

Rebuttal to “Interannual drivers of the seasonal cycle of CO₂ fluxes in the Southern Ocean”

by Gregor, Kok and Monteiro

Overview of changes

The authors would like to thank the reviewers for their recommendations to improve the manuscript. The changes are relatively substantial with the manuscript now being more succinct. The major scientific changes are: 1) removal of the two high resolution methods; 2) inclusion of uncertainty estimates. We also apologise for the multitude of typos and figure reference errors throughout the document. We hope that the reviewers now find the manuscript in a more presentable state.

In the document below we show the initial response of the reviewers in blue and the responses to each point in black. Track changes for the manuscript are shown below the response to the reviewer.

Reviewer 1

Overview

Gregor and co-authors investigate the variability of the Southern Ocean CO₂ uptake strength from 1998-2014 analysed for 9 regions (SO divided in basins and Fay and McKinley biomes). The authors combine 5 realizations to form a multi-model mean which is used to investigate seasonality and year-to-year variability of the delta pCO₂ and the CO₂ flux. 3 of the realizations are independent whereas 2 are simply higher resolution versions of 2 other methods. The authors find that the seasonal variability is the strongest mode of variability in the SO. Additionally, the authors confirm results from past studies that the SO was losing some of its uptake capacity in the early years of their analysis period, then the uptake increased in the subsequent period, whereas in the final years of their analysis period the reinvigoration of the sink stopped again. The authors investigate the cause of this variability in the sink strength by analysing anomaly periods for winter and summer season separately. From this analysis the authors conclude that the drivers are seasonally decoupled with wind being the dominant driver for winter variability and biology being the dominant driver for summer variability.

I found this study to be interesting, comprehensive and in general suitable for the journal. The authors do not only present results from new methods to confirm previous results, they also deepen the analysis by looking at anomalies rather than trends (as previously done) and investigate different seasons.

Major Issues

- The study confuses trends and variability. When do the authors talk about trends and when about variability? At the moment, these two terms are mixed up. E.g. take figure 5 all panels. There is clearly some year-to-year variability causing in some years more and in some less uptake but overarching in all panels of figure 5 and 6 one can clearly see an increasing CO₂ sink from 1998 onwards, i.e. an increasing trend throughout the entire time period. Furthermore, wording used like “decadal trends” and “interannual trends” contribute to the confusion. What is a decadal trend? Is it the slope of a regression line when considering at least 10 years of data? What are interannual trends? The same only considering 3 years? In the latter case one cannot speak of a trend at all.

We have removed most of the references to trends. We have also removed the reference to the decadal mode of variability. We do, however, make the connection between the longer modes of variability in winter and that this is likely linked to the decadal variability mentioned by Landschützer et al. (2016) linked to the SAM.

- Despite being able to do so, the authors do not add uncertainties. There are many sources of uncertainty ignored by the authors, e.g. the measurement uncertainty (which is however neglectably small), the extrapolation error of the method, the building of the

multi-model mean creates an error and finally the calculation of the air-sea flux adds another source of uncertainty (through wind and transfer velocity choice). At the moment, the results are presented overconfidently. It is not clear how much of the explored variability is significant and how much is simply statistical gibberish. I am aware that there is no “perfect” way to represent all uncertainties, but in a data sparse region like the Southern Ocean a study like this needs to add the best possible uncertainty estimate, otherwise, many of the conclusions drawn cannot simply be accepted.

Regarding the propagation of errors, we used the same approach used by Landschützer et al. (2014). However, we do note that this error is Gaussian and mechanistically consistent, thus we can make deductions about the changes in the trends we observe. We also incorporate the between-method error from transCom (as in Gurney et al., 2004) at the recommendation of Christian Rödenbeck (pers comm.). We treat this, and a variation thereof as the primary threshold of significance as in Figures 5 and 6 (new numbering).

- On page 11 line 312 I found that the authors claim statistical significance between the mean uptakes, reporting a p-value. It is not clear to the reader what test was used and how significance has been determined. Also, when adding uncertainty, the authors will notice that an uptake of -0.17 PgC/yr is unlikely to be identified as statistically significantly different from -0.19 PgC/yr in the data sparse Southern Ocean.

We have removed the trends from the FCO₂ time-series, so this is no longer an issue. Note that this figure has also moved to the supplementary materials.

- Despite the uncertainty of the CO₂ itself there are other sources of concern related to uncertainty. Chlorophyll is e.g. also presented without discussing uncertainty. How is cloud coverage and missing chlorophyll data effecting the results? Also, wind products have been shown to have different trends locally in the Southern Ocean. This has not been mentioned. I am also wondering to what extend the use of different products hampers the conclusions of the manuscript. SST from Reynolds is based – to the extent of my knowledge – from satellite and in-situ data, whereas ECCO MLD is from an assimilation model. I would expect some disagreement between these products that have nothing to do with "real world" disagreement. This is not a massive concern, but certainly needs to be mentioned as well.

This is a valid point and we agree with the reviewers concern. However, it may be beyond the scope of this study to address the uncertainties driven by the input proxies. This may be a good topic for a collaborative effort of the SOCOM intercomparison. I have to some extent addressed the reviewers points:

Chlorophyll: we include the methodology used by Gregor et al. (2017) for the missing chlorophyll, where cloud patches are filled with the climatology for that point, and missing winter values are filled with a low level Gaussian noise.

ECCO2 MLD: This is indeed assimilation model output. Our motivation here is that

using observations (most likely the de Boyer Montégut (2004) MLD climatology) would mean that MLD could not be treated as a potential driver of pCO₂. However, there may be regions (such as the MIZ) where the MLD estimates are spurious for ECCO2. Choosing between these two products is thus a choice of trade-offs.

Wind: We include our justification for using CCMP v2 only. Much of this is based on the study by Swart et al. (2015a) and personal communication with Neil Swart.

- Another source of concern is the length choice of periods P1-P4. Periods P1-P3 are all of the same length, whereas P4 is substantially shorter. The authors claim that substantial year-to-year variability occurs on various timescales (4-6 year and 10 year modes respectively), hence the variation of periods aliases this analysis.

We have changed the lengths of the periods to be more or less the same length (5, 4, 4, 4 years respectively). We hope that this approach addresses the reviewers concerns.

All the above points raised are of major concern and must be addressed before the manuscript can be considered for publication.

Minor comments:

- Title: the title only mentions CO₂ fluxes whereas in the manuscript largely discusses delta pCO₂

We have made the title more generic: CO₂

- Line 29: “paucity of observations (Landschützer et al 2015)” – This is not a good reference. Bakker et al 2016 (the SOCATv2 reference) would be a better reference for such a paucity.

We have changed this reference to Bakker et al. (2016)

- Line 62: remove 2nd that removed

- Line 95: wrong reference (Bakker et al 2016)

This reference is in fact correct for SOCAT v3. SOCAT v2 is Bakker et al. (2014)

- Table 1: How has the RMSE for the 0.25x0.25 degree product been calculated? SOCAT offers a gridded product but on 1x1 degrees. Did the authors grid the 0.25 product themselves? If yes, has this been done the “SOCAT” way, i.e per cruise weighted or differently? Same with the 16-day time step. More information is needed here.

We have removed the high resolution implementations of RFR and SVR at the request of Reviewer 2 (who felt they resulted in an ensemble biased towards these methods).

- Line 130: How different would the results be if a different transfer velocity was chosen? This may have significant effects on the uncertainty.

The fluxes are now only included in the supplementary materials.

- Line 134: where are [ice] data from? I am missing a reference here.

“...sea surface temperature (SST) and sea-ice fraction by Reynolds et al. (2007),...”

- Line 175-176: “attributed this difference to the clustering step used by the SOM-FFN that created large discrepancies in the Atlantic sector.” I have not found any convincing evidence for this in any of the cited papers.

The published version of Gregor et al. (2017) now contains a figure (A3) that the reviewer may find convincing.

- Line 236: Either the authors used the wrong wording or there is a misunderstanding, but I do not see where the authors find that the delta pCO₂ is zonally asymmetric within each biome. It looks like the other way around: Figure 4 looks like there is a strong zonal symmetry (besides indeed in panel a).

Included an additional clause that the gradient is during summer: “*Apparent also from Figure 3 is that, over and above the latitudinal gradient, $\Delta p\text{CO}_2$ is zonally asymmetric within each biome during summer (Figure 3a), when biological uptake of CO₂ increases.*”

- Lines 249-254: This paragraph is not clear. Please rephrase

We have tried to make this more clear: “*The projected summer minima (dashed lines) are calculated by subtracting the mean seasonal amplitude from the winter maxima (Figure 4, with air-sea CO₂ fluxes shown in Figure S3). The projected summer minima is the expected summer $\Delta p\text{CO}_2$ under the assumption that summer $\Delta p\text{CO}_2$ is dependent on, but not restricted to, the baseline set by winter. Differences between the summer minima and projected minima are highlighted with green and blue patches, highlighting periods of decoupling between summer and winter interannual variability. The green areas indicate periods of strong uptake (relative to winter) that enhance the mean uptake of CO₂ and amplify the seasonal cycle. Conversely, blue areas show periods where weak summer uptake (relative to winter) offsets winter outgassing, thus reducing the mean $\Delta p\text{CO}_2$ as well as suppressing the amplitude of the seasonal cycle (Figure 4).*”

- Line 273: interannual trend – what is that? Interannual variability. A 3-year trend? A trend that changes sign every year?

We have rephrase this to: “*A key feature of Figure 4 is that the mean interannual variability is the net effect of decoupled seasonal modes of variability for summer and winter.*”

- Lines 275: decadal mode: How are you able to say this. You have 1998-2014 data, i.e. 17 years of data. How can you detect a decadal mode from such a short time series?

We have removed this statement and other references to the decadal mode, unless it is associated with previous studies (Lovenduski et al., 2008; Landschützer et al., 2016).

- Line 305: “decadal trend” – what is this? A trend of at least 1 decade?

Removed decadal trend and see above comment

- Lines 311-312: “-0.19 and -0.17 PgC yr⁻¹ for the Atlantic and Pacific sectors respectively

(where the latter are significantly different with $p = 0.01$).” how was this calculated, and given the many, many uncertainties that go into such a flux number one cannot possibly believe that these numbers are indeed statistically significant.

We have moved the fluxes to supplementary materials. We have also removed the trends reported on the figure as this may detract and confuse given that the rest of the study deals with anomalies rather than trends.

- Line 340: What about acidification induced changes linked to changes in the buffer capacity (see e.g. Hauck et al 2015)? A contribution within 17 years is plausible. This is an interesting point, but would lengthen the study too much, and is thus better left for another study.

- Line 439: I suppose ENSE is ENSO – but please either way spell out abbreviations when first using them

ENS(E)O is only used once and thus written out in full

- Line 505: “The fact that Chl-a is the dominant driver of interannual ΔpCO_2 variability should not be surprising” – the authors have not proven that chlorophyll is the dominant driver. From a pool of selected variables, it showed the largest correlation – this can barely be called a “fact” in science.

Rephrased: “Our finding that Chl-a is the dominant driver of interannual ΔpCO_2 variability should not be surprising given that models and observations support this notion (Hoppema et al., 1999; Bakker et al., 2008; Mahadevan et al., 2011; Wang et al., 2012; Hauck et al., 2013; 2015; Shetye et al., 2015)”

- Figures 5 and 6: Uncertainties need to be added. Without uncertainty I do not trust that the observed variability is significant.

We have added uncertainty estimates of uncertainty as previously mentioned. We keep these relatively simple in Figure 4 (old 5) by using time averages of the between-method errors. We do however include uncertainty thresholds in the final anomaly analysis. We feel that this is perhaps a more pertinent place to show the uncertainties.

- Figures 7 and 8: Wind stress anomalies are interesting, but direction would be equally interesting and provide more evidence.

We include the wind direction for each of the anomaly transitions in the supplementary materials. We find that the wind anomalies do not increase the understanding of the changes in ΔpCO_2 significantly to justify the addition in Figures 5, 6 (old 7 and 8).

Interannual drivers of the seasonal cycle of CO₂ fluxes in the Southern Ocean

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Abstract. Machine learning methods (support vector regression and random forest regression) were used as become a useful tool to map gridded estimates interpolate ship measurements of $\Delta p\text{CO}_2$ in the Southern Ocean from (SOCAT-v3) to a gridded map using satellite data. A low ($1^\circ \times$ monthly) and high ($0.25^\circ \times$ 16-day) resolution implementation of each of these methods as well as In this study we use an ensemble of three machine learning methods: Support Vector Regression (SVR) and Random Forest Regression (RFR) from Gregor et al. (2017); and the SOM-FFN method from Landschützer et al. (2014) were added to a five member ensemble. (2016). The ensemble mean $\Delta p\text{CO}_2$ was used to calculate $F\text{CO}_2$ (air-sea CO₂ flux). Data was interpolated data were separated into nine domains regions defined by basin (Indian, Pacific and Atlantic) and biomes (as defined by Fay and McKinley (2014, 2014a)). The regional approach showed large a meridional gradient and zonal asymmetry in the magnitude of $\Delta p\text{CO}_2$ and $F\text{CO}_2$ estimates. Importantly, there was a seasonal decoupling of the modes for summer and winter interannual variability. Winter trends interannual variability had a larger 10-year longer mode of variability compared to summer trends, which had varied on a shorter 4–6 year mode time scale. To understand this variability of $F\text{CO}_2$ $\Delta p\text{CO}_2$, we separately assessed investigated changes in summer and winter $\Delta p\text{CO}_2$ and the drivers thereof. The dominant winter changes were are driven by wind stress variability. Summer variability correlated well This is consistent with the temporal and spatial characteristics of the Southern Annular Mode (SAM), which has a decadal mode of variability (Lovenduski et al., 2008; Landschützer et al., 2016). Interannual trends in summer variability of $p\text{CO}_2$ are consistent with chlorophyll-*a* variability where the latter had high mean seasonal concentrations. In regions of low chlorophyll-*a* concentrations, wind stress and sea surface temperature were lower order emerged as stronger drivers of $\Delta p\text{CO}_2$. In summary we propose that sub-decadal variability is explained by summer drivers, while winter variability contributes to the long term changes associated with the SAM.

30 1 Introduction

The Southern Ocean plays a key role in the uptake of anthropogenic CO₂ (Khatiwala et al., 2013; DeVries et al., 2017). Moreover, it has been shown that the Southern Ocean is sensitive to anthropogenically influenced climate variability, such as the intensification of the westerlies (Le Quéré et al., 2007; Lenton et al., 2009; Swart and Fyfe, 2012; DeVries et al., 2017). Until recently, the research community has not been able to accurately measure the contemporary changes, let alone understand the drivers, of CO₂ in the contemporary Southern Ocean due to a paucity of observations (Landschützer et al., 2015). Empirical models provide an interim solution to this challenge until prognostic ocean biogeochemical models are able to represent the Southern Ocean CO₂ seasonal cycle accurately (Lenton et al., 2013; Rödenbeck et al., 2015; Mongwe et al., 2016). There is an agreement in the research community agrees on large changes in CO₂ fluxes in the Southern Ocean from a source in the 1990's to a sink in the 2000's; however, there is disagreement in the drivers of the changes in CO₂ uptake (Lovenduski et al., 2008; Landschützer et al., 2015; DeVries et al., 2017). This study aims to understand the drivers of the changing CO₂ sink in the Southern Ocean based on an ensemble of empirical estimates withusing a seasonal analysis framework.

Empirical methods estimate CO₂ by extrapolating the sparse ship based CO₂ measurements using satellite observable proxies. This approach has allowed for a better understanding of the drivers of CO₂ by providing improved spatial and temporal resolution of the variability. Landschützer et al. (2015) usedshowed, using an artificial neural network (ANN) to show, that there was significant strengthening of the Southern Ocean CO₂ uptake during the period 2000-2010 is part of a decadal internal variability in the natural CO₂ flux dynamics. The authors found that the strengthening sink was not due to changes in overturning circulation associated with wind stress as suggested in other studies (Lenton and Matear, 2007; Lovenduski et al., 2007; Lenton et al., 2009; DeVries et al., 2017). Rather, they suggested that atmospheric circulation has become more zonally asymmetric since the mid 2000's. This led to an oceanic dipole of cooling and warming whose net impact together with changes in the DIC/TA (Dissolved Inorganic Carbon/Total Alkalinity) was to increase the uptake of CO₂ (Landschützer et al., 2015). During this period, in the Atlantic basin, southward advection reduced upwelled DIC in surface waters overcoming the effect of the concomitant warming in the region. Conversely, in the Eastern Pacific sector of the Southern Ocean, strongerstrong cooling overwhelmed increased upwelling (Landschützer et al., 2015). Munro et al. (2015) supported this mechanism, with data from the Drake Passage showing that $\Delta p\text{CO}_2$ decreased between 2002 and 2014.

