

1 **The Seasonal Cycle of pCO<sub>2</sub> and CO<sub>2</sub> fluxes in the Southern Ocean:**  
2 **Diagnosing Anomalies in CMIP5 Earth System Models**

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9

10 **Abstract**

11

12 The Southern Ocean forms an important component of the earth system as a major sink of CO<sub>2</sub> and  
13 heat. Recent studies based on the Coupled Model Intercomparison Project version 5 (CMIP5) Earth  
14 System Models (ESMs) show that CMIP5 models disagree on the phasing of the seasonal cycle of the  
15 CO<sub>2</sub> flux (FCO<sub>2</sub>) and compare poorly with available observation products for the Southern Ocean.  
16 Because the seasonal cycle is the dominant mode of CO<sub>2</sub> variability in the Southern Ocean, its  
17 simulation is a rigorous test for models and their long-term projections. Here we examine the  
18 competing roles of temperature and dissolved inorganic carbon (DIC) as drivers of the seasonal cycle  
19 of pCO<sub>2</sub> in the Southern Ocean to explain the mechanistic basis for the seasonal biases in CMIP5  
20 models. We find that despite significant differences in the spatial characteristics of the mean annual  
21 fluxes, the intra-model homogeneity in the seasonal cycle of FCO<sub>2</sub> is greater than observational  
22 products. FCO<sub>2</sub> biases in CMIP5 models can be grouped into two main categories i.e. group-SST and  
23 group-DIC. Group-SST models show an exaggeration of the seasonal rates of change of sea surface  
24 temperature (SST) in autumn and spring during the cooling and warming peaks. These higher-than-  
25 observed rates of change of SST tip the control of the seasonal cycle of pCO<sub>2</sub> and FCO<sub>2</sub> towards SST and  
26 result in a divergence between the observed and modelled seasonal cycles, particularly in the Sub-  
27 Antarctic Zone. While almost all analyzed models (9 out of 10) show these SST-driven biases, 3 out of  
28 10 (namely NorESM1-ME, HadGEM-ES and MPI-ESM, collectively the group-DIC models) compensate  
29 the solubility bias because of their overly exaggerated primary production, such that biologically-  
30 driven DIC changes mainly regulate the seasonal cycle of FCO<sub>2</sub>.

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## 35 **1. Introduction**

36

37 The Southern Ocean (south of 30°S) takes up about a third of the total oceanic CO<sub>2</sub> uptake, slowing  
38 down the accumulation of CO<sub>2</sub> in the atmosphere (Fung et al., 2005; Le Quere et al., 2016; Takahashi et  
39 al., 2012). The combination of upwelling deep ocean circumpolar waters (which are rich in carbon and  
40 nutrients) and the subduction of fresh colder mid-latitude waters makes it a key region in the role of  
41 sea-air gas exchange and heat uptake (Barbero et al., 2011; Gruber et al., 2009; Sallée et al., 2013). The  
42 Southern Ocean supplies about a third of the total nutrients responsible for biological production  
43 north of 30°S (Sarmiento et al., 2004), and accounts for about 75% of total ocean heat uptake  
44 (Frölicher et al., 2015). Recent studies suggest that the Southern Ocean CO<sub>2</sub> sink is expected to change  
45 as a result of anthropogenic warming, however, the sign and magnitude of the change is still disputed  
46 (Leung et al., 2015; Roy et al., 2011; Sarmiento et al., 1998; Segschneider and Bendtsen, 2013). While  
47 some studies suggest that the Southern Ocean CO<sub>2</sub> sink is weakening and will continue to do so (e.g. Le  
48 Quéré et al., 2007; Son et al., 2010; Thompson et al., 2011), other recent studies infer an increasing CO<sub>2</sub>  
49 sink (Landschutzer et al., 2015; Takahashi et al., 2012; Zickfeld et al., 2008).

50

51 Although the Southern Ocean plays a crucial role as a CO<sub>2</sub> reservoir and regulator of nutrients and  
52 heat, it remains under-sampled, especially during the winter season (JJA) (seasonal cycle in the  
53 Southern Hemisphere) (Bakker et al., 2014; Monteiro et al., 2010). Consequently, we largely rely on  
54 Earth System Models (ESM), inversions and ocean models for both process understanding and future  
55 simulation of CO<sub>2</sub> processes in the Southern Ocean. The Coupled Model Intercomparison Project  
56 (CMIP) provides an example of such a globally organized platform (Taylor et al., 2012). Although  
57 recent studies based on CMIP5 ESMs, forward and inversions models show that CMIP5 models agree  
58 on the CO<sub>2</sub> annual mean sink, they disagree with available observations on the phasing of the seasonal  
59 cycle of sea-air CO<sub>2</sub> flux (FCO<sub>2</sub>) in the Southern Ocean (e.g. Anav et al., 2013; Lenton et al., 2013).

60

61 The seasonal cycle is a major mode of variability for chlorophyll (Thomalla et al., 2011) and CO<sub>2</sub> in the  
62 Southern Ocean (Monteiro et al., 2010; Lenton et al., 2013). The large-scale seasonal states of sea-air  
63 CO<sub>2</sub> fluxes (FCO<sub>2</sub>) in the Southern Ocean comprise of extremes of strong summer in-gassing with a  
64 weaker in-gassing or even out-gassing in winter (Metzl et al., 2006). These extremes are linked by the  
65 autumn and spring transitions. In autumn CO<sub>2</sub> in-gassing weakens linked to the increasing  
66 entrainment of sub-surface waters, which are rich in dissolved inorganic carbon (DIC), (Lenton et al.,  
67 2013; Metzl et al., 2006; Sarmiento and Gruber, 2006). During spring, the increase of primary  
68 production consumes DIC at the surface and increases the ocean's capacity to take up atmospheric CO<sub>2</sub>  
69 (Gruber et al., 2009; Le Quéré and Saltzman, 2013; Pasquer et al., 2015; Gregor et al., 2017). The  
70 increase of sea surface temperature (SST) in summer reduces surface CO<sub>2</sub> solubility, which counteracts

71 the biological uptake and reduces the CO<sub>2</sub> flux from the atmosphere (Takahashi et al., 2002; Lenton et  
72 al., 2013).

73

74 FCO<sub>2</sub> is also spatially variable in the Southern Ocean at the seasonal scale. North of 50°S is generally  
75 the main CO<sub>2</sub> uptake zone (Hauck et al., 2015; Sabine et al., 2004). This region forms a major part of  
76 the sub-Antarctic Zone and is characterized by the confluence of upwelled, colder and nutrient-rich  
77 deep circumpolar water and mid-latitudes warm water (McNeil et al., 2007; Sallée et al., 2006). It is  
78 characterized by enhanced biological uptake during spring and solubility-driven CO<sub>2</sub> uptake due to  
79 cool surface waters (Marinov et al., 2006; Metzl, 2009; Takahashi et al., 2012). South of 60°S towards  
80 the marginal ice Zone, CO<sub>2</sub> fluxes are largely dominated by out-gassing, driven by the upwelling of  
81 circumpolar waters, which are rich in DIC (Matear and Lenton, 2008; McNeil et al., 2007).

82

83 The inability of CMIP5 ESM to simulate a comparable FCO<sub>2</sub> seasonal cycle with available observations  
84 estimates in the Southern Ocean has been the subject of recent literature (e.g. Anav et al., 2013;  
85 Kessler and Tjiputra, 2016) and the mechanisms associated with these biases are still not well  
86 understood. This model-observations disagreement highlights that the current ESMs might not  
87 adequately capture the dominant seasonal processes driving the FCO<sub>2</sub> in the Southern Ocean. It also  
88 questions the sensitivity of models to adequately simulate the Southern Ocean century-scale CO<sub>2</sub> sink  
89 and its sensitivity to climate change feedbacks (Lenton et al., 2013). Efforts to improve simulations of  
90 CO<sub>2</sub> properties with respect to observations in the Southern Ocean are ongoing using forced ocean  
91 models (e.g. Pasquer et al., 2015; Rodgers et al., 2014; Visinelli et al., 2016; Rosso et al., 2017).  
92 However, it remains a challenge for fully coupled simulations. In a previous study, we developed a  
93 diagnostic framework to evaluate the seasonal characteristics of the drivers of FCO<sub>2</sub> in ocean  
94 biogeochemical models (Mongwe et al., 2016). We here apply this approach to 10 CMIP5 models  
95 against observation product estimates in the Southern Ocean. The subsequent analysis is divided as  
96 follows; the methods section (section 2) explains our methodological approach, followed by results  
97 (section 3), which comprise four subsections. Section 3.1 explores the spatial variability of the annual  
98 mean representation of FCO<sub>2</sub> in the 10 CMIP5 models against observation product estimates; section  
99 3.2 quantifies the biases in the FCO<sub>2</sub> seasonal cycles in the 10 models. Section 3.3 investigates surface  
100 ocean drivers of FCO<sub>2</sub> changes (temperature driven solubility and primary production), and finally,  
101 section 3.4 examines the source terms in the DIC surface budget (primary production, entrainment  
102 rates and vertical gradients) and their role in surface pCO<sub>2</sub> changes. The discussion (section 4) is an  
103 examination of the mechanisms behind the pCO<sub>2</sub> and FCO<sub>2</sub> biases in the models. We conclude with a  
104 synthesis of the main findings and their implications.

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106

## 107 **2. Methods**

108

109 The Southern Ocean is here defined as the ocean south of the Sub-Tropical Front (STF, defined  
110 according to Orsi et al., (1995), 11.3°C isotherm at 100m). It is divided into two main domains, the Sub-  
111 Antarctic Zone; between the STF and the Polar Front (PF: 2°C isotherm at 200m) and the Antarctic  
112 Zone, south of the PF. Within the Sub-Antarctic Zone and Antarctic Zone, we further partition the  
113 domain into the three main basins of the Southern Ocean i.e. Pacific, Atlantic and the Indian zone.

