Constraining Southern Ocean CO2 Flux Uncertainty Using Uncrewed Surface Vehicle Observations

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Abstract

Remote, harsh conditions of the Southern Ocean challenge our ability to observe the region's influence on the climate system. Southern Ocean air-sea CO2 flux estimates have significant uncertainty due to the reliance on limited ship-dependent observations in combination with satellite-based and interpolated data products. We utilize a new approach, making direct measurements of air-sea CO2, wind speed, and surface ocean properties on an Uncrewed Surface Vehicle (USV). In 2019 the USV completed the first autonomous circumnavigation of Antarctica providing hourly CO2 flux estimates. Using this unique data set to constrain potential error in different measurements and propagate those through the CO2 flux calculation, we find that different wind speed products and sampling frequencies have the largest impact on CO2 flux estimates with biases that range from -4% to +20%. These biases and poorly-constrained interannual variability could account for discrepancies between different approaches to estimating Southern Ocean CO2 uptake.

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12 Key Points:

- The first autonomous circumnavigation of Antarctica allowed for direct measurements of
 air-sea CO₂ and wind speed in the Southern Ocean.
- Bias and error propagation of various approaches to calculating CO₂ flux could explain
 some of the discrepancies between previous estimates.
- Interannual variability that is poorly-constrained by observations are also likely
 contributing to the discrepancies in CO₂ flux estimates.
- 19

20 Abstract

- 21 Remote, harsh conditions of the Southern Ocean challenge our ability to observe the region's
- 22 influence on the climate system. Southern Ocean air-sea CO₂ flux estimates have significant
- 23 uncertainty due to the reliance on limited ship-dependent observations in combination with
- satellite-based and interpolated data products. We utilize a new approach, making direct
- 25 measurements of air-sea CO₂, wind speed, and surface ocean properties on an Uncrewed Surface
- Vehicle (USV). In 2019 the USV completed the first autonomous circumnavigation of Antarctica
- providing hourly CO_2 flux estimates. Using this unique data set to constrain potential error in different measurements and propagate those through the CO_2 flux calculation, we find that
- different measurements and propagate those through the CO_2 flux calculation, we find that different wind speed products and sampling frequencies have the largest impact on CO_2 flux
- estimates with biases that range from -4% to +20%. These biases and poorly-constrained
- interannual variability could account for discrepancies between different approaches to
- 32 estimating Southern Ocean CO_2 uptake.

33 Plain Language Summary

34 The Southern Ocean is an important part of the global climate, playing an outsized role in the

- ³⁵ uptake of heat and carbon. Yet observing the Southern Ocean is challenging due to its size,
- 36 remoteness, and harsh conditions. In 2019 we completed the first autonomous circumnavigation
- of Antarctica with an Uncrewed Surface Vehicle (USV), also known as an ocean robot, in order
- to address some of these observing challenges. By directly measuring air and surface seawater
- 39 carbon dioxide (CO_2) and wind speed on the USV, we were able to observe CO_2 exchange
- 40 between the ocean and atmosphere every hour during the mission. Using this data set, we
- 41 estimated potential errors in these measurements as well as other approaches to estimating CO_2
- 42 exchange. The use of different satellite-based wind products and sampling frequency play the
- 13 largest role in uncertainty of the uptake of CO_2 in the Southern Ocean. In order to reduce this uncertainty and provide a better understanding of the Southern Ocean, expansion of an observing
- 44 uncertainty and provide a better understanding of the Southern Ocean, expansion of an obse
 45 network made up of ships, USVs, and other autonomous devices is necessary.

46 **1 Introduction**

47 Covering only 30% of the global ocean surface, the Southern Ocean (most often defined as south of 30–35°S) plays an outsized role in the climate system. It is the meeting point of ocean 48 49 currents and a connector between the atmosphere and ocean interior for the transfer of heat and carbon, accounting for as much as 75% and 40% of global ocean heat and carbon uptake, 50 respectively (Frölicher et al., 2014; Khatiwala et al., 2009). While questions remain as to all of 51 52 the mechanisms that contribute to CO₂ flux and the overturning circulation in the Southern 53 Ocean, it is becoming clear that control of net CO₂ uptake over annual to decadal scales is dominated by wind-driven physical mixing and upwelling of carbon-rich deep water (Iudicone et 54

- 55 al., 2011; Lovenduski et al., 2008).
- 56 Southern Ocean CO₂ flux is primarily a balance between the outgassing of natural carbon
- 57 in upwelled waters not taken up by biological processes and the flux of anthropogenic carbon
- 58 into the ocean driven by increasing atmospheric CO₂. These processes occur continuously and
- 59 simultaneously as cold, carbon-rich water outgasses in upwelling regimes, and absorbs
- anthropogenic heat and carbon as the water flows north in the surface layer to warmer regimes.
- 61 These processes vary across the diversity of Southern Ocean regimes from the temperature-

- 62 dominated system in the Subtropical Zone to the sea ice- and biologically-dominated regime
- 63 closest to Antarctica.

