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Web links to the author's journal account have been redacted from the decision letters as indicated to maintain confidentiality

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14th Mar 22

Dear Dr Mackay,

Your manuscript titled "Re-examining the Southern Ocean CO₂ sink with new wintertime observations" has now been seen by 2 reviewers, and I include their comments at the end of this message. They find your work of interest, but some important points are raised. We are interested in the possibility of publishing your study in Communications Earth & Environment, but would like to consider your responses to these concerns and assess a revised manuscript before we make a final decision on publication.

We therefore invite you to revise and resubmit your manuscript, along with a point-by-point response that takes into account the points raised. Please highlight all changes in the manuscript text file. Should additional work allow you to

- address these criticisms (that is, either to incorporate the suggestions or provide a compelling argument why the point made by the reviewer is not valid, or relevant to the editorial threshold as outlined below),
- provide compelling estimates of the Southern Ocean carbon sink including clear recognition of limitations in the regional scope of your conclusions

AND

- fully explain and justify the algorithms and corrections used in your methodology or adapt these accordingly,
- then we would be happy to look at a revised manuscript.

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

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

[link redacted]

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

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

We understand that due to the current global situation, the time required for revision may be longer than usual. We would appreciate it if you could keep us informed about an estimated timescale for resubmission, to facilitate our planning. Of course, if you are unable to estimate, we are happy to accommodate necessary extensions nevertheless.

Please do not hesitate to contact me if you have any questions or would like to discuss these

revisions further. We look forward to seeing the revised manuscript and thank you for the opportunity to review your work.

Best regards,

Olivier Sulpis, PhD
Editorial Board Member
Communications Earth & Environment
0000-0002-6463-3320

Joe Aslin
Senior Editor
Communications Earth & Environment

EDITORIAL POLICIES AND FORMATTING

We ask that you ensure your manuscript complies with our editorial policies. Please ensure that the following formatting requirements are met, and any checklist relevant to your research is completed and uploaded as a Related Manuscript file type with the revised article.

Editorial Policy: [Policy requirements](https://www.nature.com/documents/nr-editorial-policy-checklist.zip)

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and also in our style and formatting guide [Communications Earth & Environment formatting guide](https://www.nature.com/documents/commsj-phys-style-formatting-guide-accept.pdf) .

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In particular, the Data availability statement should include:

- Unique identifiers (such as DOIs and hyperlinks for datasets in public repositories)
- Accession codes where appropriate

- If applicable, a statement regarding data available with restrictions
- If a dataset has a Digital Object Identifier (DOI) as its unique identifier, we strongly encourage including this in the Reference list and citing the dataset in the Data Availability Statement.

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

REVIEWER COMMENTS:

Reviewer #2 (Remarks to the Author):

This paper re-examines the Southern Ocean carbon sink by applying a method established by a subset of the co-authors to infer wintertime surface pCO₂ levels from DIC profiles collected during summer. Overall, I believe this paper represents a worthwhile effort to apply Mackay and Watson's (2021) pCO₂ reconstruction method to help gap-fill in the Polar Antarctic Zone, and then recompute the fluxes using a state-of-the-art approach with the new co-authors. In so doing, this paper makes their flux reconstruction more comparable to the standards of the field (in comparison to the previous paper's MLR approach used to reconstruct the mapped, time-variable fluxes). It is somewhat comforting that the gap-filled results are very close to the previous reconstructions; that is, adding nearly 800 new observations does not materially change the qualitative understanding of the carbon sink in the Polar Front Zone, while shifting it about 10% lower, an expected consequence of better observing wintertime outgassing. Therefore, I think there is scientific value in the work and support publication after addressing some considerable concerns.

My main concern is with the way the paper is framed, which I think may be misleading. First, the title: There are no new wintertime observations reported here, so the title is factually untrue and should be rewritten. Second, the manuscript scope seems to be the entire Southern Ocean south of 35°S, but, upon examination, it is not very convincing that the work would change anything north of the Antarctic Polar Front. The method only provides pseudo observations south of the APF, and - if I

understand correctly - a different neural net is produced for each biome (however the biomes are chosen). Again, if my understanding is correct, the only biome that will be influenced by the pseudo observations is the one south of the APF. This limitation should be made much more obvious everywhere in the paper, from the Abstract onwards. It is now hidden in the methods and obfuscated in various places. For instance, the sentence that describes the pseudo observations increasing data coverage by 22% south of 35°S using 4°x6° bins may be accurate, but it hides the fact that the data are bunched almost entirely south of 60°S. More importantly, showing the new flux averages for the region south of 35°S in Figures 2 and 3 will lead the reader to infer that flux estimates over this broad region are robust to the addition of new data. In reality, that inference is only appropriate for the highest latitude slice of the Southern ocean.

My recommendation would be to align the scope of the text with the actual capability of the method: that is, write a story about the region south of the APF. The narrower manuscript could more meaningfully explore the spatial pattern of the correction, as well as the qualitative changes in the time series, possibly diving deeper into inferred mechanisms of inter annual variability.

Below I offer a few more specific suggestions, but hold back from making too many minor comments, since my main recommendation could result in some major changes.

Figure 1: Mark the added data with a black dot so the reader can more readily discern the spatial distribution of the added data

Figure 1 caption: Is the gray shading where there are surface fCO₂ observations in non-winter?

Figure 2 shows that the pseudo observations are essentially inconsequential to the seasonal cycle and inter annual variability, which would be expected given the extremely limited spatial distribution of the results.

Is the shading 1 sigma of the Monte Carlo results?

It's unclear what Figure 3 adds to the discussion, since there is no text that deeply explores the differences between the sectors.

Ocean carbon uptake is mostly due to chemistry, not biology, so I quibble with describing it as an "ecosystem service."

"UN Stocktake" - I believe this is a shorthand for the annual Global Carbon Budget program, but it should be appropriately spelled out and referenced.

Reference 24 is not a proper reference (year? Journal?)

Methods: give the spatial and temporal resolution of the CCMP wind product used (and justify the choice)

[Type here]

Title: Re-examining the Southern Ocean CO₂ sink with new wintertime observations

Authors: Neill Mackay et al.

Journal: Communications Earth & Environment

Summary:

The authors use subsurface observations of dissolved inorganic carbon (DIC) from the GLODAPv2 data product and estimates of total alkalinity (TA) derived from a global biogeochemical algorithm (LIAR) to create pseudo-observations of surface $p\text{CO}_2$ during winter in the Southern Ocean. This effort is motivated by uncertainty in the magnitude of decadal variability in Southern Ocean CO₂ flux, which largely stems from a paucity of observations during the inclement season. This effort builds on the author's prior work, increasing the spatiotemporal coverage of Southern Ocean wintertime pseudo-observations by 22%. Additionally, this work advances the prior effort by: extending the study region to lower latitudes; implementing a marine boundary layer temperature correction to the surface $p\text{CO}_2$ values; including a variable MLD; and using a neural network gap-filling approach, rather than a multiple linear regression approach. The authors also test their methodology in a data assimilating BGC ocean model. From their reconstructed surface $p\text{CO}_2$ values they compute air-sea fluxes and conclude that there is strong decadal variability in the Southern Ocean CO₂ flux over the study period. The inclusion of wintertime observations reduces the Southern Ocean sink strength; however, implementation of a marine boundary layer thermal correction more than compensates for this reduction, leading to an overall increase in their mean estimate of the Southern Ocean carbon sink relative to prior estimates for the period of study.