114

### 115 **2.1 Observations datasets**

116

117 We used the Landschützer et al. (2014) data product ( $FCO_2$  and partial pressure of  $CO_2$  ( $pCO_2$ )) as the  
118 main suite of observations-based estimates against which to compare the models throughout the  
119 analysis. Landschützer et al. (2014) dataset is synthesized from Surface Ocean  $CO_2$  Atlas version 2  
120 (SOCAT2) observations and high resolution winds using a Self-Organizing Map (SOM) through a Feed  
121 Forward Neural Network (FNN) approach (Landschützer et al., 2013). While Landschützer et al.  
122 (2014) dataset is based on more *in situ* observations (SOCAT2, 15 million source measurements)  
123 (Bakker et al., 2014) in comparison to Takahashi et al., (2009) (3 million surface measurements), used  
124 in Mongwe et al., (2016). We are nevertheless mindful that due to paucity of observations in the  
125 Southern Ocean, this data product is still subject to significant uncertainties, as discussed in Ritter et  
126 al. (2018). To evaluate the uncertainty between data products we compare the Landschützer et al.  
127 (2014) data with Gregor et al. (2017) data product, which is based on two independent empirical  
128 models: Support Vector Regression (SVR) and Random Forest Regression (RFR) as well as against  
129 Takahashi et al. (2009) for  $pCO_2$  in the Southern Ocean. We compare  $pCO_2$  instead of  $FCO_2$  firstly,  
130 because Gregor et al., (2017) only provided fugacity and  $pCO_2$ , and being mindful that the choice of  
131 wind product and transfer velocity constant in computing  $FCO_2$  would increase the level of uncertainty  
132 (Swart et al., 2014). Secondly, while the focus of the paper is on the examination biases in the air-sea  
133 fluxes of  $CO_2$ , the major part of our analysis is based on  $pCO_2$ , which primarily determines the direction  
134 and part of the magnitude of the fluxes. We find that the three data products agree on the seasonal  
135 phasing of  $pCO_2$  in the Sub-Antarctic Zone, but they show differences in the magnitudes (Fig. S1). In the  
136 Antarctic Zone, all three datasets agree in both phasing and amplitude (Fig. S1). At this stage it is not  
137 clear whether this agreement is due to all the methods converging even with the sparse data or the  
138 reason for agreement is the lack of observations. Nevertheless, more independent *in situ* observations  
139 will be helpful to resolve this issue. In this regard float observations from the SOCCOM program  
140 (Johnson et al., 2017) and glider observations (Monteiro et al., 2015), for example, are likely to become

141 helpful in resolving these data uncertainties in addition to ongoing ship-based measurements.

142

143 We also used the Takahashi et al. (2009) in situ FCO<sub>2</sub> dataset as a complementary source for  
144 comparison of spatial FCO<sub>2</sub> properties in the Southern Ocean. Takahashi et al. (2009) data estimates  
145 are comprised of a compilation of about 3 million surface measurements globally, obtained from 1970  
146 – 2000 and corrected for reference year 2000. This dataset is used, as provided, on a 4° (latitude) x 5°  
147 (longitude) resolution. Using monthly mean sea surface temperature (SST) and salinity from the World  
148 Ocean Atlas 2013 (WOA13) dataset (Locarnini et al., 2013), we reconstructed total alkalinity (TAlk)  
149 using the Lee et al. (2006) formulation. We also use this dataset as the main observations platform in  
150 section 2.3. To calculate the uncertainty of the computed TAlk, we compared the calculated total  
151 alkalinity (TAlk<sub>calc</sub>) based on ship measurements of SST and surface salinity dataset with actual  
152 observed TAlk<sub>obs</sub> of the same measurements for a set of winter (August) data collected in the Southern  
153 Ocean. We found that TAlk<sub>calc</sub> compares well with TAlk<sub>obs</sub> (R<sup>2</sup> = 0.79) (Fig. S2, Supplementary). We  
154 then used this computed monthly TAlk and pCO<sub>2</sub> from Landschützer et al. (2014) to compute DIC  
155 using CO2SYS (Pierrot et al., 2006, [http://cdiac.ornl.gov/ftp/co2sys/CO2SYS\\_calc\\_XLS\\_v2.1](http://cdiac.ornl.gov/ftp/co2sys/CO2SYS_calc_XLS_v2.1)), using K1,  
156 K2 from Mehrbach et al. (1973) refitted by Dickson and Millero (1987). For interior ocean DIC, we  
157 used the Global Ocean Data Analysis Project version 2 (GLODAP2) annual means dataset (Lauvset et  
158 al., 2016). The Mixed Layer Depth (MLD) data was taken from de Boyer Montégut et al. (2004), on a 1°  
159 x 1° grid, the data is provided as monthly means climatology and was used as provided. We also use  
160 satellite chlorophyll dataset from Johnson et al. (2013).

161

## 162 **2.2 CMIP5 Model data**

163

164 We used 10 models from the Coupled Model Intercomparison Project version 5 (CMIP5) Earth System  
165 Models (ESM) shown in Table 1. The selection criterion for the models was based on the availability of  
166 essential variables for the analysis in the CMIP5 data portal (<http://pcmdi9.llnl.gov>) at the time of  
167 writing: i.e. monthly FCO<sub>2</sub>, pCO<sub>2</sub>, chlorophyll, net primary production (NPP), surface oxygen, surface  
168 Dissolved Inorganic Carbon (DIC), MLD, Sea Surface Temperature (SST), vertical temperature fields  
169 and annual DIC for the historical scenario. The analysis is primarily based on the climatology over  
170 1995 – 2005, which was selected to match a period closest to the available observational data product  
171 (Landschützer et al. (2014), 1998 – 2011). However, we do examine the consistency of the seasonality  
172 of FCO<sub>2</sub> over periods longer than 10 years by comparing the seasonal cycle of FCO<sub>2</sub> and temporal  
173 standard deviation of 30 years (1975 – 2005) vs 10 years (1995 – 2005) for HadGEM2-ES and  
174 CanESM2. We find that the seasonal cycle of FCO<sub>2</sub> remains consistent (R = 0.99) in both HadGEM2-ES

175 and CanESM2 over 30 years (Fig. S3). All CMIP5 model outputs were regridded into a common 1°x1°  
 176 regular grid throughout the analysis, except for annual CO<sub>2</sub> mean fluxes, which were computed on the  
 177 original grid for each model.

178

179 **Table 1:** A description of the 10 CMIP5 ESMs that were used in this analysis. It shows the ocean  
 180 resolution, atmospheric resolution, and available nutrients for the biogeochemical component, sea-ice  
 181 model, vertical levels and the marine biogeochemical component for each ESM.

182

| Full name and Source  | Model Name   | Ocean Resolution       | Atmospheric Resolution | Nutrients                         | Sea ice model | Vertical Coordinate & Levels | Ocean Biology | Reference             |
|---|--------------|------------------------|------------------------|-----------------------------------|---------------|------------------------------|---------------|-----------------------|
| Canadian Centre for Climate Modelling and Analysis, Canada  | CanESM2      | CanOM4<br>0.9°x1.4°    | 2.8125° x<br>2.8125°   | N<br>(accounts for Fe limitation) | CanSIM1       | z<br>40 levels               | NPZD          | Zahariev et al., 2008 |
| Centro Euro-Mediterraneo Sui Cambiamenti Climatici, Italy   | CMCC-CESM    | OPA8.2<br>0.5-2°x2°    | 3.8° x 3.7°            | P, N, Fe, Si                      | CICE4         | z<br>21 levels               | PELAGOS       | Vichi et al., 2007    |
| Centre National de Recherches Météorologiques-Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique, France | CNRM-CM5     | NEMOv3.3<br>1°         | 1.4°                   | P, N, Fe, Si                      | GELATO5       | z<br>42 levels               | PISCES        | Séférián et al., 2013 |
| Institut Pierre-Simon Laplace, France   | IPSL-CM5A-MR | NEMO2.3<br>0.5-2° x 2° | 2.58° x 1.25°          | P, N, Fe, Si                      | LIM2          | z<br>31 levels               | PISCES        | Séférián et al., 2013 |
| Max Plank Institute for Meteorology, Germany  | MPI-ESM-MR   | MPIOM<br>1.41°x0.89°   | 1.875° x<br>1.875°     | P, N, Fe, Si                      | MPIOM         | z<br>40 levels               | HAMOC5.2      | Ilyina et al., 2013   |

|  |            |                      |              |                             |          |                  |             |                             |
|--|------------|----------------------|--------------|-----------------------------|----------|------------------|-------------|-----------------------------|
| <b>Community Earth System Model, USA</b>                                     | CESM1-BGC  | 0.3° x 1°            | 0.9° x 1.25° | (P), N, Fe, Si              |          | z<br>60 levels   | BEC         | Moore et al., 2004          |
| <b>Norwegian Earth System Model, Norway</b>                                  | NorESM1-ME | MICOM<br>0.5° x 0.9° | 2.5° x 1.9°  | P, N, Fe, Si                | CICE4.1  | ρ<br>53 levels   | HAMOCC      | Tjiputra et al., 2013       |
| <b>Geophysical Fluid Dynamics Laboratory Earth System Model, USA</b>         | GFDL-ESM2M | 0.3° x 1°            | 2.5° x 2.0°  | N, P, SiO <sub>4</sub> , Fe | SISp2    | z<br>50 levels   | TOPAZ2      | Dunne et al., 2013          |
| <b>Meteorological Research Institute-Earth System Model Version 1, Japan</b> | MRI-ESM    | 0.5° x 1°            |              | P,N                         | MRI.COM3 | σ-z<br>51 levels | NPZD        | Adachi et al., 2013         |
| <b>Hadley Global Environment Model 2 - Earth System, UK</b>                  | HadGEM-ES  | 0.3° x 1°            | 2.5° x 2.0°  | N,Fe,S                      |          | 40 levels        | Diat-HadOCC | Palmer and Totterdell, 2001 |

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### 185 **2.3 Sea-Air CO<sub>2</sub> Flux Drivers: The Seasonal Cycle Diagnostic Framework**

186

187 The seasonal cycle of the ocean-atmosphere pCO<sub>2</sub> gradient ( $\Delta p\text{CO}_2$ ) is the main driver of the variability  
188 of FCO<sub>2</sub> over comparable periods (Sarmiento and Gruber, 2006; Wanninkhof et al., 2009; Mongwe et  
189 al., 2016). Wind speed plays a dual role as a driver of FCO<sub>2</sub>: it drives the seasonal evolution of  
190 buoyancy-mixing dynamics, which influences the biogeochemistry and upper water column physics  
191 (but these processes are incorporated into the variability of the DIC), as well as the rate of gas  
192 exchange across the air-sea interface (Wanninkhof et al., 2013). However, because winds in the  
193 Southern Ocean do not have large seasonal variation (Young, 1999), for this analysis, we neglect the  
194 role of wind as a secondary driver of the seasonal cycle of FCO<sub>2</sub>. Consequently, the seasonal cycle of  
195 FCO<sub>2</sub> is directly linked to surface pCO<sub>2</sub> variability, influenced by changes in temperature, salinity, TALK  
196 and DIC and macronutrients (Sarmiento and Gruber, 2006; Wanninkhof et al., 2009). In this analysis  
197 we use this assumption as a basis to explore how the seasonal variability of temperature and DIC  
198 regulate the seasonal cycle of pCO<sub>2</sub> in CMIP5 models relative to observational product estimates.