The combination of these diverse and variable biogeochemical regimes, sparse 64 observations, and inadequate constraint of circulation in models challenge estimates of Southern 65 Ocean CO₂ uptake. Climatological mean uptake estimates based on observations from ships 66 67 range from -0.8 to -1.0 Pg C yr⁻¹ (Landschützer et al., 2014; Takahashi et al., 2009). While the magnitude of interannual variability is unknown, the temporal variability of CO₂ flux at 68 interannual to decadal time scales is correlated with atmospheric variability as defined by the 69 Southern Annular Mode (SAM) index: the difference in mean sea level pressure between 40°S 70 and 65°S (Marshall, 2003). When the SAM index is positive, winds south of 45°S increase, 71 potentially accelerating upwelling of carbon-rich deep water and reducing net CO₂ uptake. A 72 73 negative SAM index is associated with a reduction of both upwelling and ventilation of CO₂ to the atmosphere, allowing increased net CO₂ uptake. However, there are regional variations in 74 CO₂ flux response to SAM conditions that are not fully understood (Keppler and Landschützer, 75 2019; Nevison et al., 2020). Keppler and Landschützer (2019), for example, found increased 76 upwelling and CO₂ outgassing in higher latitudes during positive SAM conditions but opposing 77 effects in other regions. Several data- (Fay et al., 2014; Landschützer et al., 2015; Takahashi et 78 al., 2012) and modeling-based (Le Quéré et al., 2007; Lovenduski et al., 2007, 2008, 2015) 79 studies suggest decadal-scale variability of Southern Ocean CO₂ uptake is within ± 0.4 Pg C yr⁻¹, 80 a significant portion of the climatological mean estimate of -0.8 to -1.0 Pg C yr⁻¹. 81 82 New observations, however, challenge whether the Southern Ocean is a strong sink.

Biogeochemical float data from 2014–2017 estimate a Southern Ocean CO₂ flux of -0.08 Pg C 83 yr⁻¹ (Gray et al., 2018), an order of magnitude less than the climatological mean estimates based 84 on ship-based surface ocean CO_2 partial pressure (pCO_2) data products (Landschützer et al., 85 2016, 2014; Rödenbeck et al., 2015; Takahashi et al., 2009). Even after correcting for a potential 86 bias of 4 µatm to the float-based calculated seawater pCO_2 , discrepancies between ship- and 87 88 float-based CO₂ flux estimates remain (Bushinsky et al., 2019). Whether recent float-based CO₂ flux estimates represent an updated understanding of the climatological mean, float-based 89 90 seawater pCO_2 requires an even larger bias correction, or 2014–2017 conditions were anomalous, is currently unresolved. 91

92 A criticism of ship-based estimates is the scarcity of data in both time and space, especially during winter months. However, surface ocean pCO_2 is measured directly on ships 93 with low uncertainty ($\pm 0.5\%$) (Pierrot et al., 2009), compared to pCO₂ calculated from float pH 94 measurements and estimated total alkalinity that has a higher uncertainty ($\pm 2.8\%$) (Bushinsky et 95 96 al., 2019; Williams et al., 2017). Unlike ships, floats are able to sample in harsh winter conditions unfit for safe ship operations as well as under ice, increasing the potential for filling 97 observational gaps. Another issue impacting the uncertainty in both float- and ship-based 98 99 climatological CO₂ flux estimates is the use of observation-derived atmospheric CO₂ products and satellite-based wind and sea level pressure products, which have been shown to add 100 significant uncertainty to CO₂ flux estimates in some regions (Chiodi et al., 2019; Roobaert et 101 al., 2018; Sutton et al., 2017). 102

103Technological advances of Uncrewed Surface Vehicles (USVs) address these104observational challenges through remote surveying in harsh conditions with direct measurements105of air-sea pCO_2 and wind speed. Here we present results from the first autonomous106circumnavigation of Antarctica, a 22,000-km, 196-day mission. A Saildrone Inc. USV with an

integrated Autonomous Surface Vehicle CO₂ (ASVCO₂TM) system was designed specifically to 107

