., Burger, E. F., Cai,
931	WJ., Castle, R. D., Chen, L., Chierici, M., Currie, K., Evans, W., Featherstone, C., Feely, R.
932	A., Fransson, A., Goyet, C., Greenwood, N., Gregor, L., Hankin, S., Hardman-Mountford, N.
933	J., Harlay, J., Hauck, J., Hoppema, M., Humphreys, M. P., Hunt, C. W., Huss, B., Ibánhez, J.
934	S. P., Johannessen, T., Keeling, R., Kitidis, V., Körtzinger, A., Kozyr, A., Krasakopoulou, E.,
935	Kuwata, A., Landschützer, 3P., Lauvset, S. K., Lefèvre, N., Lo Monaco, C., Manke, A.,
936	Mathis, J. T., Merlivat, L., Millero, F. J., Monteiro, P. M. S., Munro, D. R., Murata, A.,
937	Newberger, T., Omar, A. M., Ono, T., Paterson, K., Pearce, D., Pierrot, D., Robbins, L. L.,
938	Saito, S., Salisbury, J., Schlitzer, R., Schneider, B., Schweitzer, R., Sieger, R., Skjelvan, I.,
939	Sullivan, K. F., Sutherland, S. C., Sutton, A. J., Tadokoro, K., Telszewski, M., Tuma, M., Van
940	Heuven, S. M. A. C., Vandemark, D., Ward, B., Watson, A. J., Xu, S.: A multi-decade record
941	of high quality fCO2 data in version 3 of the Surface Ocean CO2 Atlas (SOCAT). Earth System
942	Science Data 8: 383-413.doi:10.5194/essd-8-383-2016, 2016.
943	2. Brainerd, K. E., and Gregg, M. C.: Surface mixed and mixing layer depth, Deep Sea Res., part
944	A, 42, 1521–1543, 1995.
945	3. Burkill, P. H., Edwards, E. S., Sleight, M. A.: Microzooplankton and their role in controlling
946	phytoplankton growth in the marginal ice zone of the Bellingshausen Sea, Deep Sea Research
947	Part II: Topical Studies in Oceanography, 42(4), 1277-1290, 1995.
948	4. Chen, L., Xu, S., Gao, Z., Chen, H., Zhang, Y., Zhan, J., Li, W.: Estimation of monthly air-
949	sea CO2 flux in the southern Atlantic and Indian Ocean using in-situ and remotely sensed data,
950	Remote Sensing of Environment, 115(8), 1935-1941, 2011.

951 5. Dandonneau, Y.: Sea surface partial pressure of carbon dioxide in the eastern equatorial

952		Pacific (August 1991 to October 1992): A multivariate analysis of physical and biological
953		factors, Deep Sea Research II, 42(2-3), 349-364, 1995.
954	6.	Dong, S., Sprintall, J., Gille, S. T., Talley, L.: Southern Ocean mixed layer depth from Argo
955		float profiles, Journal of Geophysical Research, 113, C06013, doi: 10.1029/2006JC004051,
956		2008.
957	7.	Edwards, A. M., Platt, T., Sathyendranath, S.: The high-nutrient, low-chlorophyll regime of
958		the ocean: limits on biomass and nitrate before and after iron enrichment, Ecological
959		Modelling, 171, 103-125, 2004.
960	8.	Friedrich, T., Oschlies, A.: Neural network-based estimates of North Atlantic surface pCO2
961		from satellite data: A methodological study, J. Geophys. Res., 114, C03020,
962		doi:10.1029/2007JC004646, 2009a.
963	9.	Friedrich, T., Oschlies, A.: Basin-scale pCO2 maps estimated from ARGO float data: A model
964		study, J. Geophys. Res., 114, C10012, doi:10.1029/2009JC005322, 2009b.