199

200 The seasonal cycle diagnostic framework was developed as a way of scaling the relative contributions

201 from the rates of change of SST- and the total DIC-driven changes to the seasonal cycle of pCO<sub>2</sub> on to a  
 202 common DIC scale (Mongwe et al., 2016). We use the framework to explore how understanding  
 203 differences emerging from the temperature- and DIC-driven CO<sub>2</sub> variability could be helpful as a  
 204 diagnostic of the apparent observations –model seasonal cycle biases in the Southern Ocean.

205

206 The total rate of change of DIC in the surface layer consists of the contribution of air-sea exchanges,  
 207 biological, vertical and horizontal transport-driven changes (Eq. 1).

208

$$209 \left( \frac{\partial DIC}{\partial t} \right)_{Tot} = \left( \frac{\partial DIC}{\partial t} \right)_{air-sea} + \left( \frac{\partial DIC}{\partial t} \right)_{Bio} + \left( \frac{\partial DIC}{\partial t} \right)_{Vert} + \left( \frac{\partial DIC}{\partial t} \right)_{Hor} \quad (1)$$

210 Because we used zonal means from medium resolution models, we assume that the horizontal terms  
 211 are negligible, though mindful that there could be a seasonal cycle in the divergence of the horizontal  
 212 transport due to a latitudinal gradient in DIC perturbed by Ekman flow in some regions of the Sub-  
 213 Antarctic Zone (Rosso et al., 2017). This leaves air-sea exchange, vertical fluxes (advection and  
 214 diffusion) and biological processes as the dominant drivers of DIC.

215 Since temperature does not affect DIC changes directly, but only pCO<sub>2</sub> through solubility, it was  
 216 necessary to scale the influence of temperature into equivalent DIC units in order to compare the  
 217 influence of temperature vs DIC control of surface pCO<sub>2</sub> variability. Thus in order to constrain the  
 218 contribution of temperature on the seasonal variability of pCO<sub>2</sub> and FCO<sub>2</sub> we derived a new synthetic  
 219 temperature-linked term “DIC equivalent” (DIC<sub>T</sub>) defined as: *the magnitude of DIC change that would*  
 220 *correspond to a change in pCO<sub>2</sub> driven by a particular temperature change.* In this way the ΔpCO<sub>2</sub>  
 221 driven solely by modelled or observed temperature change, is converted into equivalent DIC units,  
 222 which allows its contribution to be scaled against the observed or modelled total surface DIC change  
 223 (Eq.1). Shifts between temperature and DIC control of pCO<sub>2</sub> are in effect tipping points because they  
 224 reflect major shifts in the mechanisms that drive pCO<sub>2</sub> variability. We use this as the basis to  
 225 investigate the possible mechanisms behind model biases in the seasonal cycle of pCO<sub>2</sub>.

226 This calculation of DIC<sub>T</sub> is done in two steps: firstly, the temperature impact on pCO<sub>2</sub> is calculated  
 227 using the Takahashi et al. (1993) empirical expression that linearizes the temperature dependence of  
 228 the equilibrium constants.

$$229 \left( \frac{\partial pCO_2}{\partial t} \right)_{SST} = 0.0423 \times pCO_2 \times \left( \frac{\partial pCO_2}{\partial SST} \right) \quad (2)$$

230 Though this relationship between dSST and dpCO<sub>2</sub> is based on a linear assumption (Takahashi et al.,  
 231 1993), this formulation has been shown to hold and has been widely used in literature (e.g. Bakker et  
 232 al., 2014; Feely et al., 2004; Marinov and Gnanadesikan, 2011; Takahashi et al., 2002; Wanninkhof et



233 al., 2009; Landschützer et al., 2018). We show in the supplementary material that the extension of this  
 234 expression into polar temperature ranges ( $SST < 2^{\circ}C$ ) only introduces a minor additional uncertainty  
 235 of 4 -5% (SM Fig. S4).

236 Secondly, the temperature-driven change in  $pCO_2$  is converted to an equivalent  $DIC_T$  using the Revelle  
 237 factor.

$$238 \left( \frac{\partial DIC_T}{\partial t} \right)_{SST} = \frac{DIC}{\gamma_{DIC} \times pCO_2} \left( \frac{\partial pCO_2}{\partial t} \right)_{SST} \quad (3)$$

239 Here we also used a fixed value for the Revelle Factor ( $\gamma_{DIC}=14$ ), typical of polar waters in the Southern  
 240 Ocean in order to assess the error linked to this assumption. We recomputed the Revelle factor in the  
 241 Sub-Antarctic and Antarctic Zones using annual mean climatologies of TAlk, salinity, sea surface  
 242 temperature and nutrients. Firstly, we examined DIC changes for the nominal range of  $pCO_2$  change  
 243 ( $340 - 399 \mu atm:1 \mu atm$  intervals) and then used this dataset to derive the Revelle factor. The range of  
 244 calculated Revelle factors in the Southern Ocean was between  $\gamma_{DIC} \sim 12 - 15.5$  with an average of  $\gamma_{DIC} =$   
 245  $13.9 \pm 1.3$ . This justifies our use of  $\gamma_{DIC} = 14$  for the conversion of the solubility-driven  $pCO_2$  change to  
 246 an equivalent DIC ( $DIC_T$ ) throughout the analysis. We have provided the uncertainty that this  
 247 conversion makes into the temperature constraint  $DIC_T$ , by using the upper and lower limits of the  
 248 Revelle factor ( $\gamma_{DIC} = 12 - 15.5$ ) in the model framework. In the Supplementary Material (Fig. S5) we  
 249 show examples for observations in the Sub-Antarctic and Antarctic Zones, which indicate that the  
 250 extremes of the Revelle factor values ( $\gamma_{DIC} = 12 - 15.5$ ) do not alter the phasing or magnitude of the  
 251 relative controls of temperature or DIC on the seasonal cycle of  $pCO_2$ .

252 The rate of change of DIC was discretized on a monthly mean as follows:

$$254 \left( \frac{\partial DIC_T}{\partial t} \right)_{SST} \approx \left( \frac{\Delta DIC}{\Delta t} \right)_{n,l} = \frac{DIC_{n+1,l} - DIC_{n,l}}{1 \text{ month}} \quad (4)$$

255

256 Where  $n$  is time in month,  $l$  is vertical level (in this case the surface,  $l=1$ ). We here take the forward  
 257 derivative such that November rate is the difference between 15 November and 15 December, thus  
 258 being centered at the interval between the months.

259 Finally, to characterize periods of temperature or DIC dominance as main drivers of the instantaneous  
 260 (monthly)  $pCO_2$  change we subtract Eq. 1 from Eq. 4, which yields a residual indicator  $M_{T-DIC}$  Eq. 5.  $M_T$ .

261 DIC is then used as indicator of the dominant driver of instantaneous pCO<sub>2</sub> changes in this scale monthly  
 262 time scale.

263

$$264 \quad M_{T-DIC} = \left| \left( \frac{\partial DIC_T}{\partial t} \right)_{SST} \right| - \left| \left( \frac{\partial DIC}{\partial t} \right)_{Tot} \right| \quad (5)$$

265

266 M<sub>T-DIC</sub> > 0 indicates that the pCO<sub>2</sub> variability is dominated by the temperature-driven solubility and  
 267 when M<sub>T-DIC</sub> < 0, it indicates that pCO<sub>2</sub> changes are mainly modulated by DIC processes (i.e. Biological  
 268 CO<sub>2</sub> changes and vertical scale physical DIC mechanisms). We also examine the following DIC  
 269 processes; i.) Biological DIC changes using chlorophyll, NPP, export carbon, surface oxygen, and ii.).  
 270 Physical DIC mechanisms using estimated entrainment rates at the base of the mixed layer. Details of  
 271 this calculation are in section 2.4.

272 In the Southern Ocean, salinity and TAlk are considered lower-order drivers of the seasonal cycle of  
 273 pCO<sub>2</sub> (Takahashi et al., 1993). In the supplementary material (Fig. S6), we show that salinity and TAlk  
 274 do not play a major role as drivers of the local seasonal cycle of pCO<sub>2</sub>. We do so by computing the  
 275 equivalent rate of change of DIC resulting from seasonal variability of salinity and TAlk as done for  
 276 temperature (Eq. 2), i.e. still assuming empirical linear relationships from Takahashi et al. (1993):

$$277 \quad \left( \frac{\ln(pCO_2)}{\ln(TAlk)} \approx -9.4 \right) \text{ and } \left( \frac{\ln(pCO_2)}{\ln(Sal)} = 0.94 \right). \text{ By applying these relationships to the model data, we}$$

278 confirmed that indeed salinity and TAlk are secondary drivers of pCO<sub>2</sub> changes i.e.  $\left[ \left( \frac{\partial DIC}{\partial t} \right)_{Tot} \right]_{average} \approx$

$$279 \quad 5 \mu\text{mol kg}^{-1} \text{ month}^{-1}, \text{ while } \left[ \left( \frac{\partial DIC}{\partial t} \right)_{Tot} \right]_{average} \approx 0.6 \mu\text{mol kg}^{-1} \text{ month}^{-1} \text{ and } \left[ \left( \frac{\partial DIC}{\partial t} \right)_{TAlk} \right]_{maximum} \approx 0.4$$

280  $\mu\text{mol kg}^{-1} \text{ month}^{-1}$ .

281

## 282 **2.4 Entrainment mixing**

283

284 CO<sub>2</sub> uptake by the Southern Ocean has been shown to weaken during winter linked to the entrainment  
 285 of sub-surface DIC as the MLD deepens (e.g. Lenton et al., 2013; Metzl et al., 2006; Takahashi et al.,  
 286 2009). Here we estimate this rate of entrainment (RE) using Eq. 6, which estimates the advection of  
 287 preformed DIC at the base of the mixed layer:

288

$$289 \quad RE = U_e \left( \frac{\partial DIC}{\partial z} \right)_{MLD} \quad (6)$$

$$290 \quad RE_n = \left( \frac{\Delta MLD_n}{\Delta t} \right) \left( \frac{\Delta DIC}{\Delta z} \right)_{n,MLD} \quad (7)$$

$$291 \quad \left( \frac{\Delta DIC}{\Delta z} \right)_{n,MLD} = \frac{DIC_{n,MLD_{n+1}} - DIC_{n,MLD_n}}{\Delta z} \quad (8)$$

292

293 In which  $U_e$  is an equivalent entrainment velocity based on the rate of change of the MLD and  $n$  is the  
294 time in months. This approximation of vertical entrainment is necessary as it is not possible to  
295 compute this term from the CMIP5 data because the vertical DIC distribution is only available as an  
296 annual means. We use the entrainment rates to estimate the influence of subsurface/bottom DIC  
297 changes on surface DIC changes and subsequently  $p\text{CO}_2$  and  $\text{FCO}_2$ . Because we are mainly interested in  
298 the period autumn- winter, where the MLD  $\geq 60$  m in the Sub-Antarctic Zone and  $\geq 40$  m in the  
299 Antarctic Zone at this depth seasonal variations in DIC are anticipated to be minimal – these estimates  
300 can be used. The monthly and annual mean DIC from a NEMO PISCES  $0.5 \times 0.5^\circ$  model output were  
301 used to estimate the uncertainty by comparing RE computed from both (Dufour et al., 2013). We found  
302 the annual and monthly estimates to be indeed comparable with minimal differences (not shown). It is  
303 noted as a caveat that this rate of entrainment is only a coarse estimate because we were using annual  
304 means, and is intended only for the autumn-winter period when MLDs are deepened.