Recommendation:

The manuscript is well written, and the figures are clear. This study builds substantively from the work of multiple coauthors on the paper, as well as the lead author's related prior work, and reflects an important contribution, particularly by adding the marine boundary layer thermal correction. There are a few key issues that I feel need to be addressed prior to publication. My remaining comments are technical edits or suggestions to further clarify the results. I expect the authors will be able to address my major comments during revision.

Major Comment 1:

I find it perplexing that the authors are using the LIAR algorithm to estimate TA when they can simply use GLODAPv2 TA data at the locations of interest. I understand that the SOCAT observations used in their study require a TA estimate, but this is not the case for the GLODAP data. This is important because the global biogeochemical algorithms are notoriously mediocre (and sometimes bad) at reproducing the seasonality of carbonate system parameters in the surface ocean. Thus, the authors are likely introducing unnecessary uncertainty into their analysis. While surface TA variations are largely controlled by freshwater fluxes, the Southern Ocean is home to the Great Calcite belt, which may not be well captured in LIAR.

Major Comment 2:

While the premise of the manuscript is centered on Southern Ocean CO₂ flux variability, to me, the real contribution of this work comes in the updated $p\text{CO}_2$ data product. I find it strange that the authors don't spend a bit more time on this for two reasons. First, Earth System Model CO₂ flux discrepancies are largest in the high latitude regions, and this is largely caused by an inability to accurately model the $p\text{CO}_2$ seasonality. Second, there are known biases in observational wind speed products that may be introducing bias to the flux calculations. I would advocate that the authors show the $p\text{CO}_2$ seasonal cycle

[Type here]

and trends (as in figure 2) in addition to the CO₂ fluxes and release both the pCO₂ and CO₂ flux products upon publication.

Major Comment 3:

The authors focus heavily on the decadal CO₂ flux variability in the Southern Ocean; however, their work only contributes new information to the 2004-2018 period – after the Southern Ocean carbon sink reinvigoration. So, in fact, the only decadal variability they capture is the stagnation around 2010, which is rather minor compared to the early 2000s inflection. Interestingly, in their prior work, Mackay and Watson (2021) did not see such a stagnation (their Figure 6). This issue is very briefly mentioned in the manuscript introduction (Line 52) but is never returned to and seems to be an important point to address. For example, is this discrepancy due to the different spatial scales of the studies; the distribution of wintertime data added in the new study; use of the SOM-FFN method rather than an MLR approach; or something else entirely? It seems like the updates made when transitioning from your MLR approach to the SOM FFN approach had a larger impact on the decadal variability result than adding more pseudo-observations did (i.e., Figure 3), but this is not the framing used by the authors in the abstract.

Major Comment 4:

Line 164: Where does the AOU disequilibrium correction of -13.5 umol/kg come from? I see that it was used in Mackay and Watson (2021), but that paper points to Bushinsky et al. (2017), where I cannot find this number. Additionally, Carter et al., (2021: 10.1029/2020GB006623) provides a subsurface estimate of preformed oxygen (i.e., AOU corrected for disequilibrium when the water parcel subducted). The product doesn't resolve the mixed layer, so I'm not certain how shallow they go in the SO, but it might be worth checking out. The AOU disequilibrium corrections can be quite large (~200 umol/kg).

[image redacted]

Technical Comments:

- **Figure 1 caption:** “Light grey shading shows the coverage of all SOCAT fCO₂ observations for the same period on the same grid”.
 - By same period, do you mean other months from the same years?
 - It would be helpful to include a figure in the supplement like Figure 1 from Mackay and Watson 2021 to clarify the exact locations of the new GLODAP observations. It would help to see a histogram of all pseudo-observations versus month of year and versus year, and of all pCO₂ observations used to train the SOM-FFN versus month of year and versus year. The latter may already be published elsewhere, so referencing it would suffice.
- **Line 47:** The authors state that profiling floats and surface vehicles are not yet suited to diagnosing the uncertain low frequency variability they seek in the Southern Ocean. This is perplexing because on Line 51, the authors compare the method they are using with prior work based on the SOCCOM+SOCAT pCO₂ training dataset. Additionally, the authors do include the SOCCOM+SOCAT

[Type here]

trained SOM-FFN results in Mackay and Watson (2021) and the SOCCOM+SOCAT results do show the ~2010 CO₂ flux stagnation – which is the only low frequency variability the authors show in the manuscript under consideration. Perhaps I've missed something?

- **Line 80:** Please clarify what you mean by runs?
- **Line 76:** The Southern Ocean carbon sink with the pseudo-observations is reduced by 0.11 PgC/yr. The Southern Ocean carbon with the MBL correction is enhanced by 0.3 PgC/yr. So, shouldn't the sink change from -1.12 PgC/yr to -1.31 PgC/yr? On Line 82 the authors note a new sink of -1.29 PgC/yr. Is this a rounding issue?
- **Line 84:** Why not include the Long et al., (2021) aircraft data from their Figure 4a in your Figure 2a? I realize their results are from south of 45 S, so perhaps a direct comparison of this regional subset in the supplement is more appropriate. I realize this paper was very recently published, but it is a nice, independent point of comparison to consider.
- **Line 92:** Should this be updated to: "here defined by the **climatological** month of minimum (September) and maximum (February) uptake, respectively"?
- **Line 93:** This statement seems to be true for all the plots.
- **Line 96:** Is this *summertime* variability or *February* variability? Is it true that the February flux variability is reflective of the seasonal variability or could interannual phenology changes be impacting your result?
- **Line 98:** The winter and summer signals in the Indian basin also seem decoupled.
- **Line 102:** What is meant by variability here? Standard deviation or variance over period of interest?
- **Figure 3:** The differences between signals with and without pseudo-observations are hard to identify and not particularly compelling. Would an x-y plot of these data with the symbols outlined in black/red/blue and colored by year (e.g., gray scale) be more useful? It seems like the updates made when transitioning from your MLR approach to the SOM FFN approach had a larger impact on the decadal variability result than adding more pseudo-observations.
- **Data Availability:** It's not clear if the authors intend to release their data products for *p*CO₂ or CO₂ flux. I expect the pseudo-obs *p*CO₂ product would be widely used if released as a curated product.
- **References:**
 - There is an issue with how "CO 2" is formatted in the References section.
 - The Mackay and Watson (2021) paper seems to be referenced twice under numbers 14 and 24.
 - **Line 81:** Should the Watson et al., (2020) paper be referenced here?

Response to reviewers

We are grateful to both reviewers for their careful consideration of our manuscript, and their constructive comments. As a result of the major comments of both reviewers, we have made two significant changes to the structure of the manuscript. We have added a figure showing the seasonal cycle and trends of $p\text{CO}_2$ (new Figure 2) and associated discussion, and have shifted the focus from the whole Southern Ocean to the region south of the Antarctic Polar front, adding the fluxes for the smaller region as a new Figure 3. We still present the full Southern Ocean fluxes at the end of the Results section, for context. We have also removed the old Figure 3 and associated discussion that showed detrended fluxes split by basin, because as noted by both reviewers, the difference made by the pseudo observations is not particularly compelling, and these plots did not add much to the story. Please see below for detailed responses to both reviewers' comments.

Reviewer #1

Major comments

I find it perplexing that the authors are using the LIAR algorithm to estimate TA when they can simply use GLODAPv2 TA data at the locations of interest. I understand that the SOCAT observations used in their study require a TA estimate, but this is not the case for the GLODAP data. This is important because the global biogeochemical algorithms are notoriously mediocre (and sometimes bad) at reproducing the seasonality of carbonate system parameters in the surface ocean. Thus, the authors are likely introducing unnecessary uncertainty into their analysis. While surface TA variations are largely controlled by freshwater fluxes, the Southern Ocean is home to the Great Calcite belt, which may not be well captured in LIAR.