In a subsequent study Landschützer et al. (2016) proposed that interannual variability of CO₂ in the Southern Ocean is tied to the decadal variability of the Southern Annular Mode (SAM) – the dominant

65 mode of atmospheric variability in the Southern Hemisphere (Marshall, 2003). This concurs with previous studies, which suggested that the increase in the SAM during the 1990's resulted in the weakening of the Southern Ocean sink (Le Quéré et al., 2007; Lenton and Matear, 2007; Lovenduski et al., 2007; Lenton et al., 2009). The work by Fogt et al. (2012) bridges the gap between the proposed asymmetric atmospheric circulation of Landschützer et al. (2015) and the observed correlation with the SAM of
70 Landschützer et al. (2016). ~~Fogt et al. Their study shows~~(2012) show that changes in the SAM have been zonally asymmetric and ~~that~~ that this variability is highly seasonal, thus amplifying or suppressing the amplitude of the seasonal mode.

Assessing the changes through a seasonal framework may thus help shed light on the drivers of CO₂ in
75 the Southern Ocean. Southern Ocean seasonal dynamics suggest that the processes driving $p\text{CO}_2$ are complex but with two clear contrasting extremes. In winter, the dominant deep mixing and entrainment processes are zonally uniform driving an increase in $p\text{CO}_2$ with the region south of the Polar Front (PF) becoming a net source and weakening the net sink north of the PFZPF (Lenton et al., 2013). In summer, the picture is ~~much~~ more spatially heterogeneous, with NPPnet primary production being the primary
80 driver of variability (Mahadevan et al., 2011; Thomalla et al., 2011; Lenton et al., 2013). The competition between light and iron limitation results in heterogeneous distribution of Chl-*a* in both space and time, with similar implications for $p\text{CO}_2$ (Thomalla et al., 2011; Carranza and Gille, 2015). The interaction between the large-scale drivers, such as wind stress, surface heating and mesoscale ocean dynamics, are the primary cause of this complex picture (McGillicuddy, 2016; Mahadevan et al., 2012).
85 Some regions of elevated mesoscale and submesoscale dynamics, mainly in the Sub-Antarctic Zone (SAZ) are also characterized by strong intraseasonal modes in summer primary production and $p\text{CO}_2$ (Thomalla et al., 2011) ~~and $p\text{CO}_2$~~ (Monteiro et al., 2015). ~~The magnitudes of these~~ In general, the opposing ~~seasonal processes are large, resulting effects of mixing and primary production result~~ in the seasonal cycle being the dominant mode of variability in the Southern Ocean. (Lenton et al., 2013).

90 In this study we examine winter and summer interannual variability ~~in the air-sea fluxes of CO_2 and $p\text{CO}_2$~~ between 1998 – 2014 ~~through interannual changes in the characteristics of the seasonal mode of both $p\text{CO}_2$ and $f\text{CO}_2$ in the Southern Ocean. We use an ensemble of empirical estimates of CO_2 that combine *in situ* observations with remotely sensed proxies to perform this analysis~~ understand the drivers of long
95 term changes in CO₂ uptake.

2 Empirical methods and data

2.1 ~~Ensemble members~~Empirical methods and data

In this study we ~~made use of three empirical methods combined to an ensemble—these~~ machine learning methods ~~are~~: Random Forest Regression (RFR), Support Vector Regression (SVR) and Self-Organising-Maps Feed-Forward Neural Network (SOM-FFN). RFR and SVR are introduced in Gregor et al. (2017) and SOM-FFN is presented in Gregor et al. (2017). The advantage of an ensemble over Landschützer et al. (2014). In brief, the RFR approach is an ensemble of decision trees that provides non-linear regression by combining many high variance – low bias estimators (Gregor et al., 2017). SVRs are in principle similar to a single hidden layer FFN, with the difference that SVR statistically determines the complexity of the problem, which is analogous to the hidden layer structure that is typically determined heuristically. The SOM-FFN method approach is that a degree of robustness is added to the estimate, assuming that ensembles have unique biases in time and space. The other important assumption we make here is that the majority methods will be correct, while the minority will be biased. The ensemble mean contains five different $\Delta p\text{CO}_2$ estimate approaches, shown in Table 1, with low and high resolution (1° , monthly and 0.25° , 16-day respectively). The SOM-FFN method is defined by Landschützer et al. (2014) and is a two-step neural network approach (~~trained with SOCAT v2~~) that first clusters data (SOM) and then applies a regression model (FFN) to each cluster.

The SVR and RFR implementations used in this study are trained with the monthly by 1° gridded SOCAT v3 dataset (Bakker et al., 2016). ~~– 2014). The low resolution implementations of Support Vector Regression (SVR) and Random Forest Regression (RFR) methods are introduced in Gregor et al. (2017). Note that these are~~ The SOM-FFN (v2.2) used in this study was trained with SOCAT v3 data (Bakker et al. 2016). The high resolution implementations of SVR and RFR used in this study are implemented in the same way as described in Gregor et al. (v4 (Landschützer et al., 2017). The high resolution estimates of $\Delta p\text{CO}_2$ are resampled to match the low resolution data in the ensemble.

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Table 1: ~~Five~~Three empirical methods used in the ensemble. RFR-~~LR~~ and SVR-~~LR~~ are described in Gregor et al. (2017). SOM-FFN is from Landschützer et al. (~~Landschützer et al. 2014~~(2016)). SST = sea surface temperature, MLD = mixed layer depth, SSS = sea surface salinity, ADT = absolute dynamic topography, Chl-*a* = Chlorophyll-*a*, $p\text{CO}_{2(\text{atm})}$ = fugacity of atmospheric CO_2 , $x\text{CO}_{2(\text{atm})}$ = mole fraction of atmospheric CO_2 , $\Phi(\phi(\text{lat}, \text{lon})) = \frac{N\text{-vector}}{N\text{-vector}}$ transformations of latitude and longitude, $\lambda(\lambda(\text{day of year}))$ = trigonometric transformation of the day of the year. Note that SOM-FFN uses the de Boyer Montégut et al. (2004) climatology for MLD (dBM2004). The root mean squared errors listed in the last column are for the Southern Ocean from Gregor et al. (2017).

Metho d	Resol ution	Input variables	RMSE (μatm)
		Space	Time
RFR- LR	1.0 0.25°	M ϕ SST, MLD, SSS, ADT, Chl- <i>a</i> _(clim) , $p\text{CO}_{2(\text{atm})}$, $\Phi(\phi(\text{lat}, \text{lon}), t(\text{day of year}))$	17.21 <u>16.45</u>
SVR- LR	1.0 0.25°	M ϕ SST, MLD, SSS, ADT, Chl- <i>a</i> _(clim) , $p\text{CO}_{2(\text{atm})}$, $\Phi(\phi(\text{lat}, \text{lon}), t(\text{day of year}))$	21.73 <u>24.04</u>
SOM- FFN	1.0 0.25°	M ϕ SST, MLD <u>MLD_{dBM2004}</u> , SSS, Chl- <i>a</i> , $x\text{CO}_{2(\text{atm})}$	15.45 <u>14.84</u>
RFR-HR	0.25° 16-day	SST, MLD, SSS, ADT, Chl- <i>a</i> _(clim) , $p\text{CO}_{2(\text{atm})}$	12.58
SVR-HR	0.25° 16-day	SST, MLD, SSS, ADT, Chl- <i>a</i> _(clim) , $p\text{CO}_{2(\text{atm})}$, $\Phi(\text{lat}, \text{lon}), t(\text{day of year})$	19.18

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Table 1 also shows the proxy variables used for each of the methods. ~~The sources for the proxy variables are consistent for all methods ensuring a fair comparison. This is particularly important for the assimilated model variables, mixed layer depth (MLD) and sea~~Sea surface salinity (SSS) and mixed layer depth (MLD) for SVR and RFR are from Estimating the Circulation and Climate of the Ocean, Phase II (ECCO₂) (Menemenlis et al., 2008). ~~Choosing to~~The use ~~different of these~~ assimilative modelled products may in some cases produce results that are unrealistic. This may have influenced the use of the de Boyer Montégut et al. (2004) MLD climatology in the SOM-FFN, where ECCO₂ was used in previous iterations of the product. The trade-off of using the climatology is that no changes in MLD are taken into account. We acknowledge that using different proxy variables could result in ~~data driven differences (from the same variable)-~~different $\Delta p\text{CO}_2$ estimates, but comparing the different products is beyond the

scope of this study. Other data sources [that are consistent between methods](#) are: sea surface temperature (SST) [\(and sea-ice fraction by Reynolds et al. \(2007\)\)](#), Chlorophyll-*a* (Chl-*a*) [\(by Maritorena and Siegel \(2005\)\)](#), absolute dynamic topography (ADT) [\(by Duacs, xCO₂ \(CDIAC, 2016\) with pCO_{2\(atm\)} calculated from interpolated xCO₂ using NCEP2 sea level pressure \(Kanamitsu et al. 2002\), 2002\)](#). [In the case of Chl-*a* for SVR and RFR, Gregor et al. \(2017\) filled the cloud gaps with climatological Chl-*a*.](#) Note that ADT coverage is limited to regions of no to very low concentrations of [sea-ice cover](#), thus estimates for SVR and RFR methods do not extend into the ice covered regions during winter. [Our analyses are thus limit to the regions without ice cover.](#)

Seasonality of the data is preserved by transforming the day of the year (*j*) and is included in both SVR and RFR analyses:

$$t = \begin{pmatrix} \cos\left(j \cdot \frac{2\pi}{365}\right) \\ \sin\left(j \cdot \frac{2\pi}{365}\right) \end{pmatrix} \quad (1)$$

Transformed coordinate vectors [wereare](#) passed to [SVR](#) only ~~SVR~~ using *n*-vector transformations of latitude (*λ*) and longitude (*μ*) (Gade, 2010; Sasse et al., 2013), with *n* containing:

$$N = \Phi \begin{pmatrix} \sin(\lambda) \\ \sin(\mu) \cdot \cos(\lambda) \\ -\cos(\mu) \cdot \sin(\lambda) \end{pmatrix} \quad (2)$$

2.2 Air-sea CO₂ fluxes

~~Air sea CO₂ fluxes are calculated with:~~

$$FCO_2 = k_w \cdot K_0 \cdot (pCO_2^{sea} - pCO_2^{atm}) \cdot (1 - [ice]) \quad (3)$$

~~The gas transfer velocity (*k_w*) is calculated using a quadratic dependency of wind speed with the coefficients of (Wanninkhof et al. 2009). Wind speed is calculated from the *u* and *v* vectors ($\sqrt{u^2 + v^2}$) of the Cross-Calibrated Multiplatform Product v2 (Atlas et al. 2011). Coefficients from Weiss (1974) are used to calculate *K₀* and Δ*p*CO₂ is estimated by the empirical models. The effect of sea-ice cover on CO₂ flux is treated linearly (Butterworth and Miller 2016): the fraction of sea ice cover ([*ice*]) is converted to fraction of open water by subtracting one as shown in Equation (3).~~

[Wind speed, while not used in the empirical methods, is used in the assessment of the drivers of CO₂. We use CCMP v2, which is an observation based product that combines remote sensing, ship and weather buoy data \(Atlas et al., 2011\). Swart et al. \(2015a\) compared a number of wind reanalysis products with CCMP v1 \(where CCMP was the benchmark\). The authors found that the many of the reanalysis products had spurious trends, particularly in the Southern Hemisphere where data is sparse. Our choice of CCMP,](#)

75 which is based on observations, is thus one that aims to minimise the assumptions that are otherwise made
by reanalysis products.

2.2 Uncertainties

The machine learning approaches used in this study are by no means able to estimate $\Delta p\text{CO}_2$ with absolute
certainty. To account for the uncertainty we use the same approach as Landschützer et al. (2014) to
80 calculate total errors for each of the methods:

$$e_{(t)} = \sqrt{e_{meas}^2 + e_{grid}^2 + e_{map}^2} \quad (3)$$

where $e_{m(t)}$ is the total error associated with a method (m); e_{meas} is the error associated with SOCAT
measurements, which is fixed at 5 μatm (Pfeil et al., 2013); e_{grid} is the 5 μatm error associated with
gridding the data into monthly by 1° bins (Sabine et al., 2013). Lastly e_{map} is the root mean squared error
85 (RMSE) calculated for each method as shown in Table 1 taken from Gregor et al. (2017).

These errors are used to calculate the average “within-method” error as defined by Gurney et al. (2004):

$$E_w = \sqrt{\frac{1}{M} \cdot \sum_{m=1}^M (e_{m(t)})^2} \quad (4)$$

where $e_{m(t)}$ is the method specific error as defined in Equation 1 and M is the number of methods (3 in
this case). For a measure of the difference between methods we use the “between-method” approach used
90 in Gurney et al. (2004):

$$E_b = \sqrt{\frac{1}{M} \sum_{m=1}^M (S_m - \bar{S})^2} \quad (5)$$

where S_m is the method estimate of $\Delta p\text{CO}_2$ and \bar{S} is the mean of the methods. This is analogous to the
standard deviation (for a known population size). We later use an adaptation of this metric as a threshold
to determine the confidence around anomalies.

95 2.3 Regional Coherence Framework

Southern Ocean CO_2 is spatially heterogeneous both zonally and meridionally (Jones et al. 2012). In order
to understand this heterogeneity we used the three southernmost biomes defined by Fay and McKinley
(20172014a) as done in Rödenbeck et al. (2015). From north to south these are: ~~sub-tropical~~subtropical
seasonally stratified (STSS), sub-polar seasonally stratified (SPSS), seasonally ice covered region (ICE).
100 These three biomes are comparable to the SAZ, PFZ and MIZ respectively and will be used throughout
the rest of the study. The Southern Ocean is further split into basins where the boundaries are defined by
lines of longitude (70°W : Atlantic : 20°E : Indian : 145°E : Pacific : 70°W).

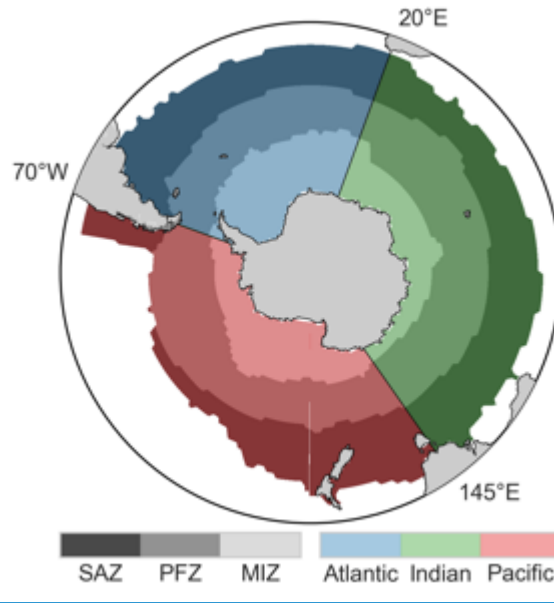


Figure 1: A map showing the regions used throughout this study. The three biomes, SAZ, PFZ and MIZ used in this study are defined by Fay and McKinley (2014a). The regions are also split by basin with boundaries shown above the map.

3 Results and discussion

Here we present and discuss the data results. The first section examines the variability uncertainties of between the ensemble and its members to understand the potential limitations of the dataset. We then look at the seasonal cycle of the ensemble mean in time and space. This is done to lay the foundation knowledge for the interpretation of the results when assessed with the regional framework, which is the following section. In the regional interpretation the data is decomposed into nine regions as shown in Figure 1. The section that follows sets out to make sense. Lastly we implement a seasonal decomposition of the trend estimates to interpret the drivers of the changes observed in the regional decomposition. $\Delta p\text{CO}_2$.