305

### 306 **3. Results**

307

#### 308 **3.1 Annual climatological sea-air $\text{CO}_2$ fluxes**

309

310 The annual mean climatological distribution of  $\text{FCO}_2$  in the Southern Ocean obtained from  
311 observational products is spatially variable, but mainly characterized by two key features: (i)  $\text{CO}_2$  in-  
312 gassing north of  $50^\circ\text{S}$ - $55^\circ\text{S}$  (Polar Frontal Zone, PFZ) within and north of the Sub-Antarctic Zone, and  
313 (ii),  $\text{CO}_2$  out-gassing between the PF ( $\sim 58^\circ\text{S}$ ) and the Marginal Ice Zone (MIZ,  $\sim 60^\circ - 68^\circ\text{S}$ ) (Fig. 1a-b).  
314 Most CMIP5 models broadly capture these features, however, they also show significant differences in  
315 space and magnitude between the basins of the Southern Ocean (Fig. 1). With the exception of CMCC-  
316 CESM, which shows a northerly-extended  $\text{CO}_2$  out-gassing band between about  $40^\circ\text{S}$  and  $50^\circ\text{S}$ , CMIP5  
317 models generally show the  $\text{CO}_2$  out-gassing zone between  $50^\circ\text{S}$ -  $70^\circ\text{S}$  in agreement with observational  
318 estimates (Fig. 1).

319

320 The analyzed 10 CMIP5 models show a large spatial dispersion in the spatial representation of the  
321 magnitudes of  $\text{FCO}_2$  with respect to observations (Fig. 1, Table 2). They generally overestimate the  
322 upwelling-driven  $\text{CO}_2$  out-gassing ( $55^\circ\text{S}$  - $70^\circ\text{S}$ ) in some basins relative to observations. IPSL-CM5A,  
323 CanESM2, MPI-ESM, GFDL-ESM2M and MRI-ESM, for example, show  $\text{CO}_2$  out-gassing fluxes reaching  
324 up to  $25 \text{ g m}^{-2} \text{ yr}^{-1}$ , while observations only show a maximum of  $8 \text{ g m}^{-2} \text{ yr}^{-1}$  (Fig. 1). Between  $40^\circ\text{S}$ -  
325  $56^\circ\text{S}$  (Sub-Antarctic Zone), observations and CMIP5 models largely agree, showing a  $\text{CO}_2$  in-gassing  
326 feature, which is mainly attributable to biological processes (McNeil et al., 2007; Takahashi et al.,  
327 2012). South of  $65^\circ\text{S}$ , in the MIZ, models generally show an excessive  $\text{CO}_2$  in-gassing with respect to

328 observations (with the exception of CanESM2, IPSL-CM5A-MR and CNRM-CM5). Note that as much as  
329 this bias south of the MIZ might be a true divergence of CMIP5 models from the observed ocean, it is  
330 also possibly due to the lack of observations in this region, especially during the winter season (Bakker  
331 et al., 2014; Monteiro, 2010).

332  
333 Table 2 shows the Pattern Correlation Coefficient (PCC) and the Root Mean Square Error (RMSE),  
334 which are here used to quantify the model spatial and magnitude performances against Landschützer  
335 et al. (2014) data product. Out of the 10 models, six show a moderate spatial correlation with  
336 Landschützer et al. (2014) (PCC = 0.40 – 0.60), i.e. CNRM-CM5, GFDL-ESM2M, HadGEM2-ES, IPSL-  
337 CM5A-MR, CESM1-BGC, NorESME-ME and CanESM2. While MPI-ESM-MR (PCC = 0.37), MRI-ESM (PCC  
338 = 0.36) and CMCC-CESM (PCC = -0.09) show a weak to null spatial correlation with observations, the  
339 latter is mainly due to the overestimated out-gassing region. Spatially, GFDL-ESM2M and NorESM1-ME  
340 are the most comparable to Landschützer et al. (2014), (RMSE < 9), while CCMC-CESM, CanESM2, MRI-  
341 ESM and CNRM-CM5 shows the most differences (RMSE > 15). The rest of the models show a modest  
342 comparison (RMSE 9 – 11).

343  
344 NorESM1-ME and CESM1-BGC are the only two of the 10 models showing a consistent spatial (RMSE  
345 < 9) and magnitude (PCC  $\approx$  0.50) performance. From Table 2, it is evident that an appropriate  
346 representation of the spatial properties of FCO<sub>2</sub> with respect to observations does not always  
347 correspond to comparable magnitudes. CanESM2 for example, shows a good spatial comparison (PCC  
348 = 0.54), yet a poor estimation of the magnitudes (RMSE = 19.5). In this case this is caused by an  
349 overestimation of CO<sub>2</sub> uptake north of 55°S ( $\approx$  - 28 g m<sup>-2</sup> yr<sup>-1</sup>) and CO<sub>2</sub> out-gassing (> 25 g m<sup>-2</sup> yr<sup>-1</sup>) in  
350 the Antarctic zone, resulting in a net total Southern Ocean annual weak sink (-0.05 Pg C m<sup>-2</sup> yr<sup>-1</sup>).

351

### 352 **3.2 Sea-Air CO<sub>2</sub> Flux Seasonal Cycle Variability and Biases**

353

354 The seasonal cycle of FCO<sub>2</sub> is shown in Fig. 2. The seasonality of FCO<sub>2</sub> in the 10 CMIP5 models shows a  
355 large dispersion in both phasing and amplitude, but mostly disagrees with observations in the phase of  
356 the seasonal cycle as well as disagreeing with each other. More quantitatively, CMIP5 models show  
357 weak to negative correlations with the Landschützer et al. (2014) data product in the Sub-Antarctic  
358 Zone and have slightly higher correlations in the Antarctic Zone (see supplementary Fig. S7). This  
359 discrepancy is consistent with the findings of Anav et al. (2013), who however used fixed latitude  
360 criteria. Based on the phasing, the seasonality of FCO<sub>2</sub> in CMIP5 models can be a priori divided in two  
361 main groups: group-DIC models, comprising of MPI-ESM, HadGEM-ES and NorESM1-ME, and group-  
362 SST models, the remainder i.e. GFDL-ESM2M, CMCC-CESM, CNRM-CERFACS, IPSL-CM5A-MR, CESM1-  
363 BGC, MRI-ESM and CanESM2. The naming convention is suggestive of the mechanism driving the

364 seasonal cycle, as will be clarified further on. A similar grouping was also identified by Kessler and  
365 Tjiputra (2016) using a different criterion. Fig. 3 shows the seasonal cycle of  $FCO_2$  of an equally-  
366 weighted ensemble of the two groups compared to observations; the shaded area shows the decadal  
367 standard deviation for the models and the Landschützer et al. (2014) data product for 1998-2014  
368 standard deviation in the various regions.

369  
370 In the Sub-Antarctic Zone, the observational products show a weakening of  $CO_2$  uptake during winter  
371 (less negative values in June-August) with values close to the zero at the onset of spring (September)  
372 in all three basins. Similarly, during the spring season, all three basins are seen to maintain a steady  
373 increase of  $CO_2$  uptake until mid-summer (December), while they differ during autumn (March-May).  
374 The Pacific basin shows an increase in  $CO_2$  uptake during autumn that is not observed in the other  
375 basins (only marginally in the Indian zone). In the Antarctic zone, the observed  $FCO_2$  seasonal cycle is  
376 mostly similar in all three basins (Fig. 3d-f). While this seasonal cycle consistency may suggest a  
377 spatial uniformity of the mechanisms of  $FCO_2$  at the Antarctic, we are also mindful that this may be due  
378 to a result of the paucity of observations in this area. In the Antarctic Zone, all three basins show a  
379 weakening of uptake or increasing of out-gassing from the onset of autumn (March) until mid-winter  
380 (June-July). The winter  $CO_2$  out-gassing is followed by a strengthening of the  $CO_2$  uptake throughout  
381 spring to summer, when it reaches a  $CO_2$  in-gassing peak.

382  
383 The differences in the seasonal cycle of  $FCO_2$  across the three basins of the Sub-Antarctic Zone found in  
384 the observational product (Fig. 2) are likely a consequence of spatial differences seen in Fig. 1. To  
385 verify this, we calculated the correlation between the seasonal cycles from the Landschützer et al.  
386 (2014) observational product in the three basins (Fig. 4). The  $FCO_2$  seasonal cycle in the Sub-Antarctic  
387 Atlantic and Indian basins are similar ( $R = 0.8$ ), while the other basins are quite different to one  
388 another ( $R = -0.1$  for Pacific – Atlantic and  $R \sim 0.4$  for Pacific – Indian). Contrary to the observational  
389 product, CMIP5 models show the same seasonal cycle phasing across all three basins in the Sub-  
390 Antarctic Zone (basin – basin correlation coefficients are always larger than 0.50 in Fig. 4 despite the  
391 spatial differences in Fig. 2, with the exception of three models (i.e. CMCC-CESM, CESM-BGC1 and  
392 GFDL-ESM2M)). Thus, contrary to Landschützer et al. (2014), CMIP5 models shows a zonal  
393 homogeneity in the seasonal cycle of  $FCO_2$ , which may suggest that the drivers of  $CO_2$  are less regional.  
394 In the Antarctic Zone, CMIP5 models agree with observations in the spatial uniformity of the seasonal  
395 cycle of  $FCO_2$  across the three basins.