It is true that LIAR has its limitations, however the alternative is not quite as simple as switching to the GLODAP in-situ TA. Since we are working with summer profiles to construct the pseudo observations, and we are aiming for wintertime $p\text{CO}_2$, the TA needs adjusting for the winter-summer changes, just as we did with DIC. We explored the DIC correction in detail for Mackay and Watson (2021), but for the winter TA we opted, in LIAR, for a product already tested. We did also explore another alkalinity product, CANYON-B, at the time, and found that LIAR gave better results for our validation. An additional complication with the suggestion to use GLODAP TA for the pseudo observations is that not all of the profiles with DIC also have TA, so in order to produce the full set of pseudo observations it would be necessary to use a combination of GLODAP and LIAR (or other TA estimate). In the light of all this, we feel that the most defensible solution is to use LIAR TA for all the pseudo observations, as we did for the first paper. We have, nonetheless, tried substituting LIAR TA for adjusted GLODAP TA in the pseudo observations and retrained the SOM-FFN for one of our ensemble configurations, and we found that it makes quite a small difference.

While the premise of the manuscript is centered on Southern Ocean CO_2 flux variability, to me, the real contribution of this work comes in the updated $p\text{CO}_2$ data product. I find it strange that the authors don't spend a bit more time on this for two reasons. First, Earth System Model CO_2 flux discrepancies are largest in the high latitude regions, and this is largely caused by an inability to accurately model the $p\text{CO}_2$ seasonality. Second, there are known biases in observational wind speed products that may be introducing bias to the flux calculations. I would advocate that the authors

show the $p\text{CO}_2$ seasonal cycle and trends (as in figure 2) in addition to the CO_2 fluxes and release both the $p\text{CO}_2$ and CO_2 flux products upon publication.

We appreciate this helpful suggestion: we have now added a new figure showing the results for $p\text{CO}_2$ (Figure 3 in the new draft), and discuss it at the beginning of the Results section (lines 70-81). We also have made arrangements to release both data products upon publication.

The authors focus heavily on the decadal CO_2 flux variability in the Southern Ocean; however, their work only contributes new information to the 2004-2018 period – after the Southern Ocean carbon sink reinvigoration. So, in fact, the only decadal variability they capture is the stagnation around 2010, which is rather minor compared to the early 2000s inflection. Interestingly, in their prior work, Mackay and Watson (2021) did not see such a stagnation (their Figure 6). This issue is very briefly mentioned in the manuscript introduction (Line 52) but is never returned to and seems to be an important point to address. For example, is this discrepancy due to the different spatial scales of the studies; the distribution of wintertime data added in the new study; use of the SOM-FFN method rather than an MLR approach; or something else entirely? It seems like the updates made when transitioning from your MLR approach to the SOM FFN approach had a larger impact on the decadal variability result than adding more pseudo-observations did (i.e., Figure 3), but this is not the framing used by the authors in the abstract.

This is a good point. We now note the limitations of the short time period of the pseudo observations in lines 147-151, and have added a discussion of the comparison between the present work and Mackay and Watson (2021) in lines 152-167. Please note, however, that our results compare comparatively well with figure D1 in the appendix of that paper, where the MLR was split and run individually on the periods 2004-2011 and 2011-2017, and this is where we have focused our comparison.

Line 164: Where does the AOU disequilibrium correction of $-13.5 \mu\text{mol/kg}$ come from? I see that it was used in Mackay and Watson (2021), but that paper points to Bushinsky et al. (2017), where I cannot find this number. Additionally, Carter et al., (2021: 10.1029/2020GB006623) provides a subsurface estimate of preformed oxygen (i.e., AOU corrected for disequilibrium when the water parcel subducted). The product doesn't resolve the mixed layer, so I'm not certain how shallow they go in the SO, but it might be worth checking out. The AOU disequilibrium corrections can be quite large ($\sim 200 \mu\text{mol/kg}$).

The $-13.5 \mu\text{mol/kg}$ correction was worked out directly from the SOCCOM float data, which contains oxygen concentration and percentage oxygen saturation values. We calculated the mean oxygen undersaturation in the top 10m over the region south of the polar front and away from sea ice, as we have defined it for calculating our pseudo observations (this is now explained in lines 193-196).

Having obtained the Carter et al. preformed oxygen estimates, we note that they are long-term averages. Given that there is a strong seasonality to the undersaturation, we feel that our approach of working out a spatial mean for September (the month to which our pseudo observations are assumed to correspond) over the whole region using the SOCCOM float data is preferable. Although we miss the small-scale spatial variability, we would argue that using values from the Carter product that apply to the annual mean is a worse option since they are biased with respect to the correction that needs applying in winter.

Minor comments

Figure 1 caption: “Light grey shading shows the coverage of all SOCAT fCO₂ observations for the same period on the same grid”. By same period, do you mean other months from the same years? It would be helpful to include a figure in the supplement like Figure 1 from Mackay and Watson 2021 to clarify the exact locations of the new GLODAP observations. It would help to see a histogram of all pseudo-observations versus month of year and versus year, and of all pCO₂ observations used to train the SOM-FFN versus month of year and versus year. The latter may already be published elsewhere, so referencing it would suffice.

We have clarified the caption on Figure 1, added the exact locations of the pseudo observations as black dots, and also added a histogram Figure S3 in the supplementary material.

Line 47: The authors state that profiling floats and surface vehicles are not yet suited to diagnosing the uncertain low frequency variability they seek in the Southern Ocean. This is perplexing because on Line 51, the authors compare the method they are using with prior work based on the SOCCOM+SOCAT pCO₂ training dataset. Additionally, the authors do include the SOCCOM+SOCAT trained SOM-FFN results in Mackay and Watson (2021) and the SOCCOM+SOCAT results do show the ~2010 CO₂ flux stagnation – which is the only low frequency variability the authors show in the manuscript under consideration. Perhaps I’ve missed something?

The reason that the SOCCOM data are not suited to looking at low frequency variability, even that since 2004 which we are able to study with our pseudo observations, is that the floats began to be deployed in 2014 (line 44), therefore miss the whole of the reinvigoration and the beginning of the stagnation. By adding pseudo observations that go back to 2004, we are in a better position to examine that variability at this point in time. Of course, when we have another decade of float data things should be much clearer at least with respect to any recent variability on the same timescale, hence ‘not yet suited’.

Line 80: Please clarify what you mean by runs?

This referred to runs of the SOM-FFN pCO₂ mapping; we have now made this clearer in the text (lines 131-132).

Line 76: The Southern Ocean carbon sink with the pseudo-observations is reduced by 0.11 PgC/yr. The Southern Ocean carbon with the MBL correction is enhanced by 0.3 PgC/yr. So, shouldn’t the sink change from -1.12 PgC/yr to -1.31 PgC/yr? On Line 82 the authors note a new sink of -1.29 PgC/yr. Is this a rounding issue?

The means quoted are for different time periods, and the difference is not related to the MBL correction. The reason for focusing on the 2004-2008 period in quoting the sink change was to highlight the difference made by the pseudo observations in this narrow window. Realising that this was a bit confusing, we now quote the difference due to the pseudo observations for the slightly longer period of 2004-2011, and explain the choice of that window in lines 92-95. The mean for the full pseudo obs period is still quoted at line 135, now for both the region south of the polar front and south of 35°S.