3.1 Ensemble member performance and variability

In this section we discuss the performance and variability. Table 2: A regional summary of the ensemble members errors for the different models. Note that the propagated errors are calculated as shown in equation (3) where the measurement and gridding errors are assumed to be constant at 5 μatm each (Pfeil et al., 2013; Sabine et al., 2013). The individual ensemble member within-model and between model errors are calculated using equations (4) and (5) respectively.

Biome	Propagated errors (μatm)			Within	Between
	SVR	RFR	SOM-FFN	model (μatm)	model (μatm)
SAZ	17.48	14.50	12.30	14.91	4.88
PFZ	15.94	12.71	13.09	13.99	4.78
MIZ	36.38	24.53	22.46	28.46	10.81
Southern Ocean	25.06	17.91	16.44	20.16	6.79

We use the RMSE scores as presented in Gregor et al. (2017) with abbreviated results shown in Table

1. The RFR is SOM-FFN method has the best performing member, with score (14.84 μatm). SVR

25 scores the lowest RMSE (12.58 μatm). The SVR members score the lowest (21.73 and 19.18 μatm for
LR and HR respectively (24.04 μatm), but ~~werewas~~ still included due to the method's sensitivity to sparse
data, which is favourable to the poorly sampled winter period (Gregor et al. 2017). This compliments the
RFR methodsmethod, which seorescores well (~~12.58 and 17.21 μatm for HR and LR respectively~~ 16.45
 μatm), but ~~areis~~ prone to being insensitive to sparse data (Gregor et al. 2017). ~~The SOM-FFN member~~
30 ~~has~~ These RMSE scores are used to calculate the best of the low-resolution scores (15.45 μatm). However,
this is because the SOM-FFN is tested with SOCAT v2 data rather than SOCAT v3; total errors for each
method and region using equation (3) where the latter has a larger standard deviation (32.85 and 36.27
 μatm respectively). When RFR-LR and SVR-LR measurement and mapping errors are tested with the
SOCAT v2 dataset, the RMSE scores are 15.15 and 19.82 μatm respectively both 5 μatm each (Pfeil et
35 al., 2013; Sabine et al., 2013). These results are shown in Table 2.

Total errors are used to calculate the within-method error, which is an estimate of the combined total
errors of the three machine learning methods (equation 4). The between-method errors are the mean of
the standard deviation between the methods (equation 5). The within-method errors are much larger
40 than the between-method errors (Table 2). However, the within-method errors are normally distributed
and are mechanistically consistent (Gregor et al., 2017).

This allows us to observe changes that are smaller than the within-method error. The between-method
error (shown in Figures 2d) serves as a better measure of whether observed variability is more than
statistical noise as it incorporates the three methodologically different approaches.

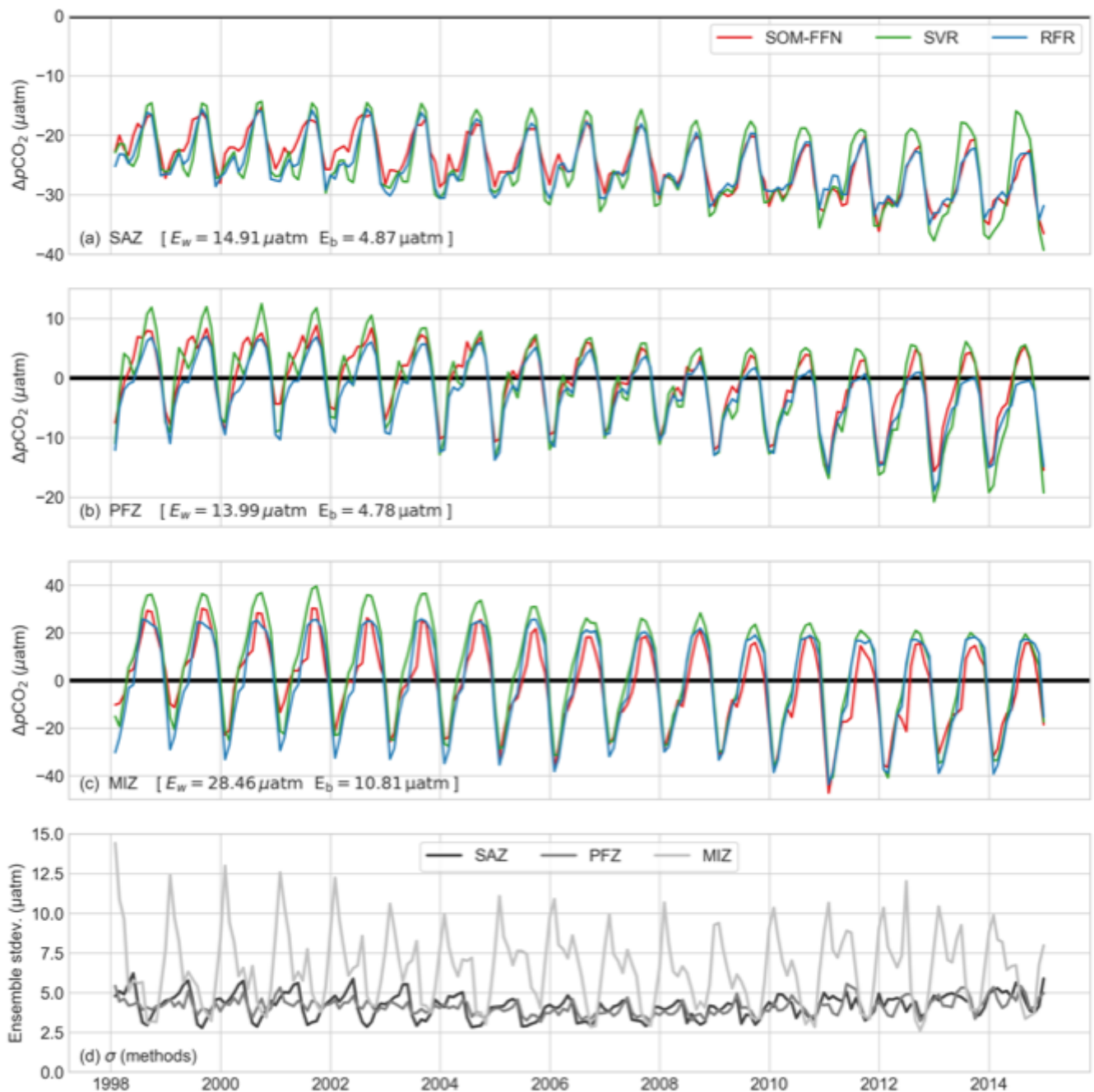


Figure 2: Time series of the five ensemble members for each biome as defined by Fay and McKinley (2014): (a) SAZ, (b) PFZ, (c) MIZ. (d) shows the standard deviation between ensemble members for the three biomes. The SOM-FFN data ends at the end within-method (E_w) and between-method (E_b) errors are shown for each biome. For a more detailed breakdown of 2011. This is indicated in (d) by the dashed line. errors see Table 2.

Figure 2 shows the ΔpCO_2 time series for each of the methods for the three Southern Ocean biomes as defined by Fay and McKinley (2014). The methodological and data driven differences between each of the approaches have been addressed in Gregor et al. (2017). In general, there is good agreement amongst the methods with a few notable exceptions. In the SAZ (Figure 2a) the SOM-FFN differs from all the other methods for summer and autumn from 1998 to 2008. Gregor et al. (2017) attributed this difference to the clustering step used by in the SOM-FFN that created large discrepancies in the Atlantic sector. The SVR-LR method overestimates the seasonal amplitude ΔpCO_2 relative to the other

methods for winter 2012 to 2014. In the PFZ (Figure 2b), the SVR methods (LR and HR) overestimate $\Delta p\text{CO}_2$ relative to the other methods during winter from 1998 to 2004, likely due to the sensitivity to sparse winter data. The spread of data in the AZ is much larger than These differences contribute to the two other regions, but the impact on the fluxes is reduced due to ice cover during winter (Ishii et al. 1998; Bakker et al. 2008; Butterworth and Miller 2016).

The seasonal amplitude

Figure 3: The mean spatial standard deviation (a) of the ensemble members (SVR-LR, SVR-HR, RFR-LR, RFR-HR and SOM-FFN) is shown to represent the “noise” of the ensemble mean. The “signal” (b) is calculated as the mean difference between the minimum and maximum values of the annually averaged $\Delta p\text{CO}_2$. This shows the signal that needs to be detected by the ensemble. The signal to noise ratio (c) shows regions where the confidence in the ensemble estimate is large, where darker shows higher confidence.

The results from Figure 2(a–c) are summarised with the standard deviation of the ensemble members over time (Figure 2d) and space (Figure 3). As noted, the AZ (Figure 2e) has the largest disagreement amongst methods shown by map (Figure 3a) and the differences between the solid and dashed lines in Figure 2d, particularly during summer and autumn. This is likely due to the inability of the methods to accurately capture the larger intra-seasonal variability and patchiness in the AZ where the rapid reduction of $p\text{CO}_2$ due to melting sea ice leads to patchy $p\text{CO}_2$ distributions (Bakker et al. 2008; Chierici et al. 2012). The ensemble members are more coherent in the SAZ and PFZ.

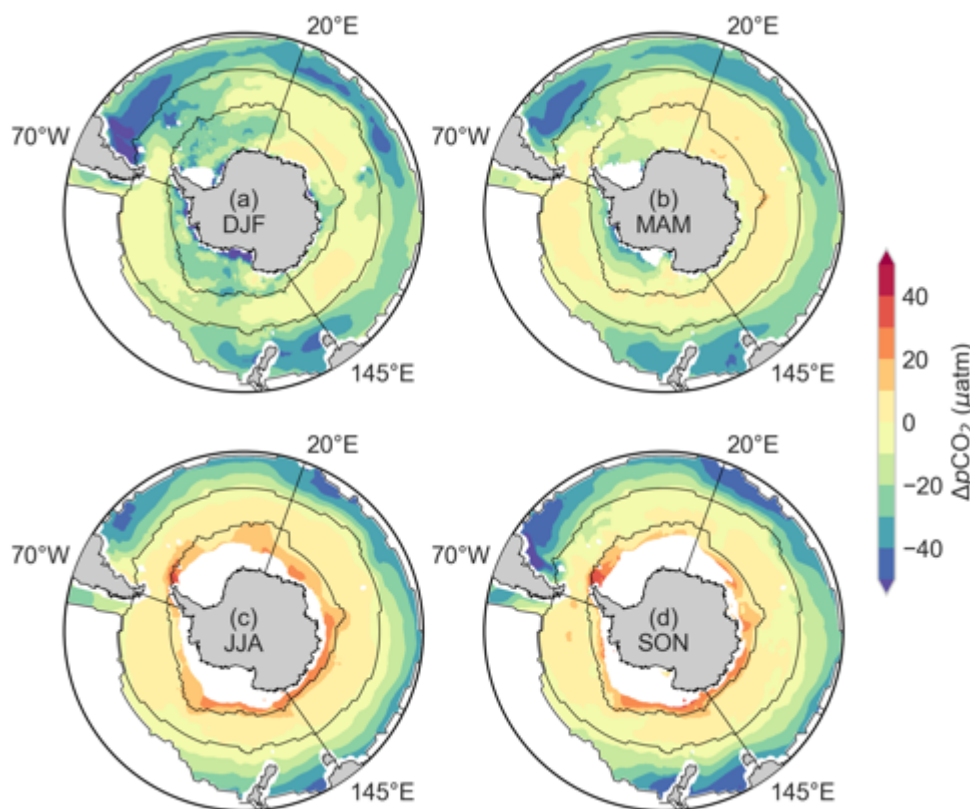
In order to ascertain a degree of coherence and confidence in the ensemble we show the signal to noise ratio in Figure 3c. We define the signal as the largest difference in the trend for a particular point. This is calculated from the largest difference of annual averages of $\Delta p\text{CO}_2$. The noise is the mean standard deviation of ensemble member estimates. A large signal to noise ratio (Figure 4c) is indicative of a large trend signal compared to the variability of the ensemble. While signal to noise ratio is > 1 for the entire domain, there are regions where the ratio is < 2 : parts of the Atlantic sector of the SAZ and the Indian sector of the PFZ.

With the established baseline of confidence in the ensemble, the ensemble mean of $\Delta p\text{CO}_2$ can be assessed. The seasonal cycle is the strongest mode of $\Delta p\text{CO}_2$ variability in the Southern Ocean (Lenton et al. 2013). It is therefore important that the ensemble mean is understood in the context of our current understanding of the seasonal cycle.

of $\Delta p\text{CO}_2$ in the MIZ is much larger than the two other regions. However, this amplitude is likely to be dampened by ice cover (Ishii et al., 1998; Bakker et al., 2008; Butterworth and Miller, 2016). Note that in this study, we do not include regions with sea-ice cover to ensure consistency between methods. Calculated fluxes for this methodologically reduced region will thus under-represent the fluxes of the full extent of the MIZ. We thus exclude the MIZ for the remainder of the study.

95 [Figure 2\(d\)](#) shows the time evolution of between-method errors for each biome. This panel highlights the seasonality of the data, specifically the increased heterogeneity of $\Delta p\text{CO}_2$ in summer and the impact that this has on $\Delta p\text{CO}_2$ estimates. This is due to the more complex competing processes affecting $p\text{CO}_2$ during summer. To gain a better understanding of the seasonal processes we look at the mean state of each season to characterise the drivers of opposing fluxes.

00 3.2 Ensemble seasonal cycle



05 **Figure 43:** The mean seasonal states of $\Delta p\text{CO}_2$ of the empirical ensemble mean. These are shown for (a) summer, (b) autumn, (c) winter and (d) spring. The black contour lines show the SAZ, PFZ and AZMIZ from north to south as defined by Fay and McKinley (2014).

The seasonal cycle of the $\Delta p\text{CO}_2$ for each biome (Figure 2a-c and Figure 4a3a-c) is coherent with expected seasonal processes based on reported in the literature (Metzl et al., 2006; Thomalla et al., 2011; Lenton et al., 2012; Lenton et al., 2013). In all biomes, uptake of CO_2 is stronger during summer than in winter giving rise to the strong seasonal cycle. This is due to the opposing influences of the dominant winter and summer drivers, partially damped by the seasonal cycle of temperature (Takahashi et al., 2002; Thomalla et al., 2011; Lenton et al., 2013). The dominant processes of mixing and entrainment in winter results result in increased surface $p\text{CO}_2$ and thus outgassing (Takahashi et al., 2009; Lenton et al., 2013; Rodgers et al., 2014). In summer, stratification also allows for increased biological production and the consequent uptake of CO_2 , thus reducing the entrained winter DIC and associated $p\text{CO}_2$ (Bakker et al., 2008; Thomalla et al., 2011). However, stratification typically limits entrainment, but does not exclude

the occurrence of entrainment during periods of intense mixing driven by storms, ~~which~~. This has an impact on ~~both~~ primary productivity, DIC and $p\text{CO}_2$ (Lévy et al., 2012; Monteiro et al., 2015; Nicholson et al., 2016; Whitt et al., 2017).