965	10 .	Gao, Z., Chen, L., Gao, Y .: Air-sea carbon fluxes and there controlling factors in the Prydz
966		Bay in the Antarctic, Acta Oceanologica Sinica, 3(27), 136-146, 2008.
967	11.	Gibsonab, J. A.E., Trullb, T. W.: Annual cycle of fCO2 under sea-ice and in open water in
968		Prydz Bay, east Antarctica, Marine Chemistry, Volume 66, Issues 3-4, 187-200, 1999.
969	12 .	Gibson, P. B., Perkins Kirkpatrick, S. E., Uotila, P., Pepler, A. S., Alexander, L. V.: On the
970		use of self-organizing maps for studying climate extremes, Journal of Geophysical Research:
971		Atmospheres, 122, 3891-3903, 2017.
972	13 .	Hales, B., Strutton, P., Saraceno, M., Letelier, R., Takahashi, T., Feely, R., Sabine, C., Chavez,
973		F.: Satellite-based prediction of pCO2 in coastal waters of the eastern North Pacific, Progress
974		in Oceanography, 103, 1–15, 2012.
975	14 .	Heil, P., I. Allison and V. I. Lytle: Seasonal and interannual variations of the oceanic heat flux
976		under a landfast Antarctic sea ice cover, J. Geophys. Res., 101(C11), 25,741-25,752, doi:
977		10.1029/96JC01921, 1996.
978	15.	Huang, J., Xu, F., Zhou, K., Xiu, P., Lin, Y.: Temporal evolution of near-surface chlorophyll
979		over cyclonic eddy lifecycles in the southeastern Pacific, Journal of Geophysical Research:
980		Oceans 122, 6165-6179, 2017a.
981	16 .	Huang, W., Chen, R., Yang, Z., Wang, B., Ma, W.: Exploring the combined effects of the
982		Arctic Oscillation and ENSO on the wintertime climate over East Asia using self-organizing
•		

983	maps, Journal of Geophysical Research: Atmospheres, 122, 9107-9129, 2017b.
984	17. Iskandar, I.: Seasonal and interannual patterns of sea surface temperature in Banda Sea as
985	revealed by self-organizing map, Continental Shelf Research, 30, 1136-1148, 2010.
986	18. Jiang, L. Q., Cai, W. J., Wanninkhof, R., Wang, Y., Lüger, H.: Air-sea CO ₂ -fluxes on the U.S.
987	South Atlantic Bight: Spatial and seasonal variability, Journal of Geophysical Research, 113
988	(2008), C07019, doi:10.1029/2007JC004366, 2008.
989	19. Jo, Y. H., Dai, M. H., Zhai, W. D., Yan, X. H., Shang, S. L.: On the variations of sea surface
990	pCO2-in the northern South China sea: A remote sensing based neural network approach,
991	Journal of Geophysical Research, 117, C08022, doi:10.1029/2011JC007745, 2012.
992	20. Kohonen, T.: Self-Organization and Associative Memory, Springer, Berlin, 1984.
993	21. Lafevre, N., Watson, A. J., Watson, A. R.: A comparison of multiple regression and neural
994	network techniques for mapping in situ pCO2 data, Tellus B, 57(5), 375-384, 2005.
995	22. Laruelle, G. G., Landschützer, P., Gruber, N., Tison, J. L., Delille, B., Regnier, P.: Global high
996	resolution monthly pCO2-climatology for the coastal ocean derived from neural network
997	interpolation, Biogeosciences, 14, 4545-4561, 2017.
998	23. Lei, R., Li, Z., Cheng, B., Zhang, Z., Heil, P.: Annual cycle of landfast sea ice in Prydz Bay,
999	East Antarctica, Journal of Geophysical Research Atmospheres, 115(C2), C02006,
1000	doi:10.1029/2008JC005223, 2010.
1001	24. Liu C., Wang Z., Cheng C., Xia R., Li B., Xie Z.: Modeling modified circumpolar deep water
002	intrusions onto the Prydz Bay continental shelf, East Antarctica, Journal of Geophysical
1003	Research, Vol. 122, Issue 7, 5198-5217. DOI: 10.1002/2016JC012336, 2017.
004	25. Liu, Y., Weisberg, R. H., He, R.: Sea Surface Temperature Patterns on the West Florida Shelf