Line 84: Why not include the Long et al., (2021) aircraft data from their Figure 4a in your Figure 2a? I realize their results are from south of 45 S, so perhaps a direct comparison of this regional subset in the supplement is more appropriate. I realize this paper was very recently published, but it is a nice, independent point of comparison to consider.

We have added a figure in the Supplementary Information (S5) and reference it in the main text at line 138.

Line 92: Should this be updated to: “here defined by the **climatological** month of minimum (September) and maximum (February) uptake, respectively”?

In the light of your comments and those of reviewer #2, we have removed Figure 3 and the discussion relating to it.

Line 93: This statement seems to be true for all the plots.

This statement has been removed.

Line 96: Is this *summertime* variability or *February* variability? Is it true that the February flux variability is reflective of the seasonal variability or could interannual phenology changes be impacting your result?

This sentence has been removed

Line 98: The winter and summer signals in the Indian basin also seem decoupled.

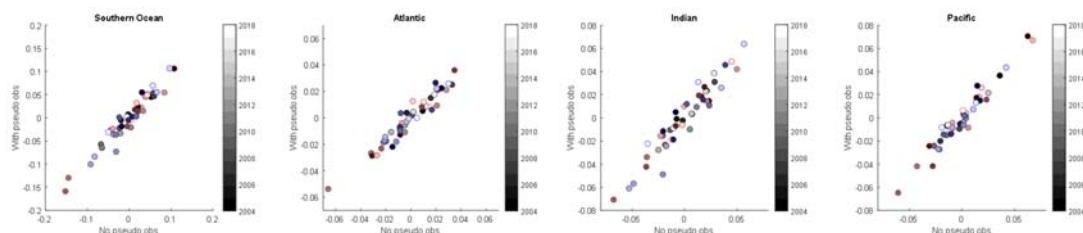
This sentence has been removed

Line 102: What is meant by variability here? Standard deviation or variance over period of interest?

This sentence has been removed

Figure 3: The differences between signals with and without pseudo-observations are hard to identify and not particularly compelling. Would an x-y plot of these data with the symbols outlined in black/red/blue and colored by year (e.g., gray scale) be more useful? It seems like the updates made when transitioning from your MLR approach to the SOM FFN approach had a larger impact on the decadal variability result than adding more pseudo-observations.

We weren't quite clear on what you meant here in terms of an alternative plot; I did try making a plot following your suggestions, and it looks like this:



In the end, however, we tend to agree with yours and the other reviewer's comments that these basin-level comparisons do not add very much to the paper, so we have removed this part of the discussion in preference for focusing on the other points you raised.

Data Availability: It's not clear if the authors intend to release their data products for $p\text{CO}_2$ or CO_2 flux. I expect the pseudo-obs $p\text{CO}_2$ product would be widely used if released as a curated product.

We will release the $p\text{CO}_2$ and CO_2 flux products on publication as you suggest; they will be housed at the NCEI OCADS national database, as now detailed in the 'Data availability' section (lines 335-338).

References:

There is an issue with how “CO 2” is formatted in the References section.

We have fixed the formatting of CO₂.

The Mackay and Watson (2021) paper seems to be referenced twice under numbers 14 and 24.

Fixed.

Line 81: Should the Watson et al., (2020) paper be referenced here?

You are correct! We have now fixed this error.

Reviewer #2

Major comments

My main concern is with the way the paper is framed, which I think may be misleading. First, the title: There are no new wintertime observations reported here, so the title is factually untrue and should be rewritten. Second, the manuscript scope seems to be the entire Southern Ocean south of 35°S, but, upon examination, it is not very convincing that the work would change anything north of the Antarctic Polar Front. The method only provides pseudo observations south of the APF, and - if I understand correctly - a different neural net is produced for each biome (however the biomes are chosen). Again, if my understanding is correct, the only biome that will be influenced by the pseudo observations is the one south of the APF. This limitation should be made much more obvious everywhere in the paper, from the Abstract onwards. It is now hidden in the methods and obfuscated in various places. For instance, the sentence that describes the pseudo observations increasing data coverage by 22% south of 35°S using 4°x6° bins may be accurate, but it hides the fact that the data are bunched almost entirely south of 60°S. More importantly, showing the new flux averages for the region south of 35°S in Figures 2 and 3 will lead the reader to infer that flux estimates over this broad region are robust to the addition of new data. In reality, that inference is only appropriate for the highest latitude slice of the Southern ocean.

My recommendation would be to align the scope of the text with the actual capability of the method: that is, write a story about the region south of the APF. The narrower manuscript could more meaningfully explore the spatial pattern of the correction, as well as the qualitative changes in the time series, possibly diving deeper into inferred mechanisms of inter annual variability.

Thank you for your suggestions; we agree with the points you made. We have renamed the manuscript to avoid using the phrase 'new observations'. We now also focus our results on the region south of the APF (new figures 2 and 3 and accompanying discussion lines 70-100), and have tweaked the other parts of the manuscript and abstract to reflect this shift (lines 50, 58, 122-124, 135, 146, 170.). We do still present the full south of 35°S fluxes at the end of the Results section (Figure 5 and lines 122-138) for context, but they are now given less prominence.

Minor comments

Figure 1: Mark the added data with a black dot so the reader can more readily discern the spatial distribution of the added data

We have added the locations of the pseudo observations as black dots on Figure 1b

Figure 1 caption: Is the gray shading where there are surface fCO₂ observations in non-winter?

Yes that's correct; we now make this clear in the caption.

Figure 2 shows that the pseudo observations are essentially inconsequential to the seasonal cycle and inter annual variability, which would be expected given the extremely limited spatial distribution of the results.

Yes, it is true that the pseudo observations do not make a huge difference, either to the whole Southern Ocean mean fluxes, or to the mean fluxes south of the polar front as shown on the new Figure 2.

Is the shading 1 sigma of the Monte Carlo results?

The shading represents the 1-sigma uncertainty, but not from Monte Carlo simulations; rather from a combination of errors due to pCO₂ gridding, mapping and the gas transfer velocity. These are described in the Methods (lines 303-318), and signposted in the Figure captions.

It's unclear what Figure 3 adds to the discussion, since there is no text that deeply explores the differences between the sectors.

On reflection, we agree that Figure 3 was not particularly helpful; we have removed it along with the discussion relating to it.

Ocean carbon uptake is mostly due to chemistry, not biology, so I quibble with describing it as an "ecosystem service."

This phrase has been removed.

"UN Stocktake" - I believe this is a shorthand for the annual Global Carbon Budget program, but it should be appropriately spelled out and referenced.

We now reference the Global Carbon Budget here (line 30).

Reference 24 is not a proper reference (year? Journal?)

Thank you for pointing this out - it was an error due to some glitches with the referencing software. We have now corrected the references including this one.

Methods: give the spatial and temporal resolution of the CCMP wind product used (and justify the choice)

We have added these details at lines 293-295.

8th Aug 22

Dear Dr Mackay,

Please allow us to apologise for the delay in sending a decision on your manuscript titled "Re-examining the Southern Ocean CO₂ sink with improved winter data coverage extrapolated from summertime observations". It has now been seen by our reviewers, whose comments appear below. In light of their advice I am delighted to say that we are happy, in principle, to publish a suitably revised version in Communications Earth & Environment under the open access CC BY license (Creative Commons Attribution v4.0 International License).