108 survive the forces of being rolled and submerged by 15-meter breaking waves in the Southern

Ocean. We calculate air-sea CO₂ flux from the USV and provide a thorough comparison of 109

potential bias in CO₂ flux calculated with direct measurements relative to recent float-based 110

methods (Bushinsky et al., 2019; Gray et al., 2018) and a ship-based data product (Landschützer 111 et al., 2020) that rely on other satellite- and observational-based data products. We then discuss

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- the potential role of flux uncertainty and interannual variability in determining the Southern 113
- Ocean carbon sink. 114

2 Materials and Methods 115

2.1 USV and sensors 116

The Saildrone USV is an ocean-going drone navigable via satellite communications with 117 wind-driven propulsion and primarily solar-powered meteorological and surface ocean physical, 118 chemical, and biological sensors. The Saildrone USV that completed the 2019 Antarctica 119 circumnavigation is similar to the standard vehicles with a 7 m hull and 2.5 m keel described by 120 Meinig et al. (2019) and Zhang et al. (2019) but includes an adapted wing to survive the extreme, 121 high winds and waves of the Southern Ocean (Figure 1). This USV design includes a lower-122 aspect square rig designed to withstand the force of being rolled and submerged by 15 m 123 breaking waves but limits navigation to sailing primarily downwind. This design has been 124

recently modified to improve maneuverability. 125

Meteorological sensors are mounted on the square wing, including a Gill WindMasterTM 126 anemometer at 3.8 m height. Through field intercomparisons, Zhang et al. (2019) found RMS 127 differences of $\pm 0.6-1.0$ m s⁻¹ between wind speed measured on Saildrone USVs with the 128 standard 5 m wing compared to both the Woods Hole Oceanographic Institute's buoy Air-Sea 129 Interaction METeorology System and the R/V Revelle. In this study, we use the higher-bound 130 wind speed error of ± 1.0 m s⁻¹ derived by Zhang et al. (2019) for the estimated error of wind 131 speed measured from the shorter wing at 3.8 m. Even though they determined that bias was 132 inconclusive, to generate conservative estimates we use the mean bias determined from Zhang et 133 al. (2019) intercomparisons of $+0.2 \text{ m s}^{-1}$. 134

The ASVCO₂TM system is packaged in a waterproof enclosure mounted in the USV hull. 135 136 The ASVCO₂ is nearly identical to the Moored Autonomous pCO_2 (MAPCO₂TM) system that has been used for over two decades on dozens of surface buoys and has a lab- and field-validated 137 uncertainty of $\pm 2 \mu$ atm or $\pm 0.5\%$ (Sabine et al., 2020; Sutton et al., 2014). These CO₂ systems 138 139 utilize an equilibrator-based gas collection system and an infrared gas analyzer (LI-820, LI-140 CORTM) calibrated in situ with reference gas traceable to World Meteorological Organization standards, a similar methodology to the underway pCO_2 system deployed on the global network 141 142 of ships of opportunity (Pierrot et al., 2009). In order to adapt the MAPCO₂ for USV deployments, the ASVCO₂ includes an equilibrator mounted to the USV hull with a fairing 143 144 added to maintain consistent water level in the equilibrator when moving at speeds greater than 4 knots (Figure 1). 145

The ASVCO₂ system collects 1-hourly measurements of sea surface and marine 146 boundary layer atmospheric xCO_2 (the mole fraction of CO_2) and sea level atmospheric pressure. 147 Each *x*CO₂ measurement is paired with sea surface temperature (SST) and salinity (SSS) 148 collected by an RBR Saildrone³ CTD customized for mounting through the Saildrone USV keel 149

- 150 at 0.5 m depth. Seawater and air pCO_2 (at in situ SST) is calculated according to standard
- operating procedures (Dickson et al., 2007; Weiss, 1974) as described in Sutton et al. (2014).
- 152 Data from the ASVCO₂ system and wind speed, SST, and SSS are archived at the National
- 153 Centers for Environmental Information (Sutton et al., 2020).
- 154 The USV was deployed from Bluff, New Zealand on 19 January 2019. Sailing
- downwind, the USV navigated east 22,000 km around Antarctica and was recovered off Bluff on
- 156 3 August 2019, 196 days later. The anemometer was damaged near the Drake Passage during an
- 157 iceberg collision at the end of March.
- 158



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Figure 1. Schematic diagram of the 2019 Southern Ocean Saildrone USV and location of the sensors used in this study. Schematic is not to scale.