396  
397 Group-DIC models are characterized by an exaggerated  $CO_2$  uptake during spring-summer (Fig. 3) with  
398 respect to observation estimates and  $CO_2$  out-gassing during winter. These models generally agree  
399 with observations in the phasing of  $CO_2$  uptake during spring, but overestimate the magnitudes. It is

400 worth noting that the seasonal characteristics of group-DIC models are mostly in agreement with the  
401 observations in the Atlantic and Indian basin in Sub-Antarctic Zone ( $R > 0.5$  in Fig. 4). The large  
402 standard deviation ( $\sim 0.01 \text{ g C m}^{-2} \text{ day}^{-1}$ ) during the winter and spring-summer seasons in the Atlantic  
403 basin shows that though group-DIC models agree in the phase, magnitudes vary considerably (Fig. 3b).  
404 For example MPI-ESM reaches up to  $0.06 \text{ g C m}^{-2} \text{ day}^{-1}$  out-gassing during winter, while HadESM2-ES  
405 and NorESM2 peak only at  $\sim 0.03 \text{ g C m}^{-2} \text{ day}^{-1}$ . Group-SST models on the other hand are characterized  
406 by a  $\text{CO}_2$  out-gassing peak in summer (Dec-Feb) and a  $\text{CO}_2$  in-gassing peak at the end of autumn (May),  
407 and their phase is opposite to the observational estimates in the Atlantic and Indian basins (Fig. 3b,c).  
408 Group-SST models only show a strengthening of  $\text{CO}_2$  uptake during spring in the Indian basin.  
409 Interestingly, group-SST models compare relatively well with the observed  $\text{FCO}_2$  seasonal cycle in the  
410 Pacific basin, whereas group-DIC models disagree the most with the observed estimates (Fig. 3a). This  
411 phasing difference within models and against observed estimates probably suggests that the  
412 disagreement of CMIP5 models  $\text{FCO}_2$  with observations is not a matter of a relative error/constant  
413 magnitude offset, but most likely points to differences in the seasonal drivers of  $\text{FCO}_2$ .

414

415 In the Antarctic Zone (Fig. 3d-f), both group-DIC and group-SST models perform better than in the  
416 Sub-Antarctic, in respect of phasing and amplitude in as shown by the correlation analysis in Fig. S7.  
417 Models reflect comparable  $\text{pCO}_2$  seasonality in the different basins of the AZ to the observational  
418 products (Fig. 4, with the exception of MRI-ESM and CanESM2 where  $R < 0$  for all three basins). Here  
419  $\text{FCO}_2$  magnitudes oscillate around zero with the largest disagreements occurring during mid-summer,  
420 where observation estimates show a weak  $\text{CO}_2$  sink ( $\approx -0.03 \text{ gC m}^{-2} \text{ day}^{-1}$ ), and group-SST show a zero  
421 net  $\text{CO}_2$  flux and a strong uptake in group DIC (e.g.  $\approx -0.12 \text{ gC m}^{-2} \text{ day}^{-1}$  in the Pacific basin). The large  
422 standard deviation ( $\approx 0.01 \text{ gC m}^{-2} \text{ day}^{-1}$ ) here indicates considerable differences among models (Fig.  
423 3d-f).

424

### 425 3.3 Seasonal Scale Drivers of Sea-Air $\text{CO}_2$ Flux

426

427 We now examine how changes in temperature and DIC regulate  $\text{FCO}_2$  variability at the seasonal scale  
428 following the method described in Sec. 2.3. Fig. 5 shows the monthly rates of change of SST ( $\text{dSST}/\text{dt}$ )  
429 for the 10 models compared with WOA13 SST. CMIP5 generally shows agreement in the timing of the  
430 switch from surface cooling ( $\text{dSST}/\text{dt} < 0$ ) to warming ( $\text{dSST}/\text{dt} > 0$ ) and vice versa; i.e. March  
431 (summer to autumn), and September (winter to spring) respectively. In both the Sub-Antarctic and  
432 Antarctic Zone CMIP5 models agree with observations in this timing (Fig. 5). However, while they  
433 agree in phasing, the amplitude of these warming and cooling rates are overestimated with respect to  
434 the WOA13 dataset with the exception of NorESM1-ME. Subsequently these differences in the  
435 magnitude of  $\text{dSST}/\text{dt}$  have important implications for the solubility of  $\text{CO}_2$  in seawater; larger

436 magnitudes of  $|dSST/dt|$  are likely to enhance the response of the  $pCO_2$  to temperature through  $CO_2$   
437 solubility changes. For example, because the observations in the Indian basin show a warming rate of  
438 about  $0.5^\circ C \text{ month}^{-1}$  lower compared to the other two basins, we expect a relatively weaker role of  
439 surface temperature in this basin.

440  
441 As described in sec. 2.3, the computed  $dSSt/dt$  magnitudes were used to estimate the equivalent rate  
442 of change of DIC driven by  $CO_2$  solubility using Eq. 2. The seasonal cycle of  $|(dDIC_T/dt)_{SST}|$  vs  
443  $|(dDIC/dt)_{Tot}|$ , for the 10 models and observations is presented in the supplementary material (Fig.  
444 S8) where we show the seasonal mean of  $M_{T-DIC}$  from (Eq. 3). As articulated in sec. 2.3,  $M_{T-DIC}$  (Fig. 6) is  
445 the difference between the total surface DIC rate of change of DIC (Eq. 1) and the estimated equivalent  
446 temperature-driven solubility DIC changes Eq. 3, such that when  $|(dDIC_T/dt)_{SST}| > |(dDIC/dt)_{Tot}|$ ,  
447 temperature is the dominant driver of the instantaneous  $pCO_2$  changes, and conversely when  $|$   
448  $(dDIC_T/dt)_{SST}| < |(dDIC/dt)_{Tot}|$ , DIC processes are the dominant mode in the instantaneous  $pCO_2$   
449 variability. The models showing the former feature are SST-driven and belong to group-SST, while the  
450 models showing the latter are DIC-driven and belong to group-SST.

451  
452 According to the  $M_{T-DIC}$  magnitudes in Fig. 6, the seasonal cycle of  $pCO_2$  in the observational estimates  
453 is predominantly DIC-driven most of the year in both the Sub-Antarctic and Antarctic Zone. Note that,  
454 however, during periods of high  $|dSST/dt|$ , i.e. autumn and spring, observations show a moderate to  
455 weak DIC control ( $M_{T-DIC} \approx 0$ ). The Antarctic Zone is mostly characterized by a stronger DIC control  
456 (mean Annual  $M_{T-DIC} > 3$ ) except for during the spring season (Fig. 6). Consistent with the similarity  
457 analysis presented in Fig. 4, the Antarctic Zone shows coherence in the sign of the temperature –DIC  
458 indicator ( $M_{T-DIC} > 0$ ) within the three basins.

459

460

### 461 **3.4 Source terms in the DIC surface budget**

462

463 To further constrain the surface DIC budget in Eq. 1, we examine the role of the biological source term  
464 using chlorophyll and Net Primary Production (NPP) as proxies. Fig. 8 shows the seasonal cycle of  
465 chlorophyll, NPP and the rate of surface DIC changes ( $dDIC/dt$ ). The observed seasonal cycle of  
466 chlorophyll (Johnson et al., 2013) shows a similar seasonal cycle within the three basins during the  
467 spring-summer seasons (autumn-winter data are removed due to the satellite limitation) in both the  
468 Sub-Antarctic and Antarctic Zone. Magnitudes are however different in the Sub-Antarctic Zone; the  
469 Atlantic basin shows larger chlorophyll magnitudes (Chlorophyll reach up to  $1.0 \text{ mg m}^{-3}$ ) compared to  
470 the Pacific and Indian basins ( $Chl < 1 \text{ mg m}^{-3}$ ).

471

472 CMIP5 models here show a clear partition between group-DIC and group-SST models. While they  
473 mostly maintain the same phase, group-DIC shows larger amplitudes of chlorophyll relative to group-  
474 SST and observed estimates in the Sub-Antarctic Zone. This difference is even clearer in NPP  
475 magnitudes, where group-DIC models show a maximum of  $NPP > 1 \text{ mmol m}^{-2} \text{ s}^{-1}$  in summer, while  
476 group-SST magnitudes shows about half of it. Except for CESM1-BGC and CMCC-CESM (and NorESM1-  
477 ME for NPP), each CMIP5 model generally maintains a similar chlorophyll seasonal cycle (phase and  
478 magnitude) in all three basins of the Southern Ocean. This is contrary to the observations, which show  
479 differences in the magnitude. Consistent with the observational product, CESM1-BGC simulates larger  
480 amplitude in the Atlantic basin. While CMCC-CESM also has this feature, it also shows an  
481 overestimated chlorophyll peak in the Indian basin. In the Antarctic Zone both observations and  
482 CMIP5 models generally agree in both phase and magnitude (except for CanESM2) of the seasonal  
483 cycle of chlorophyll in all three basins.

484  
485 We now examine the influence of the vertical DIC rate in Eq. 1, using estimated entrainment rates (RE,  
486 Eq. 5) based on MLD and vertical DIC gradients (see sec. 2.3). Fig. 7 shows the seasonal changes of  
487 MLD compared with the rate from the observational product. CMIP5 models largely agree on the  
488 timing of the onset of MLD deepening (February in the Pacific basin, and March for the Atlantic and  
489 Indian basin) and shoaling (September) in the Sub-Antarctic Zone (with the exception of NorESM1-ME  
490 and IPSL-CM5A in the Pacific basin). The Indian basin generally shows deeper winter MLD in both  
491 observations and CMIP5 models in the Sub-Antarctic Zone. Note that while CMIP5 models generally  
492 show the observed deeper MLDs in the Indian basin, they show a large variation; for example, the  
493 winter maximum depth ranges from 100 m (CMCC-CESM, Pacific basin) to 350 m (CanESM2, Indian  
494 basin) in the Sub-Antarctic Zone. In the Antarctic Zone CMIP5 models are largely in agreement on the  
495 timing of the onset of MLD deepening (February), but also variable in their winter maximum depth. It  
496 is worth noting that the observed MLD seasonal cycle might be biased due to limited in situ  
497 observations particularly in the Antarctic Zone (de Boyer Montégut et al., 2004).

498  
499 The estimated RE values in Fig. 10 show that almost all CMIP5 (with the exception of NorESM1-ME)  
500 entrain subsurface DIC into the mixed layer during autumn–winter in agreement with the  
501 observational estimates. In the Sub-Antarctic Zone, the estimates using the observational products  
502 show the strongest entrainment in the Atlantic basin in May (RE reaches up to  $10 \mu\text{mol kg}^{-1} \text{ month}^{-1}$ ),  
503 while it is lower in the other basins. In the Antarctic Zone, observed RE conversely shows stronger  
504 entrainment rates in the Pacific and Indian basin ( $RE > 15 \mu\text{mol kg}^{-1} \text{ month}^{-1}$ ) in comparison to the  
505 Atlantic basin ( $RE = 11 \mu\text{mol kg}^{-1} \text{ month}^{-1}$ ). CMIP5 models entrainment rates are variable but not  
506 showing any particular deficiency when compared with the observational estimates. Also, the group-  
507 DIC and group-SST models show no clear distinction, the major striking features being the relatively



508 stronger entrainment in MPI-ESM and CanESM2 across the three basins in the Sub-Antarctic Zone in  
509 mid to late winter ( $RE = 15 \mu\text{mol kg}^{-1} \text{ month}^{-1}$ ), and the large winter entrainment in IPSL-CM5A-MR in  
510 the Antarctic Pacific basin. The supply of DIC to the surface due to vertical entrainment is therefore  
511 generally comparable between model simulations and the available estimate.