We therefore invite you to revise your paper one last time to address the remaining concerns of our reviewers. In particular, please ensure that you:

- 1) re-set the emphasis to the new observation gap-filling method,
- 2) explain and justify the use of a Redfield carbon to oxygen ratio,
- 3) better justify your statement that "strong decadal variations remain with improved winter data coverage" or soften it accordingly.

At the same time we ask that you edit your manuscript to comply with our format requirements and to maximise the accessibility and therefore the impact of your work.

EDITORIAL REQUESTS:

Please review our specific editorial comments and requests regarding your manuscript in the attached "Editorial Requests Table". Please outline your response to each request in the right hand column. Please upload the completed table with your manuscript files.

If you have any questions or concerns about any of our requests, please do not hesitate to contact me.

SUBMISSION INFORMATION:

In order to accept your paper, we require the files listed at the end of the Editorial Requests Table; the list of required files is also available at <https://www.nature.com/documents/commsj-file-checklist.pdf>.

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Please use the following link to submit the above items:

[link redacted]

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

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

Best regards,

Olivier Sulpis
Editorial Board Member
Communications Earth & Environment

Joe Aslin
Locum Chief Editor,
Communications Earth & Environment
<https://www.nature.com/commsenv/>
Twitter: @CommsEarth

REVIEWERS' COMMENTS:

Reviewer #1 (Remarks to the Author):

Please see attached document.

Reviewer #2 (Remarks to the Author):

First, I apologize for the slow review - the second round arrived at a hectic time for me. The new version of the manuscript has addressed all of my major concerns. The new version more honestly reports on the scope of improvements to the Southern Ocean flux estimates by focusing on the region south of the APF. I believe it is a valuable contribution and should be published after attention to some minor details, explained below.

Check references. I found an issue in "n/a n/a" in ref 18 of the bibliography.

Line 28 - for the statistic of the SO absorbing 40% of the anthropogenic CO₂, give a definition of

Southern Ocean (i.e. what is the northern boundary)?

Figure 2 caption - where does the atmospheric CO₂ estimate come from?

72 - "has reduced" should "is reduced"

74 - Would it be clearer to say that the seasonal cycle of pCO₂ is anticorrelated with temperature (rather than "out of phase with the seasonal cycle of temperature"), likely because the wintertime cooling is associated with deeper mixed layers and vertical mixing that stirs high DIC water to the surface?

120-121 At least comment on how your "refinement" fits in any of these pictures. Is it consistent (or at odds) with any of the previous explanations?

146 - "modest increase in winter "pseudo-observations"

154 -Why was MLR "necessary" when the first paper was written but not now?

300 - Briefly explain where the atmospheric CO₂ product is from (besides just referencing the original paper)

315 - Explain why 20% uncertainty on K is chosen

Title: Re-examining the Southern Ocean CO₂ sink with improved winter data coverage extrapolated from summertime observations

Authors: Neill Mackay et al.

Journal: Communications Earth & Environment

Recommendation:

I want to thank the authors for addressing many of my prior concerns. However, I still find discontinuity with the manuscript framing and what the results convincingly convey. In particular, the wintertime pseudo-observation data volume is increased by only 38 GLODAP data points (from 760 to 798) relative to the prior study by Mackay and Watson (2021). This suggests that this study is less about using new wintertime observations to improve the Southern Ocean flux estimate and more about using a new gap filling technique (going from MLR to Neural Network) with primarily existing wintertime pseudo-observations. It almost seems like the title should be *Re-examining the Southern Ocean CO₂ sink with an improved method for modeling wintertime pCO₂* since the model rather than winter data addition is likely driving the change. Additionally, I have some concerns about how AOU was corrected for disequilibrium. I therefore recommend moderate revisions and potential reframing to align the content with the story.

Major Comment 1:

Considering that Antarctic winter sea ice extent reaches a maximum in September and all pseudo-observations are pinned to that month, it seems that most pseudo-observations will be under ice and will not contribute directly to air-sea CO₂ flux estimates. The authors could make this much clearer, as it implies that most of the pseudo-observations are playing an indirect role in updating the Southern Ocean CO₂ flux estimates through their influence on the pCO₂ gap-filling step – which was the major methodological change from Mackay and Watson 2021 to this paper. This is particularly relevant because areas exhibiting the largest CO₂ flux changes due to the addition of pseudo-observations (Figure 4) generally (1) do not include pseudo-observations or (2) have pseudo-observations that would likely be under sea ice and not contributing to the fluxes directly (now clear from Figure 3b). Therefore, it seems that the change in pCO₂ gap-filling approach is likely most critical to the novelty of this result. Conveying this information could be easily accomplished by creating a map of the September (or annual mean) difference in pCO₂ derived from MLR and SOM-FFN gap filling procedures when including a common subset of the pseudo-observations. The figure could include the locations of pseudo-observation (like shown in Figure 1) and the mean winter sea ice extent (as shown clearly in Mackay and Watson 2021). This would help to clarify how important the gap-filling technique is and where it is important relative to the pseudo-observations. While this is not the story the authors are trying to tell, I think it is equally valuable and better reflects what this paper contributes.

For example, Line 17: “Here, we present a new estimate of the Southern Ocean CO₂ sink that addresses historically sparse wintertime sampling through interpretation of subsurface summertime observations south of the Antarctic Polar Front (APF) to produce new and independent ‘pseudo’ wintertime observations of surface fCO₂, increasing the wintertime data coverage in that region by 68%.”

Does “new” and 68% pertain to the newly added 38 GLODAP observations that this study incorporates or does the 68% include existing pseudo-observations from the authors’ prior work? It seems like the emphasis should be on using an advanced gap-filling method with slightly more

wintertime pseudo-observations that are used to train a more sophisticated model, having an important influence on remote fluxes, relative to the pseudo-observation locations.

Major Comment 2:

Line 193: “We then adjust the concentration of dissolved inorganic carbon (DIC) from the TML for biological activity that occurred in the water mass since last winter using the apparent oxygen utilisation (AOU) and a Redfield ratio $RR_{C:O}$, obtaining an estimate for the wintertime surface DIC concentration.” **Line 219:** “We then repeated the calculation for a range of parameters a , and b , and two alternative values of $RR_{C:O}$, each time calculating the resulting RMSE between the set of model pseudo observations and their wintertime equivalents.”

I believe B-SOSE uses a fixed C:O (and fixed C:N) for biological organic matter production, so it's not clear that the authors should be using an $RR_{C:O}$ value that differs from B-SOSE to optimize their a and b parameters for the AOU disequilibrium correction. Can you please elaborate on why you are not using the B-SOSE fixed $RR_{C:O}$ – this is critical to the reconstruction of winter pseudo-observations.

Major Comment 3:

Line 150: “Here we have found instead that strong low frequency variability from 1993-2018 is robust to a modest increase in winter data coverage at high latitudes, suggesting the Southern Ocean carbon sink variability is relatively well constrained by sparse observations using this method. However, we note here the caveat that we have only boosted data coverage from 2004 onwards, and as such, our conclusions about the robustness of the variability only apply to the most recent period encompassing the reinvigoration and subsequent stagnation of the sink. A definitively constrained estimate of the variability in the most data-sparse period before 2000 remains elusive.”

For example, line 21: We show through a machine learning-based mapping method, that strong decadal variations remain with improved winter data coverage.

There is rather little variability over the 2000-2018 period, with the post 2010 stagnation being insignificant w.r.t the data product uncertainties. Thus, it's not clear that “strong decadal variations remain with improved winter data coverage.” Would a different framing be that you have achieved a similar pattern of variability with and without pseudo-observations and using two different gap-filling approaches (prior study relative to this one)?