162 2.2 Comparison data sets

163 Several data sets are used as comparisons for the USV-derived CO_2 fluxes. The first is 164 v2020 of the SOM-FFN neural network product documented in Landschützer et al. (2016),

- 165 which uses ship-based measurements of seawater pCO_2 to estimate monthly air-sea CO_2 fluxes
- 166 globally over the period 1982 to 2019 (Landschützer et al., 2020). The second product is the
- same SOM-FFN neural network, but with the addition of Southern Ocean Carbon and Climate
- 168 Observations and Modeling project (SOCCOM) float-derived pCO_2 as training datasets
- 169 (Bushinsky et al., 2019). This product is available as "SOCCOM-only" as well as
- 170 "SOCCOM+ship" for the years 2014 to 2017. To compare these two data sets with the USV, we
- subsample each product at the location and month of each USV CO_2 flux measurement and average the CO_2 fluxes over 10-day periods.
- The third comparison dataset is air-sea CO_2 fluxes estimated from calculated surface ocean pCO_2 from SOCCOM biogeochemical float data from 2015 to 2019, which is available

- online as a quality-controlled data snapshot dated 30 August 2020 (Johnson et al., 2020). All
- float profiles from 2015 to 2019 were separated by year and front locations, and subsequently
- averaged by month to create monthly pCO_2 and CO_2 flux estimates for each of the three major
- 178 zones discussed in this manuscript. The Subantarctic Zone is defined as profiles with an oxygen 179 minimum deeper than 1200 m, a salinity maximum deeper than 500 m, and surface waters
- minimum deeper than 1200 m, a salinity maximum deeper than 500 m, and surface waters
 fresher than 34.6. The Polar Frontal zone is defined as profiles with an oxygen minimum
- between 900 and 1200 m deep and a deep (>1400 m) salinity maximum. The Antarctic Zone is
- defined as profiles with an oxygen minimum between 600 and 900 m deep and a salinity
- maximum deeper than 1000 m. While there are some profiles within the Seasonal Sea Ice Zone
- 184 which fall within the definitions above, these profiles are not included in the analysis if they
- 185 occur during a calendar year when that float profiled under ice. In contrast to previous studies,
- the float profiles have not been extrapolated over time and the monthly averages only represent averages of the instantaneous fluxes at the time of the float surfacing.
- We use CO_2 flux provided by the first two comparison data sets (Bushinsky et al., 2019 and Landschützer et al., 2020). CO_2 flux for the third comparison data set (SOCCOM
- biogeochemical floats from 2015 to 2019) and the USV are calculated using established
- 191 methodologies summarized in the Supplemental.
- 192

193 **3 Results and discussion**

194 3.1 Air-sea observations

During the mission, the USV observed a large range in ΔpCO_2 (seawater – air pCO_2) of 33 to -40 µatm with a slightly negative mean of -4 µatm and a variance of ± 12 µatm (Figure 2). Although periods of negative and positive ΔpCO_2 were observed throughout the deployment, positive ΔpCO_2 indicating outgassing was prevalent during the latter part of the deployment, primarily during late fall and early winter in the Indian Ocean sector of the Antarctic Zone (Figure S1). Observed mean, variation, and range of air xCO_2 , sea pCO_2 , ΔpCO_2 , SST, SSS, and wind speed are given in Table S2.

- 202 3.2 CO₂ flux uncertainty analysis
- The uncertainty in calculated CO_2 flux can vary widely given the different options of inputs. The gas transfer velocity (*k*) uncertainty of 20% applies to all CO_2 flux estimates (Wanninkhof, 2014), leaving the choice and availability of wind speed, seawater pCO_2 , and air pCO_2 data sets the major sources of variation among different approaches.
- 207 Given the scarcity of in situ wind speed observations, the use of satellite-based wind speed in calculating CO₂ flux is common. However, in many regions, these satellite-based 208 products have biases in comparison to available in situ data (Hihara et al., 2015; Kent et al., 209 2013; Tomita et al., 2015; Wallcraft et al., 2009; Weissman et al., 2012) and can have significant 210 impacts on CO₂ flux estimates (Chiodi et al., 2019; Roobaert et al., 2018; Sutton et al., 2017). 211 Directly-measured wind speed also suffer errors due to flow distortion, platform movement, and 212 wave shadowing, resulting in uncertainties of $\pm 0.1 \text{ m s}^{-1}$ on buoys (Cronin et al., 2008; Kubota et 213 al., 2008; Weller, 2015) and up to $\pm 1.0 \text{ m s}^{-1}$ on Saildrone USVs (Zhang et al., 2019). 214
- Prior to the USV anemometer being damaged in March 2019, there is no mean difference between USV-measured and Cross-Calibrated Multi-Platform Near Real Time V2.0 (CCMP V2)