1005	Using Growing Hierarchical Self Organizing Maps, Journal of Atmospheric and Oceanic
1006	Technology, 23, 325-338, 2006.
1007	26. Lüger, H., Wallace, D. W. R., Körtzinger, A., Nojiri, Y.: The pCO2 variability in the
1008	midlatitude North Atlantic Ocean during a full annual cycle, Global Biogeochem. Cycles, 18,
1009	GB3023, doi:10.1029/2003GB002200, 2004.
1010	27. Metzl, N., Brunet, C., Jabaud-Jan, A., Poisson, A., and Schauer, B.: Sumer and winter air-sea
1011	CO2-fluxes in the Southern Ocean, Deep-Sea Research, 153: 1548-1563, 2006.
1012	28. Middleton, J. H., Humphries, S. E.: Thermohaline structure and mixing in the region of Prydz

1013 Bay, Antarctica, Deep Sea Research Part A, Oceanographic Research Papers, 36(8), 1255-

1014	1266, 1989.
1015	29. Morrison, J. M., Gaurin, S., Codispoti, L. A., Takahashi, T., Millero, F. J., Gardner, W. D.,
1016	and Richardson, M. J.: Seasonal evolution of hydrographic properties in the Antarctic
1017	circumpolar current at 170W during 1997-1998, Deep-Sea Research, 148: 3943-3972, 2001.
1018	30. Nakaoka, S., Telszewski, M., Nojiri, Y., Yasunaka, S., Miyazaki, C., Mukai, H., Usui, N.:
1019	Estimating temporal and spatial variation of ocean surface pCO2 in the North Pacific using a
1020	self-organizing map neural network technique, Biogeosciences, 10, 6093-6106, 2013.
1021	31. Nunes Vaz, R. A., Lennon, G. W.: Physical oceanography of the Prydz Bay region of Antarctic
1022	waters, Deep Sea Research Part I: Oceanography Research Papers, 43(5), 603-641, 1996.
1023	32. Pfeil, B., Olsen, A., Bakker, D. C. E., Hankin, S., Koyuk, H., Kozyr, A., Malczyk, J., Manke,
1024	A., Metzl, N., Sabine, C. L., Akl, J., Alin, S. R., Bellerby, R. G. J., Borges, A., Boutin, J.,
1025	Brown, P. J., Cai, W. J., Chavez, F. P., Chen, A., Cosca, C., Fassbender, A. J., Feely, R. A.,
1026	González-Dávila, M., Goyet, C., Hardman-Mountford, N., Heinze, C., Hood, M., Hoppema,
1027	M., Hunt, C. W., Hydes, D., Ishii, M., Johannessen, T., Jones, S. D., Key, R. M., Körtzinger,
1028	A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lenton, A., Lourantou, A., Merlivat, L.,
1029	idorikawa, T., Mintrop, L., Miyazaki, C., Murata ,A., Nakadate, A., Nakano, Y., Nakaoka, Y.
1030	Nojiri, A. M. Omar, X. A. Padin, G. H. Park, K. Paterson, F. F. Perez, S., Pierrot, D., Poisson,
1031	A., Ríos, A. F., Salisbury, J., Santana Casiano, J. M., Sarma, V. V. S. S., Schlitzer, R.,
1032	Schneider, B., Schuster, U., Sieger, R., Skjelvan, I., Steinhoff, T., Suzuki, T., Takahashi, T.,
1033	Tedesco, K., Telszewski, M., Thomas, H., Tilbrook, B., Tjiputra, J., Vandemark, D., Veness,
1034	T., Wanninkhof, R., Watson, A. J., Weiss, R., Wong, C. S., and Yoshikawa-Inoue, H.: A
1035	uniform, quality controlled Surface Ocean CO2 Atlas (SOCAT), Earth Syst. Sci. Data, 5, 125-
1036	143, doi:10.5194/essd-5-125-2013, 2013.
1037	33. Pierrot, D., Neill, C., Sullivan, L., Castle, R., Wanninkhof, R., Lüger, H., Johannessen, T.,
1038	Olsen, A., Feely, R. A., Cosca, C. E.: Recommendations for autonomous underway pCO2
1039	measuring systems and data-reduction routines, Deep-Sea Research Part II, 56, 512-522, 2009.