“...by sparse observations” do you also mean by seasonally biased observations?

Technical Comments:

Line 31: “Estimates of air-sea CO_2 fluxes from models, observation-based data products and observations show the largest disagreement in the Southern Ocean, in particular with regard to low frequency variations⁴. Given the lack of direct measurements in this remote and harsh ocean region, this disagreement does not come as a surprise.”

This seems like an odd comment since your study also does not add direct measurements, but you are attempting to argue that the pseudo-observations provide evidence that observational data products are not overestimating low frequency variability.

Line 40: “..air-sea CO_2 fluxes are then computed combining the mapped values using a simple bulk gas transfer parametrization.”

Typo?

Line 56: “In this work, we build on this novel constraint, increasing the number of pseudo observations **from 760 to 798** using the latest version of GLODAP^{17, 22}.”

Suggested text rearrangement for clarity.

Line 66: This altered the **global** ocean CO₂ sink by 0.8-0.9 PgC yr⁻¹ globally, **yet** no regional correction for the Southern Ocean exists.

Clarify global and remove “but yet”

Line 87: “However, the reduction in pCO₂ occurs **in the sea ice** (see supplementary Figure S2),...”

In the sea ice zone or below the sea ice?

Line 90: “The peak winter outgassing increases fractionally from 0.09 PgC yr⁻¹ to 0.12 PgC yr⁻¹, and is shifted from July to September; meanwhile the magnitude of the **flux** seasonal cycle increases from 0.66 to 0.69 PgC yr⁻¹.”

Is this because nearly all the new pseudo-observations for winter are during September (Figure S3)?

Line 101: “Without the pseudo observations the sink south of the APF increases by 0.22 PgC yr⁻¹ over that period; when they are added the increase is 0.25 PgC yr⁻¹.”

It would be more convincing to compare trends for this period rather than specific start and end years, given the uncertainty.

Line 141: “Our results are consistent with two atmospheric inversions (Figure 5 dashed lines), which are based on a set of independent measurements, and with a recent study that estimated the Southern Ocean sink using aircraft data³⁰ (see supplementary Figure S5).”

Your results both with and without pseudo-observations seem equally in alignment with the aircraft observations, based on the uncertainties.

Line 169: “The difference could be explained by a number of factors, including the different gap-filling methods, the longer training dataset used in the current study (1993-2018 compared to 2004-2017), a larger set of driver variables (see Supplementary Table 1; the MLR study used only temperature, salinity, mixed layer depth and atmospheric CO₂ concentration), **and perhaps least significantly, the additional pCO₂ and pseudo-data used here.**”

You seem to agree that the addition of pseudo-observations may be playing the smallest role in your results, with the revised gap-filling technique (from MLR to Neural Network) perhaps being the greatest contribution. I find that the updated results in combination with the current manuscript framing (that new winter observations help to validate the larger interannual variability found in data-based pCO₂ products) make this a rather unconvincing study – there were only 38 new wintertime observations. It seems like an altered framing around the importance of the gap-filling technique used, availability of seasonally representative training data, and how these things impact remote pCO₂ estimates and air-sea fluxes, in combination with the skin temperature adjustment, would be more valuable contribution.

Line 204: Typo in spelling alkalinity.

Reference is missing year: Mackay, N. & Watson, A. Winter air-sea CO₂ fluxes constructed from summer observations of the Polar Southern Ocean suggest weak outgassing. 1–25

Response to reviewers

We would like to thank both reviewers for their continued engagement with our work and further constructive comments. The changes we have made to address them are outlined below in blue, with line numbers referring to the revised manuscript. Please note that we have also moved the table detailing our data sources from the supplementary material to the main manuscript in order to comply with editorial requirements.

Reviewer #1

Major comments

I want to thank the authors for addressing many of my prior concerns. However, I still find discontinuity with the manuscript framing and what the results convincingly convey. In particular, the wintertime pseudo-observation data volume is increased by only 38 GLODAP data points (from 760 to 798) relative to the prior study by Mackay and Watson (2021). This suggests that this study is less about using new wintertime observations to improve the Southern Ocean flux estimate and more about using a new gap filling technique (going from MLR to Neural Network) with primarily existing wintertime pseudo-observations. It almost seems like the title should be ***Reexamining the Southern Ocean CO₂ sink with an improved method for modeling wintertime pCO₂*** since the model rather than winter data addition is likely driving the change.

Thank you for the title suggestion - we have adopted it, as we believe the phrase “improved method for modelling” incorporates both novel strengths of the manuscript, that is the addition of wintertime data, plus the refined mapping approach. We have also made a number of other changes to the abstract, introduction, and discussion, to alter the framing of the manuscript (lines 19-25, 56-60, 172-178, 198-207).

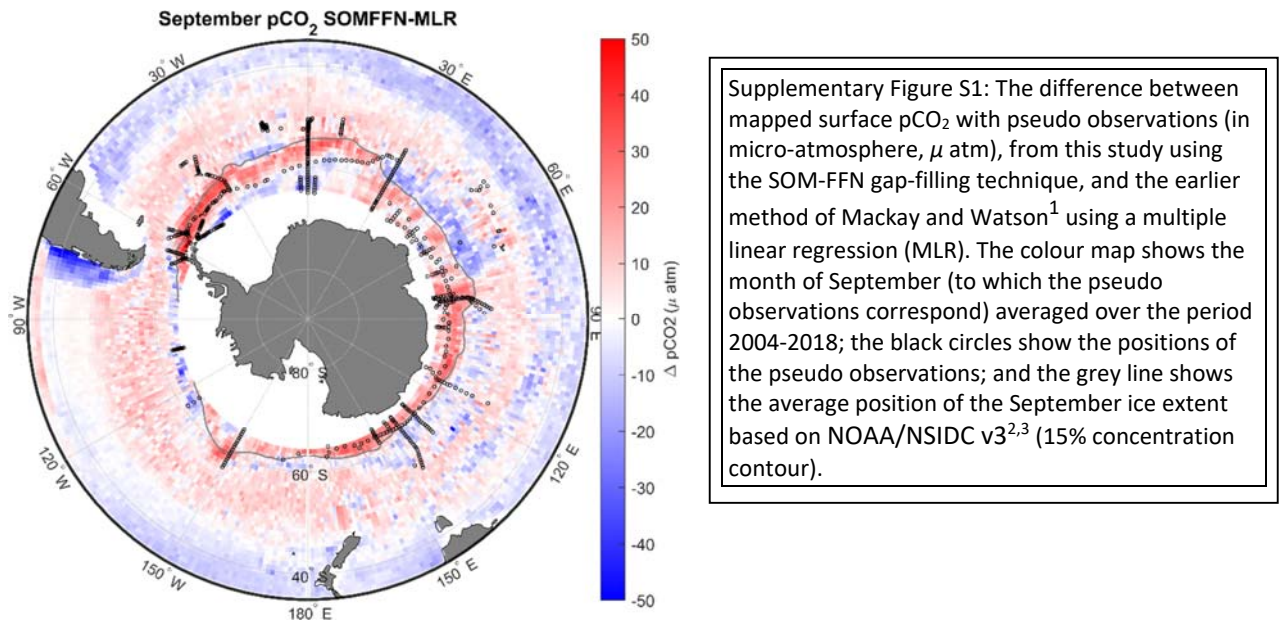
Considering that Antarctic winter sea ice extent reaches a maximum in September and all pseudo observations are pinned to that month, it seems that most pseudo-observations will be under ice and will not contribute directly to air-sea CO₂ flux estimates. The authors could make this much clearer, as it implies that most of the pseudo-observations are playing an indirect role in updating the Southern Ocean CO₂ flux estimates through their influence on the pCO₂ gap-filling step – which was the major methodological change from Mackay and Watson 2021 to this paper. This is particularly relevant because areas exhibiting the largest CO₂ flux changes due to the addition of pseudo-observations (Figure 4) generally (1) do not include pseudo-observations or (2) have pseudo-observations that would likely be under sea ice and not contributing to the fluxes directly (now clear from Figure 3b). Therefore, it seems that the change in pCO₂ gap-filling approach is likely most critical to the novelty of this result. Conveying this information could be easily accomplished by creating a map of the September (or annual mean) difference in pCO₂ derived from MLR and SOM-FFN gap filling procedures when including a common subset of the pseudo observations. The figure could include the locations of pseudo-observation (like shown in Figure 1) and the mean winter sea ice extent (as shown clearly in Mackay and Watson 2021). This would help to clarify how important the gap-filling technique is and where it is important relative to the pseudo-observations. While this is not the story the authors are trying to tell, I think it is equally valuable and better reflects what this paper contributes.