wind speed (Mears et al., 2019) or ERA-Interim Reanalysis (Dee et al., 2011) wind speed with a 217 variance around wind speed residuals of $\pm 1.8 \text{ m s}^{-1}$ and $\pm 2.0 \text{ m s}^{-1}$, respectively (Figure S2). 218 NCEP-DOE AMIP-II Reanalysis 2 (NCEP-2) (Kanamitsu et al., 2002) and ERA5 (Hersbach et 219 al., 2020) wind speeds have lower wind speed by 1.0 and 0.1 m s⁻¹, respectively, than measured 220 on the USV with a variance around the mean bias of ± 3.9 and ± 1.4 m s⁻¹, respectively. In Table 221 S1 these biases are reported relative to the "true" wind speed by correcting for the USV wind 222 speed bias of $+0.2 \text{ m s}^{-1}$ (Zhang et al., 2019). Importantly, the biases in satellite-based wind 223 speed products relative to the USV-measured wind speed are not randomly distributed. Satellite 224 and USV wind speeds tend to agree most closely at wind speeds of 10 m s⁻¹, but diverge at lower 225 and higher wind speeds (Figure S2c). These results are consistent with biases reported in other 226 intercomparisons mentioned previously and summarized by Cronin et al. (2019). 227

Uncertainties associated with ship-, USV-, and float-based sources of pCO_2 are $\pm 0.5\%$, 228 $\pm 0.5\%$, and $\pm 2.8\%$, respectively (Table S1.) Common data sources of atmospheric baseline xCO_2 229 are the NOAA Greenhouse Gas Marine Boundary Layer (MBL) Reference CO₂ product 230 (Dlugokencky et al., 2019) or observations from nearby atmospheric observatories, like at Cape 231 Grim. Monthly mean xCO_2 from these two sources and the USV tend to agree within 0.2 ppm; 232 however, shorter-term variability indicating terrestrial biosphere influence is prevalent within the 233 hourly USV observations (Figure S3) and the hourly in situ Cape Grim observations (data not 234 235 shown). Converting these sources of xCO_2 to pCO_2 requires atmospheric pressure at sea level, which if using satellite-based products such as NCEP 2, ERA-Interim, or ERA5 introduces 236 another possible source of error (Table S1). 237

Various sampling frequencies of these data sources can also introduce error into the CO₂ 238 flux calculation. Monthly CO₂ flux calculated from subsampling the hourly USV Δp CO₂ data set 239 at 6-hourly intervals, which is the common temporal frequency of satellite-based products, 240 results in nearly identical values to monthly flux calculated from the hourly observations (Figure 241 S4). However, subsampling the hourly data set at all possible 10-day sampling frequencies, the 242 timescale for float observations, results in an integrated bias in CO_2 flux of +0.05 g C m⁻² mo⁻¹ or 243 +23% (less uptake/more outgassing) over the 7-month comparison period with large variation 244 around the monthly means due to the high temporal variability of the data set at a scale of less 245 than 10 days. 246

Propagated bias of USV-derived CO₂ flux is -4% (less outgassing/more uptake) driven by 247 the potential bias in USV-measured wind speed (Table 1). In this case, USV, CCMP V2, and 248 ERA-Interim wind speed bias are equivalent and have the same impact on calculated CO₂ flux. 249 Replacing directly-measured air pCO_2 with pCO_2 calculated from MBL or Cape Grim values and 250 251 NCEP 2, ERA-Interim, or ERA5 sea level pressure does not significantly impact flux bias. Taking into consideration the potential bias of subsampling at 10-day intervals combined with 252 the ERA-Interim wind speed bias results in an overall positive bias of +20% (more 253 outgassing/less uptake) in calculated CO₂ flux primarily due to the bias in subsampling the 2019 254 USV data set at 10-day intervals. Monteiro et al. (2015) found that a 10-day sampling period in 255 spring-summer in the Subantarctic Zone resulted in a 10-25% increase in uncertainty in CO₂ flux 256 257 relative to hourly sampling due to mixed layer responses to storm events, which may explain a similar magnitude sampling bias observed with the USV results. 258 259

Table 1. Estimated bias for different approaches of calculating CO₂ flux by applying mean bias

from Table S1 to conditions observed during the 2019 USV deployment. Resulting biases are

additive based on mean biases reported in Table S1. A negative bias suggests less

outgassing/more uptake; positive suggests more outgassing/less uptake. The USV CO_2 flux bias

results from the estimated USV wind speed bias of $+0.2 \text{ m s}^{-1}$ (Zhang et al., 2019).