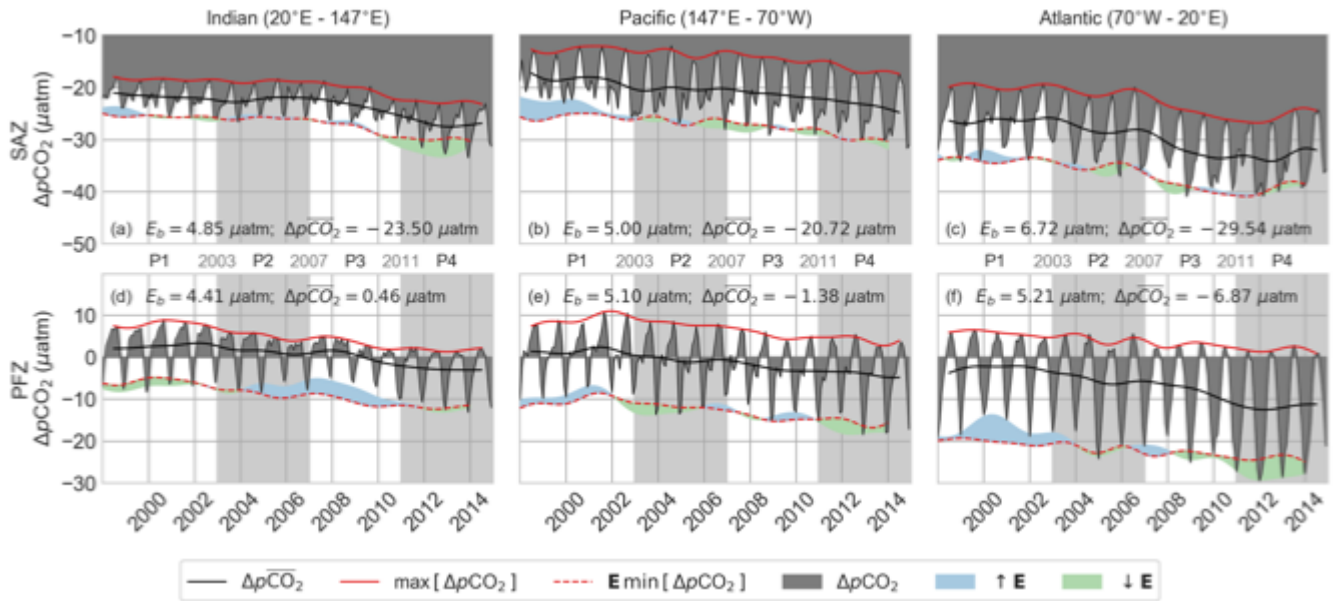
20 The SAZ (Figure 2a) is a continuous sink where summer uptake (Figure 4a3a) is enhanced by biological production and winter (Figure 4e3c) mixing results in a weaker sink (Metzl et al., 2006; Lenton et al., 2012; Lenton et al., 2013). ~~These~~ The same processes produce a similar seasonal amplitude in the PFZ (Figure 2b), but ~~the seasonal fluxes are~~ stronger upwelling and weaker biological uptake result in a positive shift of the mean. This results in an opposing: ~~a sink in net~~ summer ($< 0 \mu\text{atm}$) sink and ~~a source in~~ winter ($> 0 \mu\text{atm}$) source. However, this is according to the mean state in the PFZ and winter estimates of $\Delta p\text{CO}_2$ do in fact approach $0 \mu\text{atm}$ toward the end of the time series (Figure 2b). The AZMIZ has the strongest seasonal cycle due to upwelling of CO_2 during winter and strong biological uptake in summer. However, much of this is dampened by sea ice cover during winter and weaker winds during summer (Ishii et al., 1998; Bakker et al., 2008).

30 It ~~Apparent also from Figure 3~~ is ~~important to note~~ that, ~~over and above the latitudinal gradient~~, $\Delta p\text{CO}_2$ is zonally asymmetric within each biome, ~~particularly~~ during summer (Figure 4a3a) when biological uptake of CO_2 increases. Zonal integration of $\Delta p\text{CO}_2$ ~~and $f\text{CO}_2$~~ could thus dampen ~~magnitudes of~~ regional signals $\Delta p\text{CO}_2$. A regional approach is therefore needed to examine the regional characteristics of seasonal and interannual variability of $\Delta p\text{CO}_2$ and ~~$f\text{CO}_2$ and~~ to understand ~~their~~ drivers.

3.3 Regional $\Delta p\text{CO}_2$ ~~and $f\text{CO}_2$~~ Variability: Zonal variability: zonal and basin contrasts

Here $\Delta p\text{CO}_2$ ~~and $f\text{CO}_2$ are~~ is decomposed into nine domains by biome and basin with the boundaries shown in Figure 1, ~~but note only six are shown in Figure 4~~. The data are plotted as time series for $p\text{CO}_2$ (Figure 5) ~~and $f\text{CO}_2$ (Figure 6)~~ showing: ~~the~~ mean annual trends of $p\text{CO}_2$ ~~and $f\text{CO}_2$~~ (black lines), the maximum winter values (red line) and the projected summer minima (dashed red line) ~~based on adjusting the winter maxima each year by the mean of the difference between the winter maxima and the summer minima (Figures 5, 6)~~. The projected summer minima ~~implies that there is an~~ are calculated by subtracting the mean seasonal amplitude from the winter maxima (Figure 4, with air-sea CO_2 fluxes shown in Figure S3). The projected summer minima sets the expectation that summer $\Delta p\text{CO}_2$ is dependent on, but not restricted to, the baseline set by ~~the~~ winter maxima. Differences between the ~~ensemble~~ summer minima and projected minima are highlighted with green and blue patches, highlighting periods of decoupling between summer and winter interannual variability. The green areas indicate periods of strong uptake (relative to winter) that enhance the mean uptake of CO_2 ~~and amplify the seasonal cycle~~. Conversely, blue areas show periods where weak summer uptake (relative to winter) offsets winter

50 ~~trend~~outgassing, thus reducing the mean ~~trend~~- $\Delta p\text{CO}_2$ as well as supressing the amplitude of the seasonal cycle (Figure 4).



55 Figure 54: Figures (a-i) show $\Delta p\text{CO}_2$ (dark grey) and (j-r) show FCO_2 (dark grey) plotted by biome (rows) and basin (columns). Biomes are defined by Fay and McKinley (2014, 2014a). The solid red line shows the maximum for each year (winter outgassing) and the dashed line shows the same line less the average difference between the minimum and maximum seasonal amplitude – this is the expected amplitude. The shaded blue (green) area shows when the annual minimum is less (greater) than the expected amplitude. $\Delta p\text{CO}_2 E_b$ is the average between-method error and $\Delta p\text{CO}_2$ is the average for plots (g-i) was normalised to sea ice cover, but under ice $\Delta p\text{CO}_2$ estimates were still used to find the expected amplitude the entire time series. Light grey shading in (a-i) shows the proposed periods used in Figure 9 and Figure 10. Light grey shading in (j-r) shows the “saturation” period (1998 to 2001) and the “reinvigoration” period (2002 to 2011). 5 and Figure 6.

65 The data for $\Delta p\text{CO}_2$ and FCO_2 (Figures 5 and 6), show (Figure 4) shows that the Southern Ocean sink strengthened from 2002 to 2011 in all domains, a period identified as the *reinvigoration* by Landschützer et al. (2015). This was preceded by a period of a net weakening sink in the 1990’s referred to as the *saturation* period after Le Quéré et al. (2007). These two periods are highlighted by the grey fill in Figure 6. The saturation of the Southern Ocean CO_2 sink is not as strong in the ensemble, occurring in only five of the nine domains (see the positive trend slopes between 1998 and 2002 in Figure 6). In the last period (from 2012 to 2014) of the ensemble, three domains (Figure 4a,c,f) go from growing uptake to reducing uptake; however, our confidence in the increasing trends from 2012 to 2014 changing trend is low due to lack of coherence between methods (Figure 2a,b) and only three years of data, with very sparse few data in 2014.

75 Importantly, these A key feature of Figure 4 is that the mean interannual trends are variability is the integrated net effect of decoupled seasonal modes of variability: for summer and winter. This is particularly evident in the PFZ (Figures 5d, 4d-f). Here, and in the other biomes, there is a net

strengthening of the CO_2 sink ~~due is mainly linked~~ to a reduction of $\Delta p\text{CO}_2$ in winter ~~on roughly a decadal mode for the majority of the time series~~. This corresponds with the findings of Landschützer et al. (2016), who linked the ~~decadal variability reinvigoration~~ to ~~the decadal variability of~~ the Southern Annular Mode (SAM) – the dominant mode of atmospheric variability in the Southern Hemisphere (Marshall, 2003). In ~~comparison contrast~~, summer $\Delta p\text{CO}_2$ variability is ~~sub-decadal or shorter~~ (roughly 4 – 6 years), thus ~~impacting the short term providing inter-annual modulation of longer time-scale winter variability of the annually integrated trend~~. This is demonstrated well in the Indian sector of the PFZ where a decrease in winter $\Delta p\text{CO}_2$ from 2002 to 2011 is offset by weakening of the summer sink from 2006 to 2010 (Figure ~~5d, 6d4d~~). Similarly in the Atlantic and Pacific sectors of the ~~SAZ and PFZ strong~~ decoupling occurs from ~2011 to the end of 2014 with a rapid increase in the strength of the summer sink.

The mean amplitude of the seasonal cycle of $\Delta p\text{CO}_2$, the mean difference between the summer minima and the winter maxima, is ~~perhaps~~ a better means of understanding the ~~magnitude strength~~ of the seasonal drivers ~~for each domain~~ than the mean $\Delta p\text{CO}_2$ (~~Table A1~~). For example the Atlantic sectors of the SAZ and PFZ (Figures ~~5e4c~~,f) have the strongest seasonal variability (~~20.5714.11~~ and ~~27.6725.83~~ μatm respectively). This contrasts the relatively weak seasonal amplitude in the Indian sector of the Southern Ocean which has mean amplitudes of ~~8.857.06~~ and ~~13.3164~~ μatm for the SAZ and PFZ respectively (Figures ~~5b4b~~,e). This contrast can also be seen by comparing the mean seasonal maps of $\Delta p\text{CO}_2$ in Figures ~~4a3a~~ and ~~4e3c~~. In summer, strong uptake in the eastern Atlantic sector of the southern ocean is indicative of large biological drawdown of CO_2 by phytoplankton (Thomalla et al., 2011). Conversely, relatively low primary production in the Indian sectors of the SAZ and PFZ result in a small seasonal amplitude (Thomalla et al., 2011). This large discrepancy in biological primary production is related to the availability of iron, a micronutrient required for photosynthesis. The lack of large land masses, a source of iron, in the Indian sector of the Southern Ocean could be a contributing factor to the lack of biomass (Boyd and Ellwood, 2010; Thomalla et al., 2011).

~~The seasonal amplitude in the AZ is much larger due to strong contrast of the upwelling of CO_2 rich deep water contained beneath winter sea ice and the strong biological drawdown in the beginning of summer (Ishii et al. 1998, Bakker et al. 2008). Rapid stratification and iron supply by melting sea ice provide the environment for phytoplankton to proliferate in the AZ. This results in large seasonal amplitudes of 46.72, 75.46 and 64.29 μatm for the Indian, Pacific and Atlantic.~~

~~The air-sea fluxes of CO_2 ($F\text{CO}_2$) have decadal trends that are coherent with the $p\text{CO}_2$ (Figure 6), but there are notable differences that emerge from the impact of wind on the rate of exchange as well as the surface area of each domain (Figure A1). Most prominent are the changes in the seasonal cycle and the~~

mean seasonal sink of FCO_2 relative to pCO_2 with amplification in the Indian sector (Figures 5a,d and 6a,d) and weakening in the Atlantic Ocean (Figures 5c,f and 6c,f) of the Southern Ocean. The Indian sector of the SAZ (Figure 6a) dominates the uptake of CO_2 with an annual mean flux of $-0.25 PgC\ yr^{-1}$ compared to -0.19 and $-0.17 PgC\ yr^{-1}$ for the Atlantic and Pacific sectors respectively (where the latter are significantly different with $p = 0.01$). The seasonality of wind stress (see Figure A1) results in a damped seasonal cycle of FCO_2 in the SAZ and increasing intra-seasonal variability (compared to ΔpCO_2), with stronger winter winds compensating for a weaker ΔpCO_2 gradient (Monteiro et al. 2015).

Figure 6: Figures (a-i) show ΔpCO_2 (dark grey) and (j-r) show FCO_2 (dark grey) plotted by biome (rows) and basin (columns). Biomes are defined by Fay and McKinley (2014). The solid red line shows the maximum for each year (winter outgassing) and the dashed line shows the same line less the average difference between the minimum and maximum — this is the expected amplitude. The shaded blue (green) area shows when the annual minimum is less (greater) than the expected amplitude. ΔpCO_2 for plots (g-i) was normalised to sea ice cover, but under ice ΔpCO_2 estimates were still used to find the expected amplitude. Light grey shading in (a-i) shows the proposed periods used in Figure 9 and Figure 10. Light grey shading in (j-r) shows the “saturation” period (1998 to 2001) and the “reinvigoration” period (2002 to 2011).

This contrasts the PFZ, where opposition of summer uptake and winter outgassing of CO_2 is amplified by stronger wind stress (Figure 6d-f). Interannual variability is also enhanced, particularly during winter in the Indian sector of the PFZ, where a reduction in outgassing of $0.18 PgC\ yr^{-1}$ is observed. The decoupling between summer and winter FCO_2 also becomes more pronounced in this region (Figure 6d), resulting in a lag in the decreasing trend. In other words, the trend of FCO_2 for the reinvigoration (2002 through 2011: $-10.85 PgC\ yr^{-1}$) would have been stronger if the decoupling had not occurred. Similarly, the seasonal decoupling in the Pacific sector of the SAZ and PFZ results in a stronger growing sink from 2012 to 2014. In the Atlantic sector of the SAZ and PFZ the earlier onset of the seasonal decoupling (Figure 5c,f) also means that re-coupling occurs sooner, resulting in a positive flux trend (Figure 6c,f). Lastly, FCO_2 in the MIZ is damped during winter due to ice cover and weaker winds during summer when ΔpCO_2 is low due to the short-lived intense biological uptake of CO_2 (Ishii et al. 1998; Bakker et al. 2008).

3.4 Seasonal deconstruction of interannual variability

Figure 4 gives us insight into the magnitude of FCO_2 and ΔpCO_2 interannual ΔpCO_2 variability as well as the character of these changes; *i.e.* decoupling of decadal winter and sub-decadal summer interannual modes of variability. This alludes to the factpoint that ΔpCO_2 and FCO_2 are is responding to different adjustments of seasonal large scale atmospheric forcing and/or responses of internal ocean dynamics in the Southern Ocean (Landschützer et al., 2015, 2016; DeVries et al., 2017). In the study by Landschützer et al. (2015) it was advanced that the explanation for the reinvigoration of ΔpCO_2 uptake in the 2000s decade was linked to the net thermal control driven by a response of DIC and temperature to asymmetric atmospheric forcing over the Southern Ocean. More recently, a study by DeVries et al. (2017) proposed that the Southern Ocean uptake was due to the global deceleration of the

Meridional Overturning Circulation (MOC). They suggested that the MOC was increasing the oceanic storage and reducing the losses of CO₂ to the atmosphere, particularly in the Southern Ocean. The mechanism proposed by DeVries et al. (2017) is the same as that put forward by Le Quéré et al. (2007) and Lovenduski et al. (2008) amongst others, where the changes in outgassing are related to the strength of the westerly winds over the Southern Ocean. These studies have linked the wind stress variability to SAM.

In order to capture the decoupled short term variability observed during summer, the data are broken down into four interannual periods (P1 to P4), where P1 is five years and the remaining periods (P2 to P4) are four years as shown by the light grey fills in Figure 5. The first period is the saturation period (P1: 1998–2002) by Le Quéré et al. (2007). The second and third periods are informed by the reinvigoration period (2002 through 2011) split around the start of 2007 an early, weaker reinvigoration (P2: 2002–2006) and a late, stronger reinvigoration (P3: 2007–2011). The last period incorporates the three years of new data (P4: 2012 to 2014). The small discrepancy in the length of the periods is due to the uneven length of the time series (17 years).

These four periods are too short for trend analyses (Fay and McKinley, 2014a, 2014b), but the intention here is to identify periods that are short enough to resolve interannual changes in the large-scale drivers of the winter and summer mean values for pCO₂ and fCO₂ that would otherwise be averaged out over longer periods. We then calculate the relative anomaly between each successive period rather than a trend analysis (for which inflections of $\Delta p\text{CO}_2$ would be more suitable delimiters). The relative anomalies in an anomaly of the drivers are their differences between two adjacent periods mean state (e.g. P2 – P1). As a result four periods give rise to three sub-decadal-scale transition anomalies for summer and winter: A (P2 – P1), B (P3 – P2) and C (P4 – P3). We do this separately for each method rather than using the ensemble mean (see S4 for calculations). The mean of the method anomalies for each transition is then taken. These anomalies are considered significant if the absolute estimate of the anomaly is larger than the standard deviation between the methods for each period. These calculations along with plots for the standard deviation between methods are shown in the supplementary materials in S4.