For example, Line 17: “Here, we present a new estimate of the Southern Ocean CO₂ sink that addresses historically sparse wintertime sampling through interpretation of subsurface summertime observations south of the Antarctic Polar Front (APF) to produce **new** and independent ‘pseudo’ wintertime observations of surface fCO₂, increasing the wintertime data coverage in that region by

68%.”

Does “new” and 68% pertain to the newly added 38 GLODAP observations that this study incorporates or does the 68% include existing pseudo-observations from the authors’ prior work? It seems like the emphasis should be on using an advanced gap-filling method with slightly more wintertime pseudo-observations that are used to train a more sophisticated model, having an important influence on remote fluxes, relative to the pseudo-observation locations.

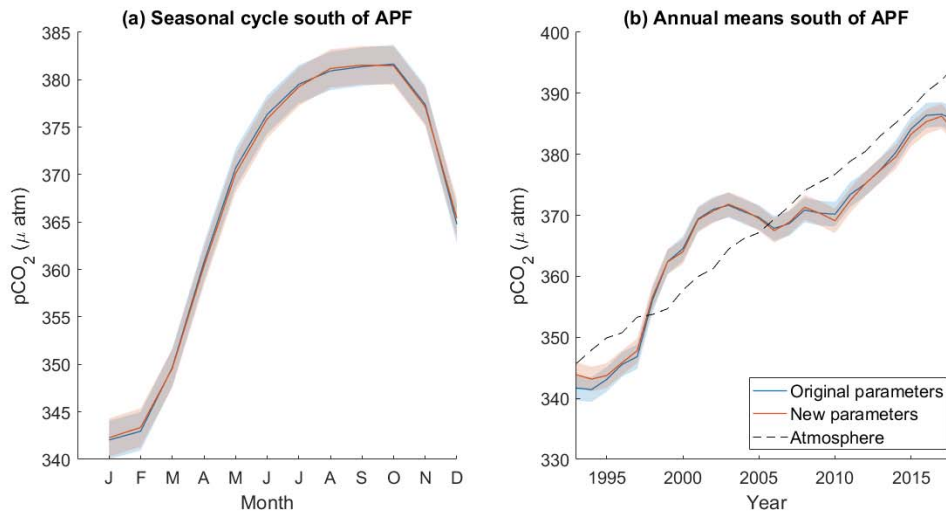
We have added the figure you suggest to the supplementary information (Figure S1 and see below), and highlighted the point about the pseudo observations having largely an indirect effect on the fluxes in lines 67-72. We have also modified the abstract (line 23) and the introduction (lines 66-67) to clarify the fact that our coverage improvement is quoted compared to the direct SOCAT data, and to emphasise the switch to a more sophisticated gap-filling method (lines 57-58).



Line 193: “We then adjust the concentration of dissolved inorganic carbon (DIC) from the TML for biological activity that occurred in the water mass since last winter using the apparent oxygen utilisation (AOU) and a Redfield ratio RRC:O, obtaining an estimate for the wintertime surface DIC concentration.” **Line 219:** “We then repeated the calculation for a range of parameters a, and b, and two alternative values of RR_{C:O}, each time calculating the resulting RMSE between the set of model pseudo observations and their wintertime equivalents.”

I believe B-SOSE uses a fixed C:O (and fixed C:N) for biological organic matter production, so it’s not clear that the authors should be using an RR_{C:O} value that differs from B-SOSE to optimize their a and b parameters for the AOU disequilibrium correction. Can you please elaborate on why you are not using the B-SOSE fixed RR_{C:O} – this is critical to the reconstruction of winter pseudo observations.

We agree with the referee that it using the B-SOSE RR_{C:O} appears more logical when optimising our ‘a’ and ‘b’ parameters; we therefore checked the effect of adopting the B-SOSE ration and we found that the effects are very small. This becomes evident when looking at the seasonal cycle and long term variability of the sea surface pCO₂ illustrated below, particularly compared to the effect of adding pseudo observations (see Figure 2 in the main manuscript for comparison)



To inform the reader that the choice of ratio is not fundamental in this case, we have added this detail in lines 254-257.

Line 150: “Here we have found instead that strong low frequency variability from 1993-2018 is robust to a modest increase in winter data coverage at high latitudes, suggesting the Southern Ocean carbon sink variability is relatively well constrained by sparse observations using this method. However, we note here the caveat that we have only boosted data coverage from 2004 onwards, and as such, our conclusions about the robustness of the variability only apply to the most recent period encompassing the reinvigoration and subsequent stagnation of the sink. A definitively constrained estimate of the variability in the most data-sparse period before 2000 remains elusive.”

For example, line 21: We show through a machine learning-based mapping method, that strong decadal variations remain with improved winter data coverage. There is rather little variability over the 2000-2018 period, with the post 2010 stagnation being insignificant w.r.t the data product uncertainties. Thus, it’s not clear that “strong decadal variations remain with improved winter data coverage.” Would a different framing be that you have achieved a similar pattern of variability with and without pseudo-observations and using two different gap-filling approaches (prior study relative to this one)?

We have altered text in a number of places to further soften our assertions about constraining the decadal variability and reframe the paper in the manner you suggest (lines 23-25, 44-45, 50, 113, and 172-174, and 198-207).

“...by sparse observations” do you also mean by seasonally biased observations?

Yes; sparse and seasonally biased; we have altered the text (lines 200-201).

Minor comments

Line 31: “Estimates of air-sea CO₂ fluxes from models, observation-based data products and observations show the largest disagreement in the Southern Ocean, in particular with regard to low frequency variations⁴. Given the lack of direct measurements in this remote and harsh ocean region, this disagreement does not come as a surprise.”

This seems like an odd comment since your study also does not add direct measurements, but you are attempting to argue that the pseudo-observations provide evidence that observational data products are not overestimating low frequency variability.

We have rephrased this to 'observational coverage' (line 37)

Line 40: "...air-sea CO₂ fluxes are then computed combining the mapped values using a simple bulk gas transfer parametrization."

Typo?

Fixed (lines 42-43)

Line 56: "In this work, we build on this novel constraint, increasing the number of pseudo observations from 760 to 798 using the latest version of GLODAP¹⁷."

Suggested text rearrangement for clarity.

We have rearranged the text as suggested (line 59).

Line 66: This altered the **global** ocean CO₂ sink by 0.8-0.9 PgC yr⁻¹²² globally, **yet** no regional correction for the Southern Ocean exists.