1040	34. Rangama, Y., Boutin, J., Etcheto, J., Merlivat, L., Takahashi, T., Delille, B., Frankignoulle,
1041	M., Bakker, D. C. E .: Variability of the net air-sea CO2-flux inferred from shipboard and
1042	satellite measurements in the Southern Ocean south of Tasmania and New Zealand, Journal
1043	of Geophysical Research: Oceans (1978-2012), 110(C9), doi: 10.1029/2004JC002619, 2005.
1044	35. Roden, N. P., Shadwick, E. H., Tilbrook, B., Trull, T. W.: Annual cycle of carbonate chemistry

045	and decadal change in coastal Prydz Bay, East Antarctica, Marine Chemistry, 155(4), 135-
046	147, 2013.
047	36. Rubin, S.I., Takahashi, T., Goddard, J.G.: Primary productivity and nutrient utilization ratios
048	in the Pacific sector of the Southern Ocean based on seasonal changes in seawater chemistry,
049	Deep-Sea Research I 45, 1211-1234, 1998.
050	37. Sabine, L., Feely, R. A., Gruber, N., Key, R. M., Lee, K., Bullister, J. L., Wanninkhof, R.,
051	Wong, S., Wallace, D. W. R., Tilbrook, B., Millero, F. J., Peng, TH., Kozyr, A., Ono, T.,
052	and Rios, A. F.: The oceanic sink for anthropogenic CO2, Science, 305, 367-371,
053	doi:10.1126/science.1097403, 2004.
054	38. Sarma, V. V. S. S., Saino, T., Sasaoka, K., Nojiri, Y., Ono, T., Ishii, M., Inoue, H. Y.,
055	Matsumoto, K.: Basin-scale pCO2-distribution using satellite sea surface temperature, Chl a,
056	and climatological salinity in the North Pacific in spring and summer, Global Biogeochemical
057	Cycles, 20, GB3005, doi:10.1029/2005GB002594, 2006.
058	39. Shadwick, E. H., Trull, T. W., Thomas, H., Gibson, J. A. E.: Vulnerability of polar oceans to
059	anthropogenic acidification: comparison of Arctic and Antarctic seasonal cycles, Scientific
060	Reports, 3: 2339, doi: 10.1038/srep02339, 2013.
061	40. Silulwane, N. F., Richardson, A. J., Shillington, F. A., Mitchell Innes, B. A.: Identification
062	and classification of vertical chlorophyll patterns in the Benguela upwelling system and
063	Angola-Benguela front using an artificial neural network, South African Journal of Marine
064	Science, 23, 37-51, 2001.
065	41. Smith, N. R., Zhaoqian, D., Kerry, K. R., Wright, S.: Water masses and circulation in the
066	region of Prydz Bay Antarctica, Deep-sea-research, 31, 1121-1147, 1984.
067	42. Smith, N., Tréguer, P.: Physical and chemical oceanography in the vicinity of Prydz Bay,
068	Antarctica, Cambridge University Press, Cambridge, 1994.
069	43. Spreen, G., Kaleschke, L., Heygster, G.: Sea ice remote sensing using AMSR-E 89 GHz
070	channels, J. Geophys. Res., 113, C02S03, doi:10.1029/2005JC003384, 2008.
071	44. Sun, W. P., Han, Z. B., Hu, C. Y., Pan, J. M.: Particulate barium flux and its relationship with
072	export production on the continental shelf of Prydz Bay, east Antarctica, Marine Chemistry,
073	157, 86-92, 2013.
074	45. Sweeney, C., Hansell, D. A., Carlson, C. A., Codispoti, L. A., Gordon, L. I., Marra, J., Millero,
075	F. J., Smith, W. O., Takahashi, T.: Biogeochemical regimes, net community production and

1076	carbon export in the Ross Sea, Antarctica, Deep Sea Research II, 47(15-16), 3369-3394, 2000.
1077	46. Sweeney, C .: The annual cycle of surface water CO2 and O2 in the Ross Sea: a model for gas
1078	exchange on the continental shelves of Antarctic, Biogeochemistry of the Ross Sea, Antarctic
1079	Research Series, 78, 295-312, 2002.
1080	47. Takahashi, T., Sutherland, S. C., Feely, R. A., and Wanninkhof, R.: Decadal change of the
1081	surface water pCO2 in the North Pacific: A synthenesis of 35 years of observations, J.