Note that, although only summer and winter anomalies are discussed, it is recognised that autumn and spring could be equally mechanistically important. Winter anomalies of $\Delta p\text{CO}_2$, wind stress, SST and MLD are shown in Figure 75. Summer anomalies of $\Delta p\text{CO}_2$, wind stress, SST and Chl-*a* are shown in Figure 86 where MLD, in winter, is replaced with Chl-*a* for summer as it is potentially a more

important driver than the generally shallow ~~MLD in~~ summer ~~MLD~~ (the omitted plots are shown in Figures ~~A2S5~~ and ~~A3S6~~).

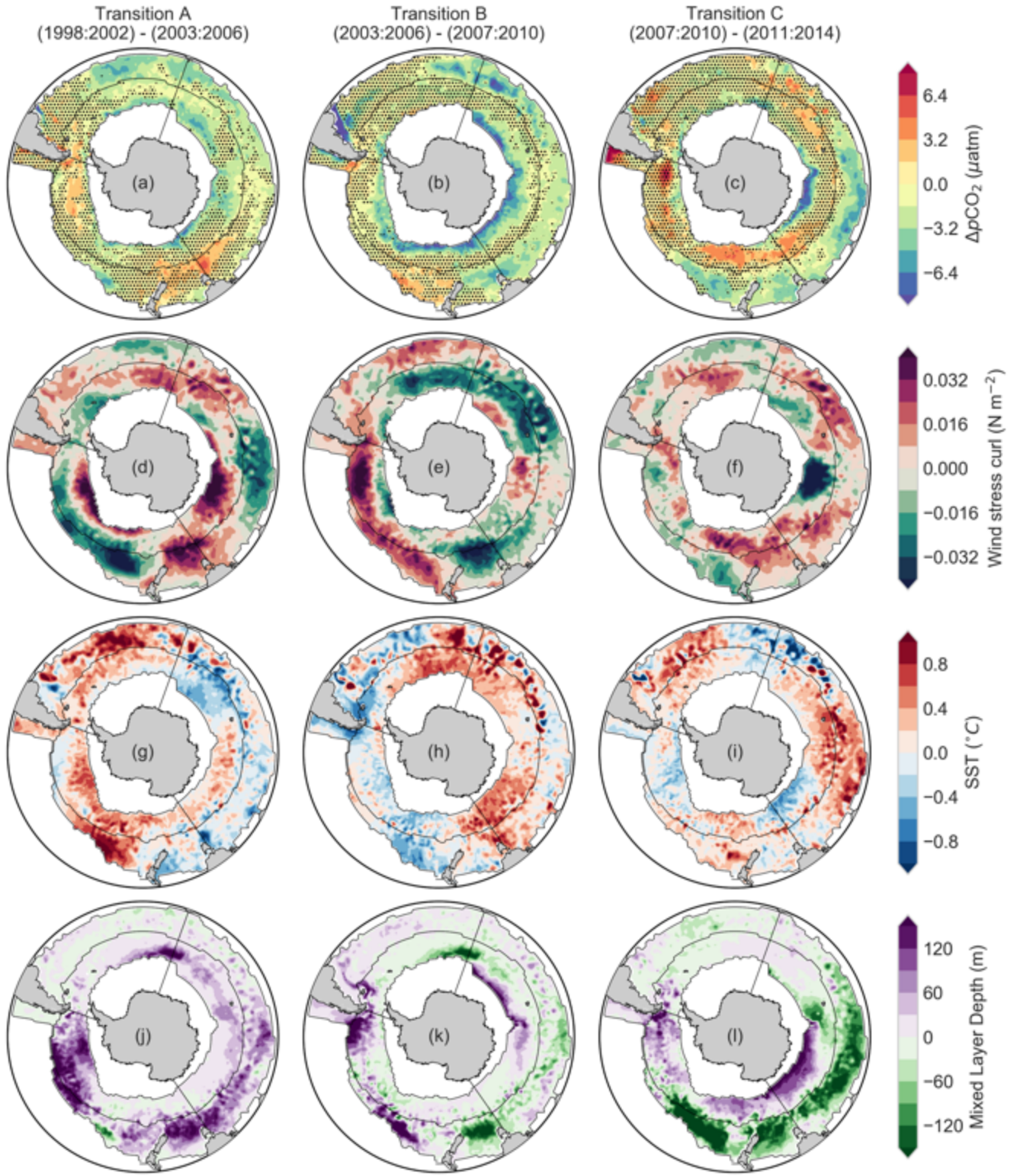


Figure 7: Transitions of winter $\Delta p\text{CO}_2$, wind stress, SST and MLD. Transitions (relative anomalies) of winter $\Delta p\text{CO}_2$ (a-c), wind stress (d-f), sea surface temperature (g-i) and mixed layer depth (j-l) for four periods (as shown above each column). The thin black lines show the boundaries for each of the nine regions described by the biomes (Fay and McKinley 2014) and basin boundaries (Fay and McKinley 2014a) and basin boundaries. Regions with dots in (a-c) are where the anomalies are not significant ie: standard deviation of the anomalies between models is greater than the absolute mean of method anomalies as described in equations S1 to S3.

3.5 Drivers of ~~the decadal~~ winter trends in $\Delta p\text{CO}_2$ and $f\text{CO}_2$ variability

There are two features of interest in the anomalies of winter $\Delta p\text{CO}_2$ and its drivers (Figure 7). First, there is a zonally asymmetric dipole for wind stress between the Pacific and Indian sectors of the Southern Ocean that dominates transitions A and B. Second, $\Delta p\text{CO}_2$, SST and MLD cohere roughly to the spatial variability of wind stress anomalies, mirroring the wind dipole. These features will be expounded on in the paragraphs that follow.

We will limit the interpretation of the changes to the regions where the anomaly is larger than the between-method error of anomalies (see S4 for calculations and maps). This masks out large regions, but three key points still arise from the significant anomalies. Firstly, $\Delta p\text{CO}_2$ is often spatially roughly coherent with wind stress and the inverse of SST. Secondly, there is a dipole in the wind anomalies in the Indian and Pacific between transitions A and B. This is confirmed by the u - and v -components of wind shown in the supplementary materials (Figure S5). Lastly, the Indian sector of the Southern Ocean dominates the reinvigoration of the CO_2 sink. These points are now addressed in more detail.

Transition A (~~the transition from P1, the saturation period, to P2, the start of the reinvigoration – P1~~) shows a relative increase of $\Delta p\text{CO}_2$ in the east Indian and Pacific sectors of the SAZ – suggesting a delay in the onset of the reinvigoration for these basins. This regional sustained saturation corresponds to a shift towards stronger winds and/or deeper MLDs west of the Tasman Sea (Pacific sector of the SAZ) and surrounds (Figure 7d5d,j). In contrast, CO_2 uptake in the east Atlantic and west Indian sectors of the SAZ, and the south-eastern Indian sector of the PFZ show a reinvigoration of CO_2 uptake. In the central Pacific, weaker wind stress (green in Figure 7d) start to strengthen, which roughly corresponds with relative warming and shoaling or stagnation of MLD. This is consistent with an invigoration of the Southern Ocean CO_2 sink (P1 – P2: 1998 – 2007) initiated by a weakening of the mean westerly wind stress in the Pacific and W Indian Oceans, which we are suggesting, reduced winter entrainment and possibly upwelling of CO_2 -rich deep waters (Marshall, 2003; DeVries et al. 2017); the weaker winds.

Transition B, which corresponds to anomalies between (P3 – P2 to P3 (the two reinvigoration periods), is characterized by ~~an~~ a further intensification of the invigoration of $\Delta p\text{CO}_2$ (~~ve~~(negative shift) ~~in all basins, but particularly primarily~~ in the Indian basin (Figure 7b). This5b). Once again the strengthening of the CO_2 uptake corresponds with weaker wind stress, a warming trend in surface waters and shoaling MLDs in the SEastern Atlantic and Indian Ocean sectors ~~in~~of the winterSAZ and PFZ (Figure 7b5b,e,h,k). ~~In the Pacific, the~~The opposing effects of the dipole are: observed east of New Zealand where stronger wind stress, deeper MLD, and cooler surface waters. ~~These changes are associated~~ corresponds with the

~~persistence of a neutral to weak reduction of positive shift in $\Delta p\text{CO}_2$ compared to the Indian sector. All the changes in transitions A and B are coherent to changes in the Pacific-Indian wind stress dipole.~~

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~~In transition C (P4 – P3: 2012 – 2015), when we propose the invigoration trend starts to weaken,) $\Delta p\text{CO}_2$ sink strengthens further in the northern and southern extremes of the east Indian and west Pacific basins, albeit in a more spatially heterogeneous way. In the Atlantic sector the previous invigoration trend reverses completely and the CO_2 sink in the winter is shown to weaken. This negative shift corresponds well with strong shoaling of the MLD (Figure 7b,e51). The previously well characterized west Pacific-Indian dipole is not apparent, suggesting that transition A and B capture well established phases in the decadal variability, while transition C may be capturing a transition into the following phase sector of the PFZ shows a positive shift in $\Delta p\text{CO}_2$, which could take the system back to the same configuration as P1. The notion that this period is a snapshot between two distinct phases is supported by the relatively heterogeneous spatial structure of is coherent with an increase in the wind stress in both the Atlantic and Indian Oceans and deepening MLD.~~

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3.5.1 Wind dominated interannual variability of $p\text{CO}_2$ in winter

~~We~~Based on the observations outlined above, we propose that ~~the~~ interannual variability of ~~seasonal the regional (basin-scale) characteristics of winter~~ wind stress ~~in winter~~ may be the dominant driver of the saturation and reinvigoration periods. ~~Moreover, the suggested Pacific-Indian wind dipole may be linked to the decadal variability of $\Delta p\text{CO}_2$ observed in the Southern Ocean (Landschützer et al. 2016).~~

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~~Increasing~~These findings suggest that ~~increasing~~ or decreasing interannual winter wind stress variability impacts $\Delta p\text{CO}_2$ (and thus $F\text{CO}_2$) by driving ~~stronger~~changes in turbulent mixing- ~~that set the magnitudes of winter entrainment~~. In the transition to and during winter, this mixing is associated ~~with changes in rates of~~ heat loss ~~resulting in that drive~~ loss of buoyancy or weaker stratification (Abernathey et al., 2011). Weaker buoyancy facilitates deepening of the MLD, thus entraining DIC-rich deep waters (Abernathey et al., 2011; Lenton et al., 2013). Conversely, decreased wind stress and mixing during winter (on seasonal or interannual time scales) reduces the rate of heat loss (represented as warm anomalies in Figure 75). This results in stronger stratification and shallower winter MLD limits entrainment of DIC, which strengthens the CO_2 winter disequilibrium and leads to a stronger CO_2 sink anomaly (Figure 7). ~~This is~~5). These are the ~~mechanism~~mechanisms that ~~results~~we propose result in decreasing or increasing fluxes with ~~interannual and basin-scale~~ changes in wind. ~~However, the direct link between this wind stress mechanism and the reinvigoration was not made by Landschützer et al. (2015).~~ ~~This may be, in part, due to the seasonal decoupling that may lead to biased interpretation of wind stress and SST.~~

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We propose the link between spatial changes in wind stress and uptake of CO₂ as an alternative hypothesis to temperature being a driver as suggested by Landschützer et al. (2015). Typically an increase in ocean temperature, which reduces CO₂ solubility, results in an increase in $\Delta p\text{CO}_2$ (Takahashi et al., 1993). However, seasonal – regional analysis shows that the observed relationship between $p\text{CO}_2$ and SST is counterintuitive (Figure 5a-c,g-i). On this basis we propose that SST is not a driver of $p\text{CO}_2$ in winter. We suggest that this relationship is a product of weaker mixing and Ekman transport that allows warmer waters to shift southward. This also has the impact of strengthening buoyancy that would otherwise bring CO₂ to the surface. In summary, our results suggest that, like $p\text{CO}_2$, the SST changes are also a response to the wind stress not in themselves the drivers of $p\text{CO}_2$ changes.

Given the hypothesis that wind stress is the dominant driver of interannual – decadal $\Delta p\text{CO}_2$ in winter, it is of interest to understand its potential mechanisms. Past studies have used the SAM as a proxy for wind stress variability over the Southern Ocean, where the multi-decadal increasing trend has been cited as a reason for the saturation in the 1990's (Marshall, 2003; Le Quéré et al., 2007; Lenton and Matear, 2007; Lovenduski et al., 2008). While Landschützer et al. (2016) identified the SAM as being a driver of global CO₂ variability, the index does not explain the reinvigoration of the Southern Ocean CO₂ sink in the 2000s. The SAM is often represented as a zonally integrating index (Marshall, 2003), but more recent studies have shown that the SAM, as the first empirical mode of atmospheric variability, is zonally asymmetric (Fogt et al., 2012). The zonal asymmetry of the SAM is linked with **ENSENSO** and is strongest in winter, particularly over the Pacific sector of the Southern Ocean during a positive phase, thus in accord with the Pacific–Indian winter wind stress dipole observed in Figures 5d,e (Barnes and Hartmann, 2010; Fogt et al., 2012). Fogt et al. (2012) noted that the SAM has become more zonally symmetric in summer since the 1980's, matching the wind stress anomalies seen in Figure 76d-f.

~~DeVries et al. (2017) proposed that slowing down of Meridional Overturning Circulation (MOC) as an alternate mechanism for the reinvigoration of the Southern Ocean CO₂ sink in the 2000's. The authors explain that weaker overturning reduces the natural CO₂ brought from the deep to the surface ocean. Moreover, they suggest that this mechanism may continue to drive intensification of the global CO₂ sink. The longer modes of MOC variability makes it difficult to attribute the change in flux to changes in overturning.~~

~~This poses an interesting question for the Southern Ocean carbon sink when we consider that weakening MOC may counteract the intensification of winds over the Southern Ocean (encapsulated by the increasing SAM). Meredith et al. (2012) found that this question is made more complex by the compensatory effect of increased eddy activity (measured by eddy kinetic energy – EKE) to enhanced~~

northward Ekman transport driven by intensified winds (Meredith and Hogg, 2006; Abernathey et al. 2011; Marshall and Speer, 2012). Moreover, the inclusion of these eddies in a high resolution model reduced CO₂ outgassing driven by increased Ekman transport by one third by entraining alkalinity to the surface water (Dufour et al. 2013). As it stands, this is an unresolved question and more work will have to be undertaken to understand the effect of these two counteracting mechanisms of CO₂ transport.

In summary, we propose that interannual variability of wind stress and its regional expression in winter is the dominant interannual driver of $\Delta p\text{CO}_2$ variability in the Southern Ocean. The interannual variability of wind stress is linked to the SAM, but this relationship is nuanced by the zonally (regional) asymmetric variability of the SAM— as observed by zonal asymmetry of wind stress in the Pacific and Indian sectors of the Southern Ocean.

3.6 Trends in the anomalies Anomalies of $\Delta p\text{CO}_2$ and its summer drivers ~~in summer~~

The most ~~important~~ marked difference between the summer and winter anomalies, is that $\Delta p\text{CO}_2$ (Figures 6a-c) does not correlate with wind stress (Figures ~~8d6d-f) does not correlate to~~ $\Delta p\text{CO}_2$ (Figures 8a-e), thus ruling out wind as a first order driver of summer CO₂. Rather, $\Delta p\text{CO}_2$ has the strongest coherence with Chl-*a* (an inverse relationship), which suggests that primary production may be a first order driver of the observed $\Delta p\text{CO}_2$ variability. Another difference between summer and winter is that the magnitudes of the transition anomalies are much larger in summer, and thus there are larger regions of significant anomalies (Figure 6a-c).