512  
513 However, our RE estimates are estimated at the base of the mixed layer, which is not necessarily a  
514 complete measure of the vertical flux of DIC at the surface. We therefore investigate the annual mean  
515 vertical DIC gradients in Fig. 10 as an indicator of where the surface uptake processes occur. The  
516 simulated CMIP5 profiles are similar to GLODAP2, but some differences arise. In the Sub-Antarctic  
517 Zone, GLODAP2 shows a shallower surface maximum in the Atlantic basin consistent with higher  
518 biomass in this basin ( $(dDIC/dz)_{\text{max}} = 0.55 \mu\text{mol kg}^{-1} \text{ m}^{-1}$ , at 50 m) compared to the Pacific  
519 ( $(dDIC/dz)_{\text{max}} = 0.60 \mu\text{mol kg}^{-1} \text{ m}^{-1}$ , at 80 m) and Indian basin ( $(dDIC/dz)_{\text{max}} = 0.40 \mu\text{mol kg}^{-1} \text{ m}^{-1}$ , at  
520 80 m). CMIP5 models generally do not show this feature in the Sub-Antarctic Zone, except for CESM1-  
521 BGC1 ( $(dDIC/dz)_{\text{max}} = 0.50 \mu\text{mol kg}^{-1} \text{ m}^{-1}$ , at 50 m). Instead, they show the surface maxima at the same  
522 depth in all three basins. In the Antarctic Zone both CMIP5 models and observations show larger  
523  $(dDIC/dz)_{\text{max}}$  magnitudes and nearer surface maxima (with the exception of CanESM2 and CESM1-  
524 BGC). This difference in the position and magnitude of the DIC maxima between the Sub-Antarctic and  
525 Antarctic Zone has important implications for surface DIC changes and subsequently  $p\text{CO}_2$  seasonal  
526 variability. Because of the nearer surface DIC maxima in the Antarctic Zone, surface DIC changes are  
527 mostly influenced by these strong near-surface vertical gradients than MLD changes. This implies that  
528 even if the entrainment rates at the base of the MLD are comparable between the Sub-Antarctic and  
529 the Antarctic, the surface supply of DIC may be larger in the Antarctic Zone.

530

531

## 532 **4. Discussion**

533

534 Recent studies have highlighted that important differences exist between the seasonal cycle of  $p\text{CO}_2$  in  
535 models and observations in the Southern Ocean (Lenton et al., 2013; Anav et al., 2015; Mongwe, 2016).  
536 Paradoxically, although the models may be in relative agreement for the mean annual flux, they  
537 diverge in the phasing and magnitude of the seasonal cycle (Lenton et al., 2013; Anav et al., 2015;  
538 Mongwe, 2016). These differences in the seasonal cycle raise questions about the climate sensitivity of  
539 the carbon cycle in these models because they may reflect differences in the process sensitivities to  
540 drivers that are themselves climate sensitive.

541

542 In this study we expand on the framework proposed by Mongwe et al. (2016), which examined the  
543 competing roles of temperature and DIC as drivers of pCO<sub>2</sub> variability and the seasonal cycle of pCO<sub>2</sub> in  
544 the Southern Ocean, to explain the mechanistic basis for seasonal biases of pCO<sub>2</sub> and FCO<sub>2</sub> between  
545 observational products and CMIP5 models. This analysis of 10 CMIP5 models and one observational  
546 product (Landschutzer et al., 2014) highlighted that although the models showed different seasonal  
547 cycles (Fig. 2), they could be grouped into two categories (SST- and DIC-driven) according to their  
548 mean seasonal bias of temperature or DIC control (Fig. 3 & 6).

549  
550 A few general insights emerge from this analysis. Firstly, despite significant differences in the spatial  
551 characteristics of the mean annual fluxes (Fig. 1), models show unexpectedly greater inter-basin  
552 coherence in the phasing seasonal cycle of FCO<sub>2</sub> and SST-DIC control than observational products (Fig.  
553 3 & 6). Clear inter-basin differences have been highlighted in studies on the climatology and  
554 interannual variability that examined pCO<sub>2</sub> and CO<sub>2</sub> fluxes based on data products (Landschutzer et al.,  
555 2015; Gregor et al., 2017), as well as phytoplankton chlorophyll based on remote sensing (Thomalla et  
556 al., 2011; Carranza et al., 2016). Briefly, the Atlantic basin shows the highest mean primary  
557 production in contrast to the Pacific basin, which has the lowest (Thomalla et al., 2011). Similarly,  
558 strong inter-basin differences for pCO<sub>2</sub> and FCO<sub>2</sub> have been highlighted and ascribed to SST control  
559 (Landschützer et al., 2016) and wind stress - mixed layer depth (Gregor et al., 2017). The combined  
560 effect of these regional differences in forcing of pCO<sub>2</sub> and FCO<sub>2</sub> would be expected to be reflected in the  
561 CMIP5 models as well. A quantitative analysis of the correlation of the phasing of the seasonal cycle of  
562 FCO<sub>2</sub> between basins for different models shows that all the models except three (CMCC-CESM, GFDL-  
563 ESM2M CESM1-CESM) are characterized by strong inter-basin correlation in both the SAZ and the AZ  
564 (Fig. 4). This suggests that the carbon cycle in these CMIP5 models is not sensitive to inter-basin  
565 differences in the drivers as is the case for observations. This most likely implies that CMIP5 models  
566 are not sensitive to regional FCO<sub>2</sub> variability at the basin scale, so FCO<sub>2</sub> seasonal biases are zonally  
567 uniform.

568  
569 Secondly, an important part of this analysis is based on the assumption that the observational  
570 products that are used to constrain the spatial and temporal variability of pCO<sub>2</sub> and FCO<sub>2</sub> reflect the  
571 correct seasonal cycles of the Southern Ocean. This assumption requires significant caution not only  
572 due to the limitations in the sparseness of the *in situ* observations but also due to limitations of the  
573 empirical techniques in overcoming these data gaps (Landschutzer et al., 2014; Rödenbeck et al., 2015;  
574 Gregor et al., 2017a, b; Ritter et al., 2018). The uncertainty analysis from these studies suggests that,  
575 while the seasonal bias in observations may be less in the SAZ and PFZ, it is the highest in the AZ  
576 where access is limited mostly to summer, and winter ice cover results in uncertainties that may limit  
577 the significance of the data-model comparisons. It is important to note that though the observation

578 product that we use here (Landschützer et al., (2014) is based on more surface measurement (10  
579 millions, SOCAT v3) compared to previous datasets (e.g. Takahashi et al., 2009, 3 millions), the data  
580 are still sparse in time and space in the Southern Ocean. Thus, in using this data product as our main  
581 observational estimates for this analysis we are mindful of the limitations in the discussion below.

582  
583 Thirdly, the seasonal cycle of  $\Delta p\text{CO}_2$  is the dominant mode of variability in  $\text{FCO}_2$  (Mongwe et al., 2016;  
584 Wanninkhof et al., 2009). Though winds provide the kinematic forcing for air-sea fluxes of  $\text{CO}_2$  and  
585 indirectly affect  $\text{FCO}_2$  through mixed layer dynamics and associated biogeochemical responses  
586 (Mahadevan et al., 2012; du Plessis et al., 2017),  $\Delta p\text{CO}_2$  sets the direction of the flux. Surface  $p\text{CO}_2$   
587 changes are mainly driven by DIC and SST (Hauck et al., 2015; Takahashi et al., 1993). Subsequently  
588 the sensitivity of CMIP5 models to how changes in DIC and SST regulate the seasonal cycle of  $\text{FCO}_2$  is  
589 fundamental to the model's ability to resolve the observed  $\text{FCO}_2$  seasonal cycle. Thus, here we  
590 examined the influence of DIC and SST on  $\text{FCO}_2$  at seasonal scale for 10 CMIP5 models with respect to  
591 observed estimates. Because temperature does not directly affect DIC changes, we first scaled up the  
592 impact of SST changes on  $p\text{CO}_2$  through surface  $\text{CO}_2$  solubility to equivalent DIC units using the Revelle  
593 factor (section 2.3). In this way, we can distinguish the influence of surface solubility and DIC changes  
594 (i.e. biological and physical) on  $p\text{CO}_2$  and hence on  $\text{FCO}_2$ .

595  
596 Fourthly, using this analysis framework (sec 2.3, summarized in Fig. 6) we found that CMIP5 models  
597  $\text{FCO}_2$  biases cluster in two groups, namely group-DIC ( $M_{\text{T-DIC}} < 0$ ) and group-SST ( $M_{\text{T-DIC}} > 0$ ). Group-DIC  
598 models are characterized by an overestimation of the influence of DIC on  $p\text{CO}_2$  with respect to  
599 observations estimates, which instead indicate that physical and biogeochemical changes in the DIC  
600 concentration mostly regulate the seasonal cycle of  $\text{FCO}_2$  (in short, DIC control). Group-SST models  
601 show an excessive temperature influence on  $p\text{CO}_2$ ; here surface  $\text{CO}_2$  solubility biases are mainly  
602 responsible for the departure of modelled  $\text{FCO}_2$  from the observational products. While CMIP5 models  
603 mostly show a singular dominant influence of these extremes, observations show a modest influence  
604 of both, with a dominance of DIC changes as the main driver of seasonal  $\text{FCO}_2$  variability. Below we  
605 discuss the seasonal cycle characteristics and possible mechanisms for these two groups of CMIP5  
606 models in the Sub-Antarctic and Antarctic Zones of the Southern Ocean.