1082	Geophys. Res., 111, C07S05, doi: 10.1029/2005JC003074, 2006.
1083	48. Takahashi, T., Sweeney, C., Hales, B., Chipman, D. W., Newberger, T., Goddard, J. G.,
1084	Iannuzzi, R. A., Sutherland, S. C.: The changing carbon cycle in the Southern Ocean,
1085	Oceanography, 25, 26-37, 2012.
1086	49. Telszewski, M., Chazottes, A., Schuster, U., Watson, A. J., Moulin, C., Bakker, D. C. E.,
1087	González-Dávila, M., Johannessen, T., Körtzinger, A., Lüger, H., Olsen, A., Omar, A., Padin,
1088	X. A., Ríos, A. F., Steinhoff, T., Santana-Casiano, M., Wallace, D. W. R., Wanninkhof, R.:
1089	Estimating the monthly pCO ₂ distribution in the North Atlantic using a self-organizing neural
1090	network, Biogeoscience, 6, 1405-1421, 2009.
1091	50. Thomson, R. E., and Fine, I. V.: Estimating mixed layer depth from oceanic profile data, J.
1092	Atmos. Oceanic Technol., 20, 319-329, 2003
1093	51. Ultsch, A., Röske, F.: Self organizing feature maps predicting sea levels, Information
1094	Sciences, 144, 91-125, 2002.
1095	52. Vesanto, J.: Data Exploration Process Based on the Self-Organizing Map: the Finnish
1096	Academies of Technology, 2002.
1097	53. Wanninkhof, R.: Relationship between wind speed and gas exchange over the ocean revisited,
1098	Limnology and Oceanography: Methods, 12, 351-362, 2014.
1099	54. Wong, C. S., Christian, J. R., Emmy Wong, S. K., Page, J., Xie, L., and Johannessen, S.:
1100	Carbon dioxide in surface seawater of the eastern North Pacific Ocean (Line P), 1973-2005,
1101	Deep Sea Res., I, 57(5), 687-695, doi: 10.1016/j.dsr.2010.02.003, 2010.
1102	55. Wu, L., Wang, R., Xiao, W., Ge, S., Chen, Z., Krijgsman, W.: Productivity-climate coupling
1103	recorded in Pleistocene sediments off Prydz Bay (East Antarctica), Palaegeography,
1104	Palaeoclimatology, Palaeoecology, 485, 260-270, 2017.
1105	56. Xu, S., Chen, L., Chen, H., Li, J., Lin, W., Qi, D.: Sea-air CO ₂ -fluxes in the Southern Ocean
1106	for the late spring and early summer in 2009, Remote Sensing of Environment, 175, 158-166,
1	

1107	2016.
1108	57. Yabuki, T., Suga, T., Hanawa, K., Matsuoka, K., Kiwada, H., and Watanabe, T.: Possible
1109	source of the Antarctic Bottom Water in Prydz Bay region, J. Oceanogr., 62, 649-655, doi:
1110	10.1007/s10872-006-0083-1, 2006.
1111	58. Zeng, J., Nojiri, Y., Murphy, P. P., Wong, C. S., Fujinuma, Y.: A comparison of $\triangle pCO_2$
1112	distributions in the northern North Pacific using results from a commercial vessel in 1995-
1113	1999, Deep Sea Res., Part II, 49, 5303-5315, 2002.
1114	59. Zeng, J. Nojiri, Y., Nakaoka, S., Nakajima, H., Shirai, T.: Surface ocean CO2 in 1990-2011
1115	modelled using a feed-forward neural network, Geoscience Data Jounal, 2, 47-51, doi:
1116	10.1002/gdj3.26, 2015.
1117	60. Zeng, J., Mtsunaga, T., Saigusa, N., Shirai, T., Nakaoka, S., Tan, Z.: Technical note:
1118	Evaluation of three machine learning models for surface ocean CO2 mapping, Ocean Sci., 13,
1119	303-313, <u>http://doi.org/10.5194/os-13-303-2017, 2017.</u>
1120	