Looking more specifically at the significant variability of $\Delta p\text{CO}_2$, ~~Transition~~ transition A (P2 – P1 in Figure 8a6a) is marked by ~~patchy decreases—a decrease of~~ CO₂ in ~~regions of high EKE (Agulhas retroflection and the SAZ (Tasman shelf) in the SAZ and AZ, region),~~ mirrored by an increase in Chl-*a*. The Atlantic and Indian sectors of the PFZ remain mostly neutral/weak sources marked by a reduction in phytoplankton biomass (Figure 8j6j). Transition B (P3 – P2 in Figure 8b6b), shows invigoration of CO₂ uptake in: the Atlantic sector of the SAZ and PFZ; ~~the Indian sector and in parts~~ of the ~~AZ; and patchy strengthening in the~~ Pacific Ocean. Once again, the reduction of $\Delta p\text{CO}_2$ ~~from P2 to P3 in the~~ aforementioned regions correlate correlates well with Chl-*a* increases. In transition C (P4 – P3 in Figure 8e6c) the reduction of the $\Delta p\text{CO}_2$ is widespread in the Indian and Pacific Oceans in all three biomes, ~~though this does not necessarily correspond with as the increase in~~ Chl-*a*. ~~There is a strong decrease~~ similarly widespread. Conversely, there is a reduction in Chl-*a* and concomitant increase in $\Delta p\text{CO}_2$ along Polar front in the Atlantic sector, coinciding with position of the ACC₂ which has high EKE (Meredith, 2016). These examples demonstrate that $\Delta p\text{CO}_2$ is driven primarily by Chl-*a* in summer. However, understanding Chl-*a* variability is ~~perhaps~~ more complex as there is seemingly no set rule between Chl-*a*, SST and wind stress (Thomalla et al., 2011).

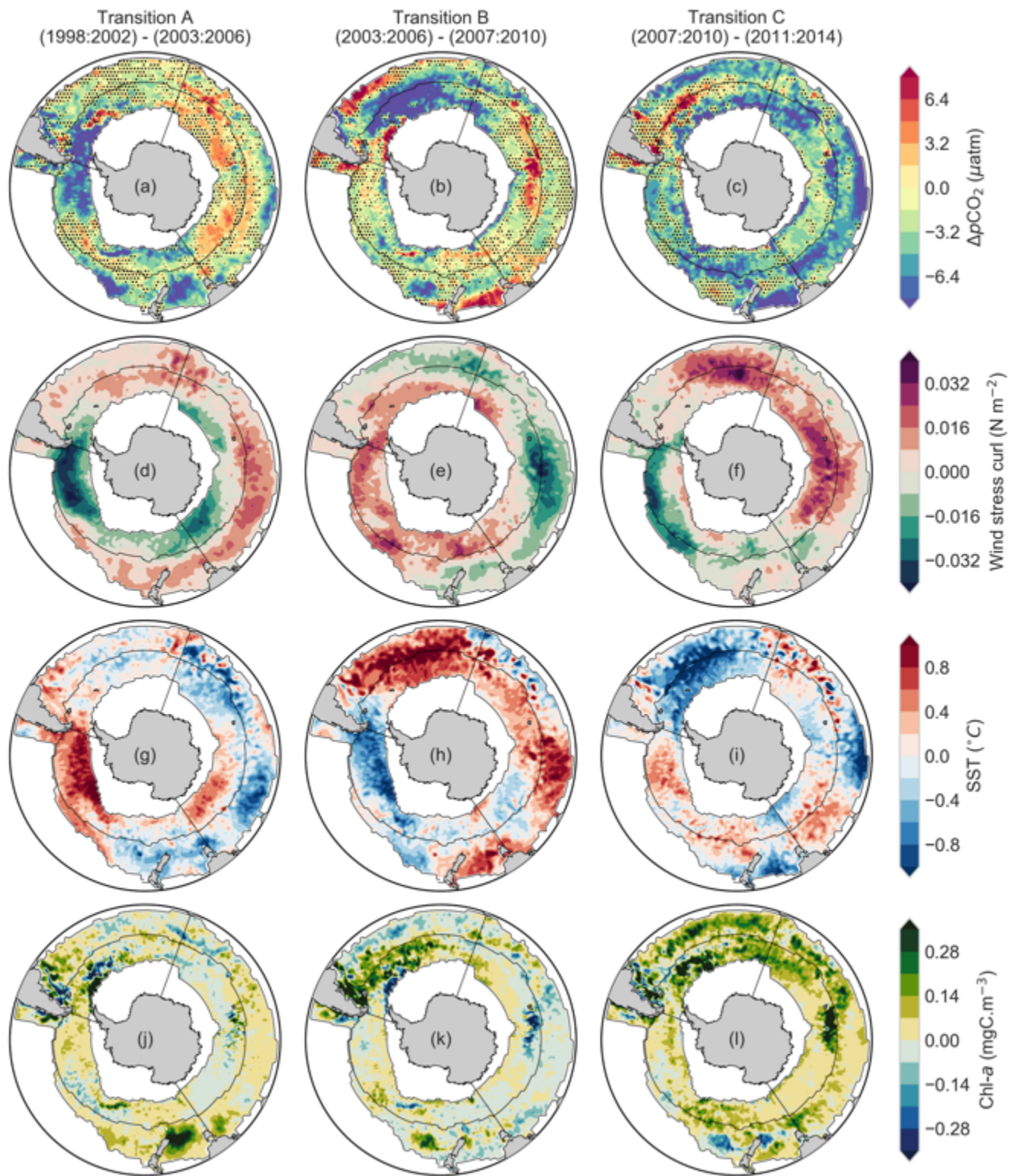


Figure 8: Transitions of summer $\Delta p\text{CO}_2$, wind stress, SST and Chl-*a* for four periods (as shown above each column). The thin black lines show the boundaries for each of the nine regions described by the biomes (Fay and McKinley 2014, 2014a) and basin boundaries.

There are regions in the Southern Ocean where summer Chl-*a* variability does not coincide with $\Delta p\text{CO}_2$ variability, particularly in the Indian and Pacific sectors of the SAZ (Figures 8a6a-c and 8j6j-l). This may be due to the fact that low chlorophyll concentrations, and anomalies thereof, are low in these regions (Thomalla et al., 2011). This may As a result in the other variables, SST and wind stress, becoming may

be higher order drivers [in low chlorophyll regions](#), as found by Landschützer et al. (2015) and Munro et al. (2015).

It is thus important to understand the variability of SST and wind stress in summer. Large SST anomalies between the western Atlantic and eastern Pacific sectors vary as [ana](#) zonally asymmetric dipole. As in winter, there is a summer wind stress anomaly dipole, but rather than being zonally asymmetric (e.g. Pacific–Indian), the dipole has annular, north-south variability (Figures [7,8d5,6d-f](#)). We suggest that these dipoles in the variability may indicate that the Southern Ocean, as a system, transitions between different states forced by atmospheric variability (Landschützer et al. [2015](#)).

~~Lastly, there~~An important note is ~~seasonal variability in that~~ the magnitudes of $\Delta p\text{CO}_2$ and ~~the its~~ drivers. ~~The have different magnitudes seasonally. For example, the~~ anomalies of $\Delta p\text{CO}_2$ and SST ~~have aare~~ larger ~~magnitude in summer~~ than ~~the in~~ winter ~~anomalies~~. Conversely, the wind stress anomalies are [larger](#) for winter than in summer. This is an important consideration for analyses that aim to understand the driving mechanisms, where annual averaging would make it difficult to decompose the true drivers of change.

3.6.1 Chlorophyll dominated interannual anomalies of $p\text{CO}_2$ in summer

~~The fact~~Our finding that Chl-*a* is the dominant driver of interannual $\Delta p\text{CO}_2$ variability should not be surprising given that models and observations support this [notion](#) (Hoppema et al. [2019](#); Bakker et al. [2008](#); Mahadevan et al. [2011](#); Wang et al. [2012](#); Hauck et al. [2013](#); [2015](#); Shetye et al. [2015](#)). However, our data show that the dominance of interannual Chl-*a* variability over $\Delta p\text{CO}_2$ is largely limited to regions where Chl-*a* is high, such as the Atlantic, the Agulhas retroflection and south of Australia and New Zealand (Figure [97](#)).

~~However, the~~The spatial variability of high Chl-*a* regions in the Southern Ocean is complex due to the dynamics of light and iron limitation (Arrigo et al. [2008](#); Boyd and Ellwood [2010](#); Thomalla et al. [2011](#); Tagliabue et al. [2014](#); [2017](#)). This complexity is highlighted in Thomalla et al. (2011), where the Chl-*a* is characterized into regions of concentration and seasonal cycle reproducibility (Figure [97](#)). The seasonal cycle reproducibility (SCR) is calculated as the correlation between the mean annual seasonal cycle and the observed chlorophyll time series. Here we use the approach of Thomalla et al. (2011), in Figure [97](#), as a conceptual framework to understand the interannual variability of $\Delta p\text{CO}_2$.

3.6.2 High chlorophyll regions

While regions of high SCR (dark green in Figure [97](#)) do not correspond with the interannual variability of Chl-*a* (Figure [8j6j-l](#)), the framework by Thomalla et al. (2011) does present a hypothesis by which the

variability of Chl-*a* and its drivers can be interpreted. This is, that the variability of Chl-*a* in a region is a complex interaction of the response of the underlying physics (mixing vs buoyancy forcing, which modulate light ([via the MLD](#)) and iron supply, to the interannual variability in the drivers (SST and wind stress). This complexity is exemplified by strong warming in the Atlantic during transition B, which results in both an increase and decrease in Chl-*a*, with inverse consequences for $\Delta p\text{CO}_2$. The effect is even stronger transition C, where strong cooling in the Atlantic results in both a decrease and increase of Chl-*a* (Figure [8+61](#)). In both transition A and B the respective increase and decrease of Chl-*a* occur roughly over the ACC, while the opposing effects during transitions A and B occur roughly to the north and south of the ACC region. These temperature changes may impact the stratification of the region, but complex interaction with the underlying physics results in variable changes in Chl-*a*.

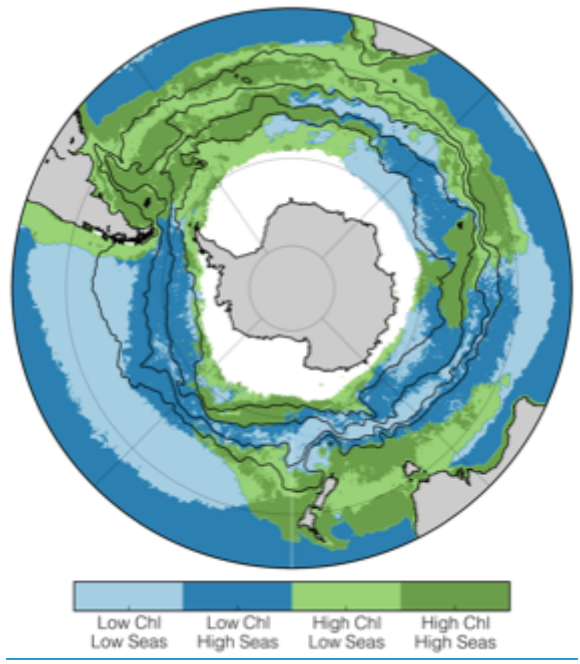


Figure 9: Chl-*a* seasonal cycle reproducibility and iron supply mechanisms in the Southern Ocean (a) Regions of chlorophyll biomass and seasonal cycle reproducibility from Thomalla et al. (2011) (using SeaWiFS data). Seasonality is calculated as the correlation between the mean annual seasonal cycle compared to the observed chlorophyll time series. A correlation threshold of 0.4 was applied to each time series to distinguish between regions of high and low seasonality; similarly, a threshold of 0.25 mg m^{-3} was used to distinguish between low or high chlorophyll waters. Black lines showing the fronts are the same as described in figure.

It is clear that, while there is a relationship between Chl-*a* and $p\text{CO}_2$ as well as a relationship between wind stress and SST in summer, the relationship between wind forcing and Chl-*a* and $p\text{CO}_2$ is not as strong as in the winter anomalies (Figure 7). The reason for this is likely to be that enhanced summer buoyancy forcing resulting from summer warming and mixed layer eddies drives a more complex response to wind stress in the form of vertical velocities (w) and mixing (K_z), which influence the iron supply and the depth of mixing depth (McGillicuddy, 2016; Mahadevan et al., 2012).

Mesoscale and sub-mesoscale processes may have a part to play in these dynamic responses of Chl-*a* to changes in SST and wind stress (amongst other drivers). For example, eddy-driven slumping is a sub-

~~mesoscale process that acts could act~~ to rapidly shoal the mixed layer (Mahadevan et al., 2012; Swart et al., 2015b; du Plessis et al., 2017). This allows phytoplankton to remain within the euphotic zone and thus grow (while iron is not limiting). Similarly, Nicholson et al. (2016) and Whitt et al. (2017) demonstrated that ~~a combination of high and low frequency oscillation of down-front winds are able to enhance nutrient entrainment (including submesoscale processes could supply iron) into to~~ the mixed layer ~~on the less dense side of a front. This has important implications for Southern Ocean fronts, where Chl-*a* may benefit from this entrainment mechanism combined with eddy driven slumping that could subsequently rapidly shoal the mixed layer (Du Plessis et al. by submesoscale 2017).~~

~~Storm driven, intra-seasonal mixing is another sub-mesoscale process that could alleviate iron limitation through shear driven mixing along the base of the mixed layer (Nicholson et al. 2016).~~ Importantly, ~~both storm driven entrainment and the oscillatory enhancement of entrainment, these mechanisms~~ rely on a mixing transition layer that has sufficient iron that is able to sustain growth – weak dissolved iron gradients in the Pacific and east Indian sectors of the Southern Ocean ~~would could~~ explain the lack of phytoplankton in these regions (Tagliabue et al., 2014; Nicholson et al., 2016). Much of the spatial character of the transition anomalies occurs at mesoscale, which strengthens the view that these mesoscale and sub-mesoscale processes may be key to explain changes in Chl-*a* (Figure 8j-l). ~~This level of mechanistic detail was not part of this study. 6j-l).~~

3.6.3 Low chlorophyll regions

Entrainment and stratification can explain much of the variability in the eastern Pacific and Indian sector of the PFZ (with the exception of the wake of the Kerguelen Plateau). For example, in the eastern Pacific in transition A (Figure 8a6a,d,g), strong warming and weaker winds have little impact on Chl-*a*, but a decrease in $\Delta p\text{CO}_2$ is observed. Conversely, cooling in the west Indian sector of the PFZ results in a weak increase in $\Delta p\text{CO}_2$ during the same transition. In both these cases, the effect of cooling or warming on $\Delta p\text{CO}_2$ is negligible relative to the impact of entrainment or stratification respectively. The effect is reversed in the eastern Pacific during transition B where strong cooling results in a weak reduction of $\Delta p\text{CO}_2$ rather than the increase that would be expected from entrainment. This is the mechanism that Landschützer et al. (2015) ~~describe in the Pacific, where enhanced entrainment of DIC and TA is compensated for by cooling. This emphasises that the balance between SST (as a driver of stratification) and wind stress is far more important than in winter~~ (2015) ascribed to the reduction of $\Delta p\text{CO}_2$ in the Pacific, but the effect observed in 6b is weak.

In summary, regions with high biomass, Chl-*a* integrates the complex interactions between SST, wind stress, MLD and sub-mesoscale variability resulting in large interannual $p\text{CO}_2$ variability compared to

low biomass regions. In low Chl-*a* regions, wind driven entrainment/stratification are ~~in general dominant over thermally driven changes~~more likely drivers of $\Delta p\text{CO}_2$.

4 Synthesis

In this study, ~~an~~ ensemble means~~mean~~ of empirically estimated $\Delta p\text{CO}_2$ ~~and $f\text{CO}_2$ were~~is used to investigate the trends and the drivers of these trends in the Southern Ocean. The ~~ensemble mean of estimated~~ $\Delta p\text{CO}_2$ ~~showed~~shows that the seasonal cycle is the dominant mode of variability imposed upon ~~a~~ weaker interannual ~~and decadal trends~~variability. The data ~~were~~are separated into ~~nine~~ domains defined by functional biomes and oceanic basins to account for the roughly basin scale zonal asymmetry observed in preliminary analyses of $\Delta p\text{CO}_2$ (Fay and McKinley, ~~2014~~2014a). A seasonal decomposition ~~was~~is applied to the ~~nine~~ domains, revealing that winter and summer ~~interannual trends are~~variability is decoupled for each region. ~~The decadal trend was~~increase and subsequent decrease of $p\text{CO}_2$ (and air-sea CO_2 fluxes) is in accordance with recent studies showing a saturation of the Southern Ocean CO_2 sink in the 1990's followed by the reinvigoration in the 2000's (Le Quéré et al., 2007; Landschützer et al., 2015).