607

#### 608 **4.1 Sub-Antarctic Zone (SAZ)**

609

610 Our diagnostic analysis indicates that the seasonal cycle of  $p\text{CO}_2$  in the observational product  
611 (Landschützer et al., 2014) is mostly DIC controlled across all three basins of the SAZ ( $M_{\text{T-DIC}} < 0$  in Fig.  
612 6). The Atlantic basin shows a stronger DIC control (Annual mean  $M_{\text{T-DIC}} \geq 2$ ) compared to the Pacific  
613 and Indian basin (Annual mean  $M_{\text{T-DIC}} \approx 1$ ). This stronger influence of DIC on  $p\text{CO}_2$  in the Atlantic basin

614 is consistent with higher primary production in this basin (Graham et al., 2015; Thomalla et al., 2011),  
615 here shown by the larger mean seasonal chlorophyll from remote sensing in the Atlantic basin with  
616 respect to the Pacific and Indian basin (Fig. 8). This significant basin difference is most likely linked to  
617 the fact that the Atlantic basin has longer periods of shallow MLD compared to the Pacific and Indian  
618 basins (Fig. 7a-c, Nov – Mar & Nov - Feb respectively) and has been shown to have higher supplies of  
619 continental shelves and land-based iron (Boyd and Ellwood, 2010; Tagliabue et al., 2012; 2014). These  
620 conditions are more likely to enhance primary production that translates into a higher rate of change  
621 of surface DIC (Fig. 8), which becomes the major driver of  $FCO_2$  variability. In contrast, shorter periods  
622 of shallow MLD and lower iron inputs in the Pacific basin (Tagliabue et al., 2012), likely account for a  
623 lower chlorophyll biomass and hence the weaker DIC control evidenced in our analysis ( $M_{T-DIC} \approx 0$  in  
624 Fig. 6). In the Indian basin, the winter mixed layer is deeper than in the Atlantic and deepens earlier in  
625 the season (Fig. 7c). These conditions limit chlorophyll concentration (Fig. 8) and possibly contribute  
626 to the lower rates of surface temperature change because of the enhanced mixing (cf Fig. 5a-c). As a  
627 consequence, the resulting net driver in the Indian and Pacific basins is a weaker DIC control, because  
628 both biological DIC and solubility changes are relatively weaker and they oppose each other. Because  
629 of this, when the magnitudes of the rate of change of SST are larger during cooling and warming  
630 seasonal peaks (autumn and spring respectively), DIC control is weaker ( $M_{T-DIC} \approx 0$ ) during these  
631 seasons.

632  
633 CMIP5 models do not capture these basin-specific features as demonstrated with the correlation  
634 analysis in Fig. 4, with the exception of three group-SST models (i.e. CESM1-BGC, GFDL-ESM2M and  
635 CMCC-CESM). These, in contrast, mostly show comparable  $FCO_2$  phasing in the three basins. The  
636 seasonal cycle of  $CO_2$  flux in the Southern Ocean (3,4) is both zonally and meridionally uniform for  
637 most CMIP5 models, in contrast to observational data product (Fig. 3). This suggests that CMIP5  
638 models show equal sensitivity to basin scale  $FCO_2$  drivers, suggesting that  $pCO_2$  and  $FCO_2$  driving  
639 mechanisms are less local than for observations. Thus the understanding of fine-scale (mesoscale and  
640 sub-mesoscale) processes responsible for basin-scale  $FCO_2$  variability will be an important  
641 contribution to the next generation of ESM. Studies based on new available data from higher  
642 resolution autonomous platforms like Monteiro et al., (2015), Williams et al., (2017). Briggs et al.,  
643 (2018) and Rosso et al., (2017) may be useful constraints to these dynamics in ESMs.

644  
645 The major feature of group-SST models in the SAZ is the out-gassing during summer and in-gassing  
646 mid-autumn to winter (Fig. 3a-c, Apr-Aug), which our diagnostics in Fig. 6 attribute to temperature  
647 (solubility) control. The summer period coincides with the highest warming rates ( $dSST/dt$ , Fig 5a-c),  
648 and associated reduction in solubility of  $CO_2$ . Similarly, exaggerated cooling rates at the onset of  
649 autumn (Fig. 5a-c) enhance  $CO_2$  solubility causing a change in the direction of  $FCO_2$  into strengthening

650 CO<sub>2</sub> in-gassing (Fig 3a-c). Thus, while group-SST models have a seasonal amplitude of FCO<sub>2</sub>  
651 comparable to observations, they are out of phase (Fig. 3) as was the case in a previous analysis of a  
652 forced ocean model (Mongwe et al., 2016).

653  
654 In addition to increasing CO<sub>2</sub> solubility, the rapid cooling at the onset of autumn also deepens the MLD  
655 (March-June, Fig. 7), which induces entrainment of DIC, increasing surface CO<sub>2</sub> concentration and  
656 weakening the ocean-atmosphere gradient, and, in some instances, reversing the air-sea flux to out-  
657 gassing (Lenton et al., 2013a; Mahadevan et al., 2011; Metzl et al., 2006). While these processes  
658 (cooling and DIC entrainment) are likely to co-occur in the Southern Ocean, in CMIP5 models they are  
659 characterized by their extremes: temperature impact of solubility exceeds the rate of entrainment  
660 (Fig. 6 & 10). Because of the dominance of the solubility effect in group-SST models, the impact of DIC  
661 entrainment on surface pCO<sub>2</sub> changes, the weakening of CO<sub>2</sub> in-gassing / out-gassing only happens in  
662 mid-late winter (June-July -August) when entrainment fluxes peak (Fig. 10) and the SST rate  
663 approaches zero (Fig. 5).

664  
665 In the spring-summer transition, primary production is expected to enhance the net CO<sub>2</sub> uptake  
666 (Thomalla et al., 2011; Le Quéré and Saltzman, 2013). However, the elevated surface warming rates  
667 during spring reduces CO<sub>2</sub> solubility in group-SST models and overwhelms the role of primary  
668 production in the seasonal cycle of pCO<sub>2</sub> and FCO<sub>2</sub> (atmospheric CO<sub>2</sub> uptake). As a consequence, these  
669 group-SST models mostly show a constant or weakening net CO<sub>2</sub> uptake flux during spring in the  
670 Pacific and Atlantic basin even though primary production is occurring and is relatively elevated (Fig.  
671 3 & 8). Though some models show chlorophyll concentrations comparable to observations (e.g. GFDL-  
672 ESM2M, CNRM-CM5, CanESM2), and sometimes greater (e.g. MRI-ESM), the impact of temperature-  
673 driven solubility still dominates due to the phasing of the rates of the two drivers (Fig. 2a-c). The  
674 Indian basin however shows the only exception to this phenomenon. Here, the amplitude of the  
675 seasonal surface warming is relatively smaller ( $\sim 0.5 \text{ }^\circ\text{C}^{-1} \text{ month}^{-1}$  lower than the Pacific and Atlantic  
676 basins), and the biologically-driven CO<sub>2</sub> uptake becomes notable and shows a net strengthening of the  
677 sink of CO<sub>2</sub> during spring (Fig. 3c).

678  
679 Though almost all analyzed CMIP5 models (with the exception of NorESM1-ME) exaggerate the  
680 warming and cooling rates in autumn and spring, group-DIC models do not manifest the expected  
681 temperature-driven solubility impact on pCO<sub>2</sub> and FCO<sub>2</sub> (Fig. 2). Instead, the seasonal cycle of pCO<sub>2</sub> and  
682 FCO<sub>2</sub> are controlled by DIC changes, which are driven by an overestimated seasonal primary  
683 production and the associated export carbon (Fig. 8). It is striking how in these models the seasonal  
684 cycle of chlorophyll and FCO<sub>2</sub> are in phase (Fig 3a-c, 8a-c, with linear correlation coefficients always

685 larger than 0.9 not shown) but, as we discuss below, this is not because the temperature rates of  
686 change are correctly scaled but because the biogeochemical process rates are exaggerated (Fig. 8).

687  
688 Because of the particularly enhanced production in group-DIC models, the CO<sub>2</sub> sink is stronger (Fig. 8)  
689 with respect to observation estimates during spring. This is visible in the reduction of surface DIC  
690 (negative dDIC/dt in Fig. 8a, g-i), which can only be explained by drawdown due to the formation and  
691 export of organic matter (Le Quéré and Saltzman, 2013). However, note that in the same way, after the  
692 December production peak, both CMIP5 models and observations show an increase of surface DIC  
693 concentrations (positive dDIC/dt) until March (Fig. 8, g-i). These DIC growth rates are particularly  
694 enhanced in group-DIC models compared to some group-SST and observations (Fig. S9). The onset of  
695 these DIC increases also coincides with the depletion of surface oxygen (Fig. S9), which we speculate is  
696 due to the remineralization of organic matter to DIC through respiration. Unfortunately, only a few  
697 models have stored the respiration rates, therefore the full reason for this DIC rebound remains to be  
698 examined at a later stage. We would however tend to exclude other processes, because the onset of  
699 CO<sub>2</sub> out-gassing seen in March in group-DIC models occurs prior to significant MLD deepening (Fig. 7)  
700 and entrainment fluxes, therefore remineralization is likely be a key process here (Fig. 8).

701

## 702 **4.2 Antarctic Zone (AZ)**

703

704 The seasonal cycle framework summarized in Fig. 6 shows that the variability of FCO<sub>2</sub> and pCO<sub>2</sub> in the  
705 Landschützer et al. (2014) product is characterized by a stronger DIC control (annual mean  $M_{T-DIC} < -2$ )  
706 relative to the Sub-Antarctic ( $M_{T-DIC} \approx -1$ ), except in the spring season ( $M_{T-DIC} > -1$ ). This DIC control is  
707 spatially uniform in the Antarctic Zone across all three basins (Fig. 4). The available datasets indicate  
708 that the combination of weaker SST rates due to lower solar heating fluxes (Fig. 5), and stronger  
709 shallower vertical DIC maxima (Fig. 10) favour a stronger DIC control through larger surface DIC rates.  
710 The spatial uniformity in the seasonality of FCO<sub>2</sub> is also evident in the satellite chlorophyll and  
711 calculated dDIC/dt from GLODAP2 in Fig. 9. Contrary to the Sub-Antarctic this might be suggesting  
712 that FCO<sub>2</sub> mechanisms here are less local. It could be hypothesized that the seasonal extent of sea-ice,  
713 deeper mixing and heat balance differences affect this region more uniformly compared to the Sub-  
714 Antarctic Zone, and hence the mechanisms of FCO<sub>2</sub> are spatially homogeneous. However, we cannot  
715 forget that sparseness of observations in this region is a key limitation to data products (Bakker et al.,  
716 2014; Gregor et al., 2017; Monteiro et al., 2010; Rödenbeck et al., 2013) that might hamper the  
717 emergence of basin-specific features. Consequently, this highlights the importance and need to  
718 prioritize independent observations in the Southern Ocean south of the polar front and in the Marginal  
719 Ice Zone. Increased observational efforts should also include a variety of platforms such as

720 autonomous vehicles like gliders (Monteiro et al., 2015) and biogeochemical floats (Johnson et al.,  
721 2017) in addition to ongoing ship-based measurements.