Clarify global and remove "but yet"

Clarified as '1992-2018 global mean ocean CO₂ sink' and rephrased as suggested (line 77).

Line 87: "However, the reduction in pCO₂ occurs in the sea ice (see supplementary Figure S2),..."

In the sea ice zone or below the sea ice?

Below; we have rephrased this (line 102), and clarified the definition in the caption to Figure S3.

Line 90: "The peak winter outgassing increases fractionally from 0.09 PgC yr⁻¹ to 0.12 PgC yr⁻¹, and is shifted from July to September; meanwhile the magnitude of the **flux** seasonal cycle increases from 0.66 to 0.69 PgC yr⁻¹."

Is this because nearly all the new pseudo-observations for winter are during September (Figure S3)?

We attribute this signal to the new mapping method rather than the addition of September observations. In Mackay and Watson 2021 – using the MLR method and similarly distributed data, we do not see such a shift. We therefore rephrased for clarification (lines 104-107):

"The peak winter outgassing increases fractionally from 0.09 PgC yr⁻¹ to 0.12 PgC yr⁻¹, and is shifted from July to September attributed to the data interpolation method; meanwhile ..."

Line 101: "Without the pseudo observations the sink south of the APF increases by 0.22 PgC yr⁻¹ over that period; when they are added the increase is 0.25 PgC yr⁻¹."

It would be more convincing to compare trends for this period rather than specific start and end years, given the uncertainty.

We now quote linear trends rather than differences, for both the 2004-2011 and 2011-2018 periods (lines 115-118), and have added the linear fits to Figure 3.

Line 141: “Our results are consistent with two atmospheric inversions (Figure 5 dashed lines), which are based on a set of independent measurements, and with a recent study that estimated the Southern Ocean sink using aircraft data³⁰ (see supplementary Figure S5).”

Your results both with and without pseudo-observations seem equally in alignment with the aircraft observations, based on the uncertainties.

This is true; we have added a comment in lines 166-169.

Line 169: “The difference could be explained by a number of factors, including the different gapfilling methods, the longer training dataset used in the current study (1993-2018 compared to 2004-2017), a larger set of driver variables (see Supplementary Table 1; the MLR study used only temperature, salinity, mixed layer depth and atmospheric CO₂ concentration), and perhaps least significantly, the additional pCO₂ and pseudo-data used here.”

You seem to agree that the addition of pseudo-observations may be playing the smallest role in your results, with the revised gap-filling technique (from MLR to Neural Network) perhaps being the greatest contribution. I find that the updated results in combination with the current manuscript framing (that new winter observations help to validate the larger interannual variability found in data-based pCO₂ products) make this a rather unconvincing study – there were only 38 new wintertime observations. It seems like an altered framing around the importance of the gap-filling technique used, availability of seasonally representative training data, and how these things impact remote pCO₂ estimates and air-sea fluxes, in combination with the skin temperature adjustment, would be more valuable contribution.

We have altered parts of the introduction and reorganised the discussion to shift the emphasis towards the application of the more sophisticated gap-filling technique to the pseudo observations (lines 19-25, 56-60, 172-178, 198-207).

Line 204: Typo in spelling alkalinity.

Fixed.

Reference is missing year: Mackay, N. & Watson, A. Winter air-sea CO₂ fluxes constructed from summer observations of the Polar Southern Ocean suggest weak outgassing. 1–25

Fixed (now ref. 13).

Reviewer #2

Minor comments

Check references. I found an issue in "n/a n/a" in ref 18 of the bibliography.

Thank you for picking this up, it has now been corrected (ref 20).

Line 28 - for the statistic of the SO absorbing 40% of the anthropogenic CO₂, give a definition of Southern Ocean (i.e. what is the northern boundary)?

We have added this detail (line 31).

Figure 2 caption - where does the atmospheric CO₂ estimate come from?

This comes from the NOAA ESRL product - we have added the reference in the Figure 2 caption.

72 - "has reduced" should "is reduced"

Fixed (line 87).

74 - Would it be clearer to say that the seasonal cycle of pCO₂ is anticorrelated with temperature (rather than "out of phase with the seasonal cycle of temperature"), likely because the wintertime cooling is associated with deeper mixed layers and vertical mixing that stirs high DIC water to the surface?

We agree with your interpretation, and have added it along with your suggested rewording in lines 89-94.

120-121 At least comment on how your "refinement" fits in any of these pictures. Is it consistent (or at odds) with any of the previous explanations?

We cannot say anything definitive, but have added some speculations (lines 140-148).

146 - "modest increase in winter "pseudo-observations"

This sentence has been removed in the most recent version of the manuscript.

154 -Why was MLR "necessary" when the first paper was written but not now?

What we meant to say here is that the gap-filling step is necessary, and that it was carried out in the previous work using an MLR. We have modified the wording to 'having been achieved' to clarify this sentence (line 177).

300 - Briefly explain where the atmospheric CO₂ product is from (besides just referencing the original paper)

We have added a reference to the NOAA ESRL product used (line 343)

315 - Explain why 20% uncertainty on K is chosen

Since you highlighted this we have realised it is not clear why we went with 20%, and the literature suggests that a 10% value is most appropriate. We have therefore remade Figures 3, 5, S5 and S6 with the smaller error bounds and added a reference for that value (line 465). We have also updated the uncertainties on our quoted mean fluxes accordingly (lines 26-27, 163, and 181).

23rd Aug 22

**** Please ensure you delete the link to your author home page in this e-mail if you wish to forward it to your coauthors ****

Dear Ms Thapa,

Your manuscript titled "Heat flux assumptions contribute to overprediction of smoke injection for 2019 Western US wildfires" has now been seen by our reviewers, whose comments appear below. In light of their advice I am delighted to say that we are happy, in principle, to publish a suitably revised version in Communications Earth & Environment under the open access CC BY license (Creative Commons Attribution v4.0 International License).

We therefore invite you to revise your paper one last time to address the remaining concerns of Reviewer #3. At the same time we ask that you edit your manuscript to comply with our format requirements and to maximise the accessibility and therefore the impact of your work.

EDITORIAL REQUESTS:

Please review our specific editorial comments and requests regarding your manuscript in the attached "Editorial Requests Table". Please outline your response to each request in the right hand column. Please upload the completed table with your manuscript files.

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REVIEWERS' COMMENTS:

Reviewer #3 (Remarks to the Author):

Response: This is a good idea! Table 1c shows the results when we use the observed PBLH (black open circles in Supplementary Fig 1-51) to evaluate injection. From the manuscript (lines 130-131): "For this evaluation, injection occurs in 60% of cases, resulting in an accuracy of 0.68, a true positive rate of 0.88 and a false positive rate of 0.42, indicating better model performance."

Comment: The injection rate for the WRF-Chem model is reduced from about 80% using simulated PBL height to 60% using observed PBL and the FP cases from 24 to 14, indicating the substantial impact of the error in PBL simulation. Despite the reduced FP cases, the finding that the WRF-Chem model overpredicts FP cases seems acceptable.

Table 1 does not show the result using the observed PBL height for the HRRR model because "For HRRR-Smoke, uncertainties in the boundary layer are smaller and likely play less of a role in generating false injections" (Lines 133-134). However, the same FP rate of 24 between the two models (Table 1a and b) suggests that the rate depends on not only PBL height modeling but also smoke plume injection modeling. The result same to Table 1c but for the HRRR model will provide evidence that the finding that the HRRR overpredicts FP cases remains to be true after using the observed PBL height to classify injection / non-injection.