We suggest that changes in the characteristics of the seasonal cycle of the drivers of $p\text{CO}_2$ define the interannual ~~and decadal modes~~. ~~The variability $p\text{CO}_2$. In other words, the~~ mechanisms that drive ~~the~~ interannual ~~and decadal~~ modes of variability are ~~therefore~~ embedded in the seasonal cycle.

We propose that winter $\Delta p\text{CO}_2$ ~~decadal~~ variability is driven ~~by~~ primarily by changes in ~~the~~ winter wind stress, which influences the resulting convective entrainment of deep DIC-rich water masses (Lenton et al., 2009; 2013). This winter variability has a longer mode than summer inter-annual variability. We attribute this longer winter mode of variability to the Southern Annular Mode, which has a decadal mode (Lovenduski et al., 2008; Fogt et al., 2012; Landschützer et al., 2016). This mechanism is ~~strongest~~likely dominant in winter due to ~~the~~its role ~~of~~in large seasonal net heat losses ~~on that drive~~ convective overturning of the water column. ~~The $\Delta p\text{CO}_2$ winter trends, agreed with wind stress variability, where the latter corresponds with the decadal variability associated with the Southern Annular Mode (Lovenduski et al. 2008; Fogt et al. 2012; Landschützer et al. 2016).~~

~~Our findings show~~We suggest that interannual summer variability of $\Delta p\text{CO}_2$ occurs from a baseline set by an interannual winter trend ~~but~~. Moreover, the shorter time-scale summer ~~linked~~ interannual variability of $\Delta p\text{CO}_2$ (roughly 4 – 6 years) ~~was~~is driven primarily by Chl-*a*. Wind stress and sea surface temperature still ~~influenced~~influence $\Delta p\text{CO}_2$ in summer, but ~~were~~are lower order drivers. We propose that the

interannual variability of the summer seasonal peak is linked to the complex interaction of mid-latitude
'70 storms with the strong mesoscale and sub-mesoscale gradients in the Southern Ocean.

~~We~~Overall, we propose that ~~there needs to be a more concerted focus through in situ and modelling~~
~~experiment towards understanding although~~ the winter wind-stress linked mechanisms ~~that drive seasonal~~
~~and intraseasonal variability in order to improve explain~~ the ~~ability of ocean and earth systems models in~~
'75 ~~reflecting and predicting~~ decadal ~~and interannual modes~~.

A Additional Materials

A1 Mean $\Delta p\text{CO}_2$ for Southern Ocean domains

The SAZ (Figures 5a-c) accounts for trends in the majority of strengthening and weakening of CO_2 uptake in the Southern Ocean with a mean $\Delta p\text{CO}_2$ of $-25.31 \mu\text{atm}$. However, there is a relatively large difference between the three sectors of the SAZ, with mean $\Delta p\text{CO}_2$ values of -24.39 , -22.24 and $-30.48 \mu\text{atm}$ for the Indian, Pacific and Atlantic respectively. In the PFZ (Figures 5d-f) the sink is far weaker due to the opposing summer uptake and winter outgassing, with $\Delta p\text{CO}_2$ values of 0.23 , -2.06 and -6.57 again in the respective order Indian, Pacific and Atlantic. Similarly, in the AZ (Figures 5g-i) mean estimates of $\Delta p\text{CO}_2$ are muted by opposing seasonal signals with mean estimates of 4.83 , -3.01 and $-0.76 \mu\text{atm}$ by the Southern Ocean, summer drivers may explain the inter-annual variability in the decadal trends (Lovenduski et al., 2008; Landschützer et al., 2015).

Lastly the ensemble of machine learning methods shows that there is still considerable disagreement between the different approaches. This is likely driven by the lack of $p\text{CO}_2$ measurements in the Southern Ocean as found by Rödenbeck et al. (2015). Table 2: Mean $\Delta p\text{CO}_2$ for each of the Southern Ocean domains shown in Figure 5, where the domains are defined according to Figure 1.

BIOME	Indian	Pacific	Atlantic
SAZ	-24.39	-22.25	-30.48
PFZ	0.23	-2.06	-6.57
AZ	4.83	-3.01	-0.76

A2 Autonomous sampling platforms will likely play a role in closing this “observation gap”, but strategic deployment and sampling strategies will be critical to constrain and improve our understanding of CO_2 in the non-stationary context (McNeil and Matear, 2013; Monteiro et al., 2015).

S Supplementary Materials

S1 Wind speed and regional surface area

The regional magnitude of integrated air-sea CO₂ fluxes are in part determined by the wind speed and surface area of the specific region. Figure 4a shows the average wind speeds for summer and winter for each of the regions as defined in Figure 1. The wind product used is CCMP v2 (Atlas et al. 2011). Figure 4b shows the surface area of each of the regions. Note that the Indian sector of the PFZ has both the highest average wind speed and has the largest surface area. This explains the dominance of the region in the determination of interannual trends of FCO₂ (Figure S2), even though $\Delta p\text{CO}_2$ trends (Figure 4) are relatively weak.

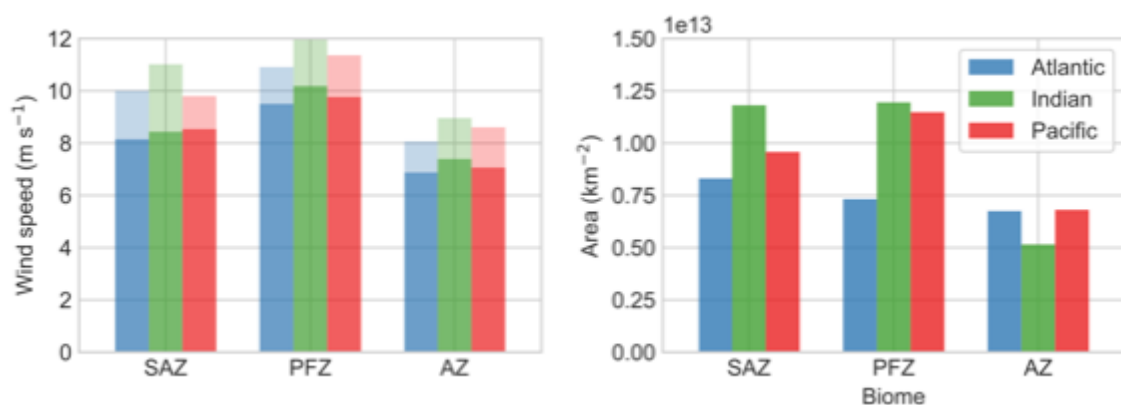


Figure A1S1: (a) Average wind speeds for each of the biomes for summer (dark) and winter (light). The ocean basins are shown by the colors as shown in the key for (b). (b) shows the size of each region separated by biome and basin.

A3 Additional transition anomaly figures

Figure A2 and A3 augment Figures 7 and 8 respectively. These were omitted from the main text figures as we found that these variables (Chl *a* in winter and MLD in summer) do little to aid our understanding of changes in $\Delta p\text{CO}_2$. These are included for the sake of completeness.

Figure A2: Winter Chl *a* transitions for each of the three anomaly periods (relating to Figure 7).

Figure A3: Summer MLD transitions

S2 Seasonal time series

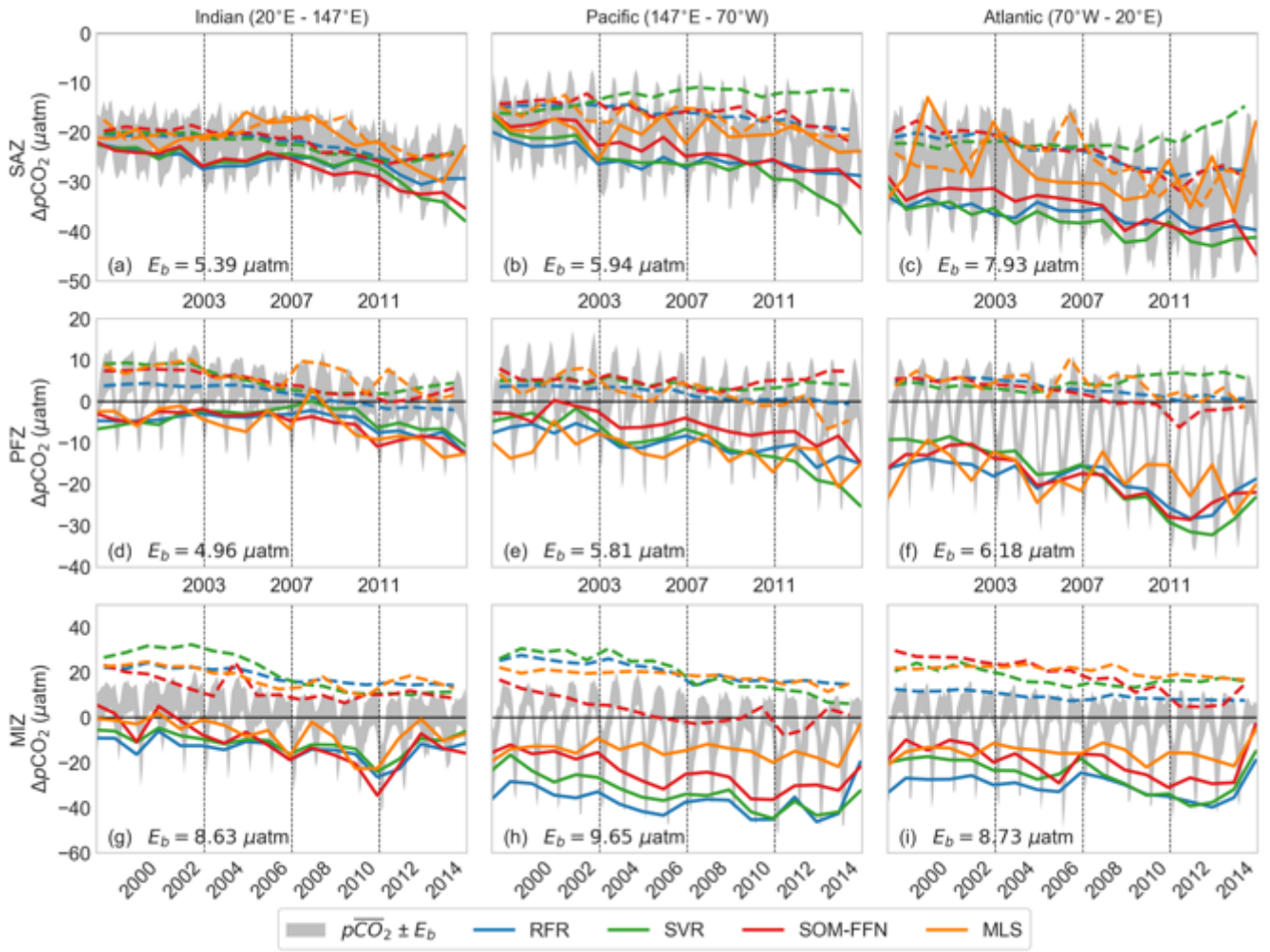


Figure S2: The regional breakdown of the seasonal averages for $\Delta p\text{CO}_2$. The seasonal mean for summer (solid) and winter (dashed) for each method is represented by the different coloured lines as shown in the key, where MLS is the Mixed Layer Scheme. The other methods are as in the main text. The grey fill is the ensemble mean $\Delta p\text{CO}_2 \pm E_b$ where E_b is the between-method error calculated as in Eq (5).

Figure S2 shows the seasonal time series for each of the three anomaly periods (relating to Figure 8)-region maintaining separate seasonal averages for each method. We also include the Marginal Ice Zone plots with all plots showing the average between-method error.

The Mixed Layer Scheme (MLS) method by Rödenbeck et al. (2013) is also included. Note that the scale of MLDMLS is not a machine learning method as it incorporates prior knowledge of the system. The method results in divergent estimates of $\Delta p\text{CO}_2$, particularly in the SAZ. The MLS fails to produce a seasonal cycle with winter and summer $\Delta p\text{CO}_2$ having the same magnitude. Further work will have to be done to understand the cause for this difference. We do not include MLS in the main ensemble as we cannot explain this difference. The methods are in much better agreement in the PFZ and MIZ.

S3 Air-Sea CO₂ Fluxes

Air sea CO₂ fluxes are calculated with:

$$FCO_2 = k_w \cdot K_0 \cdot (pCO_2^{sea} - pCO_2^{atm}) \quad (S1)$$

The gas transfer velocity (k_w) is calculated using a quadratic dependency of wind speed with the coefficients of (Wanninkhof et al., 2009). Coefficients from Weiss (1974) are used to calculate K_0 and ΔpCO_2 is estimated by the empirical models. Wind speed is calculated from the u and v vectors ($\sqrt{u^2 + v^2}$) of the Cross-Calibrated Multiplatform Product (CCMP) v2 (Atlas et al., 2011; Wentz et al., 2015). Wind speed is one of the largest contributors to the uncertainty in flux estimates, thus the choice of the wind product could have a large impact on flux estimates as well as interpretation of the drivers of CO₂ (Takahashi et al., 2009). We use the ensemble mean ΔpCO_2 from Figure 4 to calculate fluxes - note that this does not include the scale of MLDMLS shown in Figure S2.

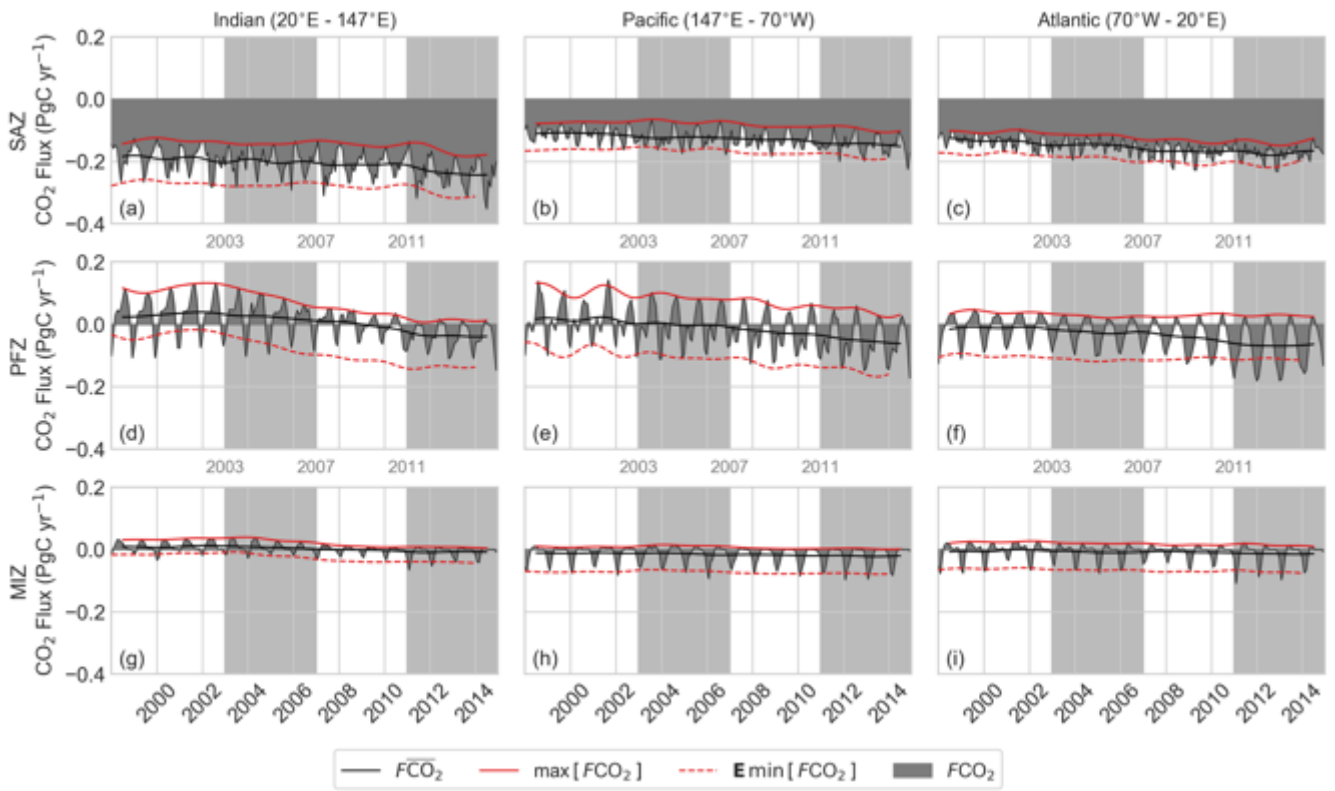


Figure S3: FCO_2 (dark grey) plotted by biome (rows) and basin (columns). Biomes are defined by Fay and McKinley (2014a). The solid red line shows the maximum for each year (winter outgassing) and the dashed line shows the same line less the average difference between the minimum and maximum – this is the expected amplitude. Lighter grey shading in (a-i) shows periods used in Figure 7–5 and 6. Note that fluxes in the MIZ are calculated from a reduced surface area to maintain consistency between methods.