722

723 In general terms, CMIP5 models are mostly in agreement (with an exception of MRI-ESM) with the  
724 observational product on the dominant role of DIC to regulating the seasonal cycle of FCO<sub>2</sub> (Fig. 6d-f),  
725 though not all models agree in the phase of the seasonal cycle of FCO<sub>2</sub> (e.g. CanESM2, Fig. 2). Though  
726 CMIP5 models still mostly show the SST rates biases in autumn and spring with respect to observed  
727 estimates, the stronger and near-surface vertical DIC maxima (Fig. 10), likely favor DIC as a dominant  
728 driver of FCO<sub>2</sub> changes. Differences between group-SST and group-DIC models are only evident in mid-  
729 summer when SST rates heighten and primary production peaks (Fig. 3 & 9). Probably because of sea  
730 ice presence, the onset of SST warming is a month later (November) here in comparison to the Sub-  
731 Antarctic (October). This subsequently allows the onset of primary production before the surface  
732 warming, which then permits the biological CO<sub>2</sub> uptake to be notable in group-SST models. Thus the  
733 two model groups here agree in the FCO<sub>2</sub> in-gassing during spring with group-SST models being the  
734 closest to the observational product. The MRI-ESM is the only model showing anomalous solubility  
735 dominance during autumn and spring as in the Sub-Antarctic Zone.

736

737 This coherence of CMIP5 models and observations in the Antarctic Zone may suggest that CMIP5  
738 models compare better to observations in this region (Fig. 4). However, because CMIP5 models also  
739 show this spatial homogeneity in the Sub-Antarctic Zone (contrary to observational estimates), it is  
740 not clear whether this indicates an improved skill in CMIP5 model to the mechanisms of FCO<sub>2</sub> in this  
741 region, or both CMIP5 models and observational product lacks spatial sensitivity to the drivers of  
742 FCO<sub>2</sub>. The sparseness of observations in the AZ points to the latter.

743

744 The cause of differences in the seasonal rates of SST change in group-SST models remains a subject of  
745 ongoing research. The Southern Ocean is a part of the global ocean (upwelling) where earth systems  
746 models show a persistent warming SST bias (Hirahara et al., 2014). Several studies point to highlight  
747 potential explanations but the main reasons remains uncertain. For example, CMIP5 models  
748 differences in the magnitude and meridional location of the peak of wind speeds in the Southern Ocean  
749 (Bracegirdle et al., 2013) and MLD differences (Meijers, 2014; Sallée et al., 2013) may be such that the  
750 net effect of change on surface turbulence and mixing leads to these amplified surface temperature  
751 rates. Other known CMIP5 models' biases that which may contribute includes; heat fluxes and storage  
752 (Frölicher et al., 2015) as well as sea-ice dynamics (Turner et al., 2013). Notwithstanding these,  
753 investigation of the reasons for sources of these dSST/dt biases is out of the scope of this study. Our  
754 aim here is to show that understanding biases in the drivers of pCO<sub>2</sub> (DIC and SST) at the seasonal  
755 scale is necessary to understand differences in the seasonal cycle of FCO<sub>2</sub> between models and

756 observational products. However we recommend that the mechanistic basis for the differences the  
757 seasonal rates of warming and cooling be a matter of urgent investigated further

758 .

759

760

761

762

## 763 **5. Synthesis**

764

765 We used a seasonal cycle framework to highlight and examine two major biases in respect of pCO<sub>2</sub> and  
766 FCO<sub>2</sub> in 10 CMIP5 models in the Southern Ocean.

767

768 Firstly, we examined the general exaggeration of the seasonal rates of change of SST in autumn and  
769 spring seasons during peak cooling and warming respectively with respect to available observations.  
770 These elevated rates of SST change tip the control of the seasonal cycle of pCO<sub>2</sub> and FCO<sub>2</sub> towards SST  
771 from DIC and result in a divergence between the observed and modelled seasonal cycles, particularly  
772 in the Sub-Antarctic Zone. While almost all analyzed models (9 of 10) show these SST-driven biases, 3  
773 of the 10 (namely NorESM1-ME, HadGEM-ES and MPI-ESM) don't show these solubility biases because  
774 of their overly exaggerated primary production (and remineralization) rates such that biologically-  
775 driven DIC changes mainly regulate the seasonal cycle of FCO<sub>2</sub>. These models reproduce the observed  
776 phasing of FCO<sub>2</sub> as a result of an incorrect scaling of the biogeochemical fluxes. In the Antarctic Zone,  
777 CMIP5 models compare better with observations relative to the Sub-Antarctic Zone. This is mostly  
778 because both CMIP5 models and observational product estimates show a spatial and temporal  
779 uniformity in the characteristics of FCO<sub>2</sub> in the Antarctic Zone. However, it is not certain if this is  
780 because model process dynamics perform better in this high latitude zone or that the observational  
781 products variability is itself limited by the lack of *in situ data*. This remains an open question that  
782 needs to be explored further and highlights the need for increased scale-sensitive and independent  
783 observations south of the Polar Front and into the sea-ice zone.

784

785 The second major bias is that contrary to observational products estimates, CMIP5 models generally  
786 show an equal sensitivity to basin scale FCO<sub>2</sub> drivers (except for CMCC-ESM, GFDL-ESM2M and  
787 CESM1-BGC) and hence the seasonal cycle of FCO<sub>2</sub> has similar phasing in all three basins of the Sub-  
788 Antarctic Zone. This is in contrast to observational and remote sensing products that highlight strong  
789 seasonal and interannually varying basin contrasts in both pCO<sub>2</sub> and phytoplankton biomass. It is not  
790 clear if this is due to inadequate carbon process parameterization or improper representation of the



791 dynamics of the physics. This should be investigated further with CMIP6 models and our analysis  
792 framework is proposed as a useful tool to diagnose the dominant drivers. Contrary to observed  
793 estimates, CMIP5 models simulate FCO<sub>2</sub> seasonal dynamics that are zonally homogeneous and we  
794 suggest that any investigation of local (basin-scale) mechanisms, dynamics and long term trends of  
795 FCO<sub>2</sub> using CMIP5 models must remain tentative and should be treated with caution. This highlights a  
796 key area of development for the next generation of models such those planned to be used for CMIP6.  
797

798

799

800

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801

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809

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## L184 **Figures and table titles**

L185

L186 **Figure. 1:** The annual mean climatological distribution Sea-Air CO<sub>2</sub> Flux (FCO<sub>2</sub>, in gC m<sup>-2</sup> yr<sup>-1</sup>) for  
L187 observations (L14: Landschützer et al., 2014 and T09: Takahashi et al., 2009) and 10 CMIP5 models over  
L188 1995 – 2005. CMIP5 models broadly capture the spatial distribution of FCO<sub>2</sub> with respect to L14 and T09,  
L189 however, they also show significant differences in space and magnitude between the basins of the  
L190 Southern Ocean with a few exceptions.

L191

L192 **Figure. 2:** Seasonal cycle of Sea-Air CO<sub>2</sub> Flux (FCO<sub>2</sub>, in gC m<sup>-2</sup> yr<sup>-1</sup>) in observations and 10 CMIP5 models in  
L193 the Sub-Antarctic and Antarctic zones of the Pacific Ocean (first column), Atlantic Ocean (second column)  
L194 and Indian Ocean (third column). The shaded area shows the temporal standard deviation over the  
L195 considered period (1995 – 2005), g-sst and g-dic shows the clustering of CMIP5 models into group-SST and  
L196 group-DIC as shown in Fig. 3 (section 3.2).

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L198 **Figure. 3.** Seasonal cycle of the equally-weighted ensemble means of FCO<sub>2</sub> (gC m<sup>-2</sup> yr<sup>-1</sup>) from Fig. 2 for group  
L199 DIC models (MPI-ESM, HadGEM-ES and NorESM) and group SST models (GFDL-ESM2M, CMCC-CESM,  
L200 CNRM-CERFACS, IPSL-CM5A-MR, CESM1-BGC, NorESM2, MRI-ESM and CanESM2). The shaded areas show  
L201 the ensemble standard deviation. The black line is the Landschützer et al. (2014) observations.

L202

L203 **Figure. 4:** The correlation coefficients (R) of basin – basin seasonal cycles of FCO<sub>2</sub> for observations  
L204 (Landschützer et al., 2014) and 10 CMIP5 models in the three basins of the Southern Ocean i.e. Pacific,  
L205 Atlantic and Indian basin.

L206

L207 **Figure. 5:** Mean seasonal cycle of the estimated rate of change of sea-surface temperature (dsST/dt, °C  
L208 month<sup>-1</sup>) for the Sub-Antarctic and Antarctic zones of the Pacific Ocean (first column), Atlantic Ocean  
L209 (second column) and Indian Ocean (third column).

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L213 **Figure. 6:** Mean seasonal and annual values of the DIC–temperature control index (M<sub>T-DIC</sub>). The increase in  
L214 the red color intensity indicates increase in the strength of the temperature driver and the blue intensity  
L215 shows the strength of the DIC driver. The models are sorted according to the annual mean value of the  
L216 indicator presented in the last column (A<sub>mean</sub>).

L217

L218 **Figure. 7:** Seasonal cycle of the Mixed Layer Depth (MLD) in the Sub-Antarctic and Antarctic zones of the  
L219 Pacific Ocean (first column), Atlantic Ocean (second column) and Indian Ocean (third column).

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L221

L222 **Figure. 8:** The seasonal cycle of chlorophyll ( $\text{mg m}^{-3}$ ), Net Primary Production ( $\text{mmol m}^{-2} \text{s}^{-1}$ ) and the surface  
L223 rate of change of DIC ( $\mu\text{mol kg}^{-1} \text{month}^{-1}$ ) in the Sub-Antarctic zone of the Pacific Ocean (first column),  
L224 Atlantic Ocean (second column) and Indian Ocean (third column).

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L226 **Figure. 9** Same as Fig. 8 for the Antarctic zone.

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L228 **Fig. 10:** (a-f) Estimated DIC entrainment fluxes ( $\text{mol kg month}^{-1}$ ) at the base of the mixed layer and (g-i)  
L229 vertical DIC gradients ( $\mu\text{mol kg}^{-1} \text{m}^{-1}$ ) in the Sub-Antarctic and Antarctic zone of the Pacific Ocean (first  
L230 column), Atlantic Ocean (second column) and Indian Ocean (third column).

L231

L232 **Table 2:** Sea-Air  $\text{CO}_2$  fluxes ( $\text{Pg C yr}^{-1}$ ) annual mean uptake in the Southern Ocean (first column), here  
L233 defined as south of the Sub-tropical front, Sub-Antarctic zone (second column) and Antarctic zone (third  
L234 column). The third and fourth column shows the Pattern Correlation Coefficient (PCC) and Root Mean  
L235 Square Error (RMSE) for the whole Southern Ocean for each model. Observations here refer to  
L236 Landschützer et al., 2014.

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