Mean FCO_2 is shown in Figure S3. Note that the apparent weak fluxes in the MIZ are due to the reduction of the surface area and thus flux to maintain equal weighting between machine learning methods. The SAZ clearly dominates the annual uptake of CO₂ in the Southern Ocean, but the interannual variability is dominated by the PFZ. An interesting point of the SAZ is that the seasonal cycle of wind speed (strong in winter, weak in summer) opposes that of ΔpCO_2 sink (weak in winter, strong in summer). The net result is that, compared to ΔpCO_2 , the seasonal amplitude of FCO_2 is reduced. The same effect shifts the

mean flux in the PFZ, but does not affect the amplitude, where outgassing is amplified in winter and the sink is weaker than if wind speed was constant. Lastly, Figures S3a,d show that the Indian sector of the Southern Ocean dominate both uptake (SAZ) and the interannual variability (PFZ).

S4 Uncertainty of the transition anomalies

The transition anomalies are not calculated from the mean of the three methods. Rather we calculate the anomalies for each individual method with:

$$a_{n(p')} = \bar{s}_{n(p)} - \bar{s}_{n(p-1)} \quad (S2)$$

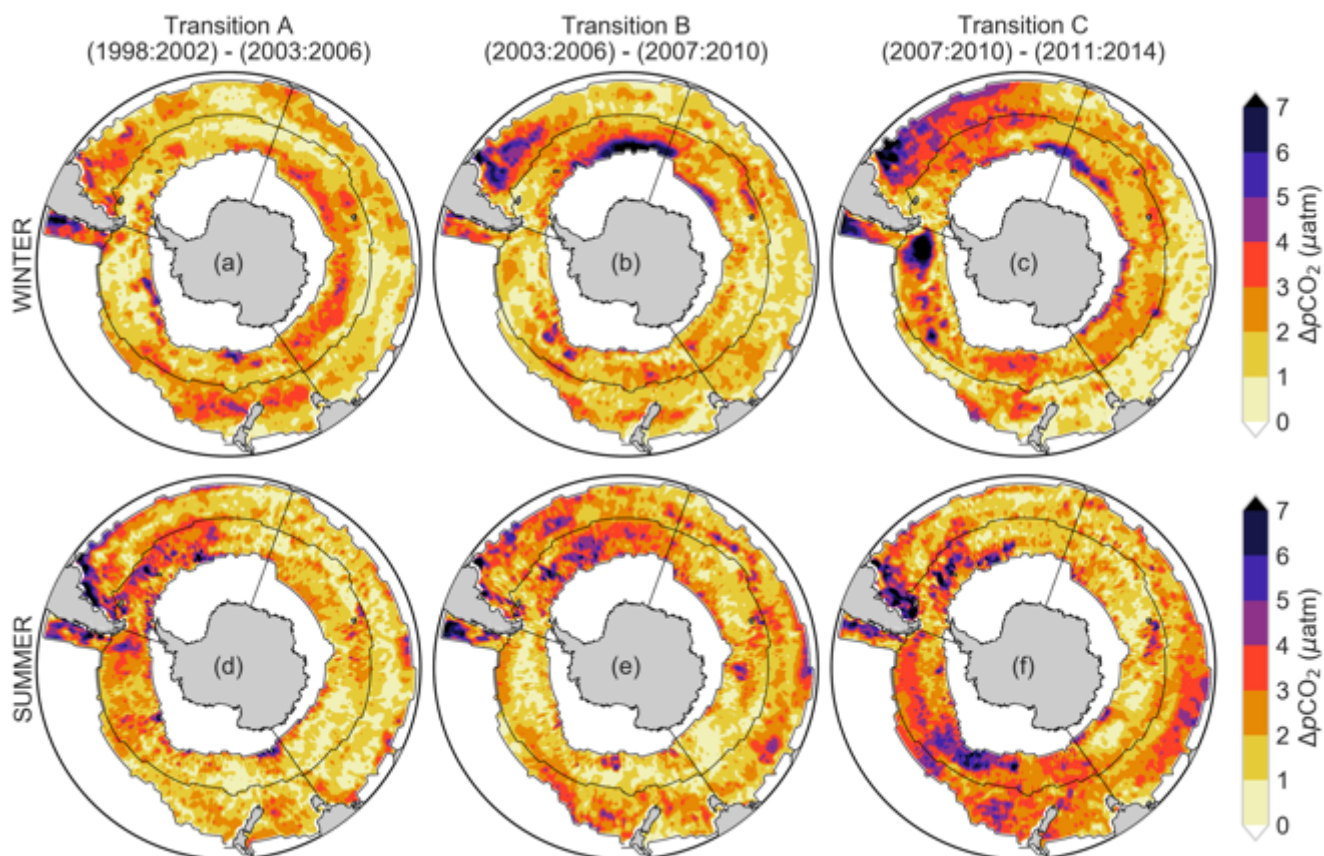
where s are the estimates for a particular model, n represents an individual model and p represents P1 to P4. The result, $a_{n(p')}$ thus represents the anomaly for two periods for a particular model. We then calculate the average of the anomalies with:

$$a_{p'} = \frac{1}{N} \cdot \sum_{n=1}^N a_{n(p')} \quad (S3)$$

where N is 3, the number of models. We then calculate the standard deviation of the three anomalies ($e_{p'}$), which is analogous to the between-model error, with:

$$e_{p'} = \sqrt{\frac{1}{N} \cdot \sum_{n=1}^N (a_{n(p')} - \bar{a}_{n(p')})^2} \quad (S4)$$

where the terms are consistent with those above. We use $e_{p'}$ as an uncertainty threshold where anomalies are only considered significant if $|a_{p'}| > e_{p'}$. These regions are masked in Figures 5a-c and 6a-c. Figure S4 shows the winter (a-c) and summer (d-f) $e_{p'}$ for each transition anomaly.



80 [Figure S4: Maps of the standard deviation between empirical methods for the anomalies. These are used as thresholds for \$\Delta p\text{CO}_2\$ in](#)
[Figures 5\(a-c\) and 6\(a-c\) for winter and summer respectively. When the standard deviation exceeds the absolute value average](#)
[anomaly, the values are masked as shown in Figures 5 and 6.](#)

85

S5 Additional driver variables

Here we show additional variables that accompany Figures 5 and 6. Figure S5 shows winter Chl-*a*, u- and v-components of wind and Figure S6 shows summer MLD, u- and v-components of wind. These variables were not included in the main analyses as they did not contribute significant information to the proxy variables already present (wind stress, SST and MLD/Chl-*a*). It is interesting to note that the u- and v- components of wind speed highlight the zonally asymmetric dipole during winter (Figures S5d,e,g,h) and the annular dipole during summer (Figures S6d,e).

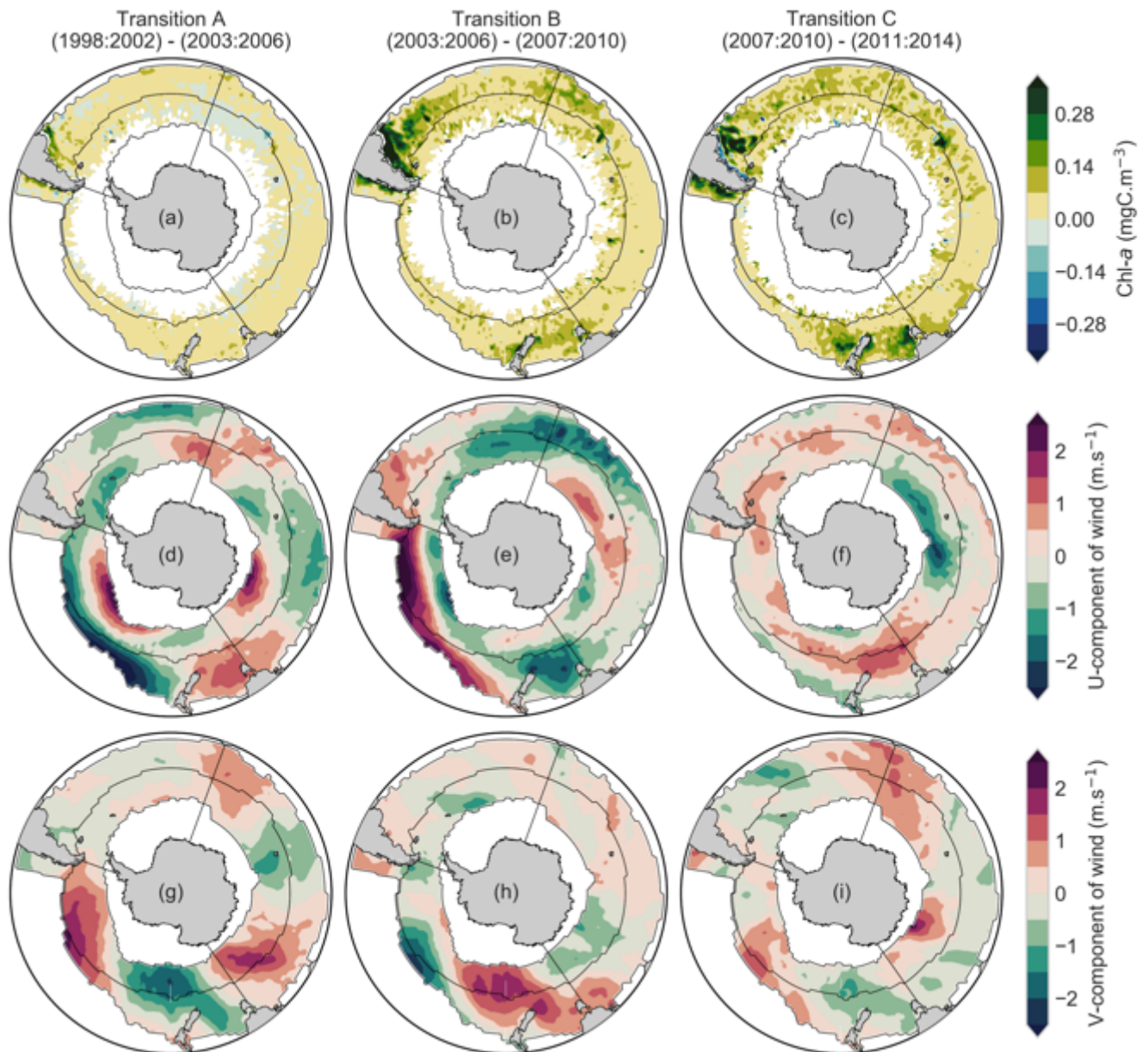


Figure S5: Relative anomalies of winter chlorophyll-*a* (a-c), u- (d-f), and v-components (g-i) of wind for four periods (as shown above each column). The thin black lines show the boundaries for each of the nine regions described by the biomes (Fay and McKinley, 2014a) and basin boundaries.

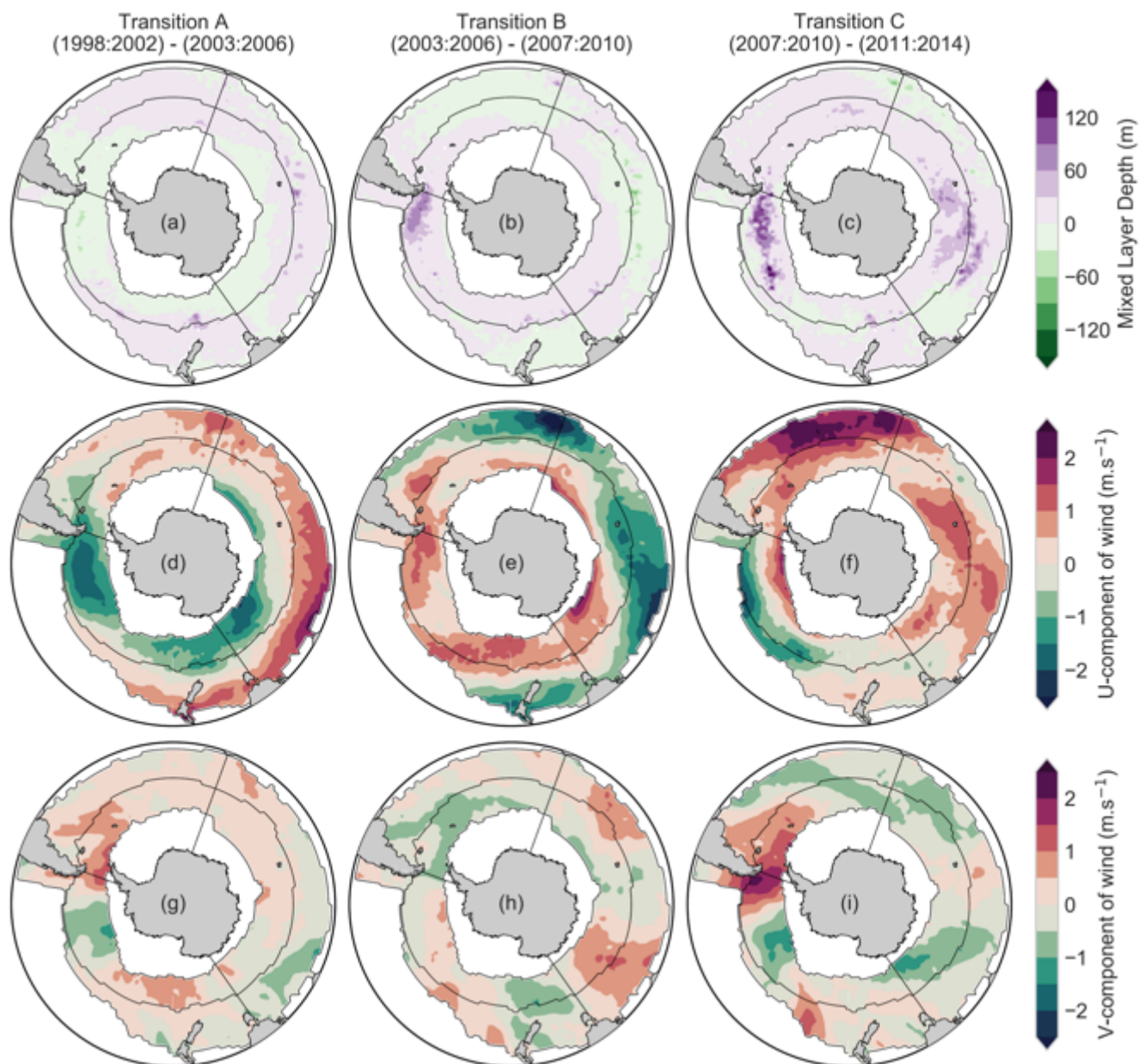


Figure S6: Relative anomalies of summer mixed layer depth (a-c), u- (d-f), and v-components (g-i) of wind for four periods (as shown above each column).. The thin black lines show the boundaries for each of the nine regions described by the biomes (Fay and McKinley, 2014a) and basin boundaries.

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