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Seawater <i>p</i> CO ₂ data source	Air pCO_2 data source	Wind speed data source	Estimated CO ₂ flux bias
USV	USV	USV	-4%
Ship or USV	Ship, USV, MBL, or Gape Grim	CCMP-NRT or ERA-Interim	-4%
Float-derived	MBL or Cape Grim	ERA-Interim	+20%

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267 3.3 CO₂ flux comparisons

Due to the loss of the wind speed sensor during the USV deployment, USV CO₂ flux 268 presented in this section is calculated using CCMP V2 wind speed. During the 2019 269 circumnavigation, the USV observed periods of strong outgassing as high as 10.5 g C m⁻² mo⁻¹ in 270 June and July in the Antarctic Zone, which was one of the zones where SOCCOM float-based 271 data from 2014–2017 showed stronger outgassing than the SOM-FFN ship-based climatology 272 273 (Figure 3a; Bushinsky et al., 2019; Gray et al., 2018). There were also periods of intense shortscale CO₂ uptake during February through April, some of which were associated with 274 phytoplankton blooms (data not shown). The periods of strong outgassing observed by the USV 275 in June and July overlap with the Bushinsky et al. (2019) 2014-2017 SOCCOM-only SOM-FFN 276 estimates of CO₂ outgassing (Figure 3a). However, the USV observations show these outgassing 277 events occur over time periods from hours to two days in length, and these short-lived outgassing 278 279 events do not lead to outgassing as strong as the SOCCOM-only SOM-FFN estimates when averaged at the 10-day scale. Mean USV CO₂ flux in June and July results in a weak net 280 outgassing of 0.7 g C m⁻² mo⁻¹, more similar to the Landschützer et al. (2020) ship-based data 281 product and the Bushinsky et al. (2019) combined SOCCOM-ship SOM-FFN product than the 282 283 SOCCOM-only SOM-FFN product. 284





Figure 2. CO_2 flux calculated from USV-measured ΔpCO_2 , SST, and SSS and CCMP-NRT wind speed. Dates and * show the location of the USV with time. Black lines indicate climatological locations of the major fronts from Orsi et al. (1995) as in Figure S1.

Focusing only on 2019 observations, USV-measured and float-estimated surface seawater 290 pCO_2 are consistent within standard deviations of monthly means within the Subantarctic Zone 291 292 and the Antarctic Zone, the two major zones sampled by the 2019 Saildrone USV (Figure S5). Within the Antarctic Zone where Gray et al. (2018) found the largest winter-time discrepancy 293 between float- and ship-based data, we find a mean difference of 0.5 ± 2.6 g C m⁻² mo⁻¹ (or no 294 significant difference) between USV and float-derived CO₂ flux in March through July 2019 295 (Figure 3b). To test the possible effect of variable float locations on the estimates of CO₂ flux in 296 297 the Antarctic Zone, the Landschützer v2020 SOM-FFN ship-based climatology was subsampled at the times and locations of each float observation. Float-based fluxes are on average 1.5 g C m⁻ 298 ² mo⁻¹ greater than the ship-based climatology in this zone for 2015–2019 with significant 299 interannual variability (2015: +3.9, 2016: +2.1, 2017: +0.6, 2018: +0.8, and 2019: -0.1 g C m⁻² 300 301 mo^{-1}).

Figure 3b illustrates this significant interannual variability in float-derived CO_2 flux in the Antarctic Zone from 2015–2019. Net CO_2 uptake observed by the USV and floats in 2019 contrasts with the strong outgassing during winter of 2015 and 2016. This interannual variability may be influenced by SAM with increased westerly wind strength during the more positive phases of SAM increasing upwelling of relatively CO_2 -rich waters. The greatest outgassing is



- 308 3b and S6). The USV data were collected during a decline in the SAM index and are similar to 309 the float-based net flux estimates for 2019 (Figure 3b).
- 310



Figure 3. a) Time series of monthly CO_2 flux calculated using all USV observations at hourly 312 (red dots) and 10-day averaged (red line) time steps; from Landschützer et al. (2020) SOM-FFN 313 ship-based climatology (orange) and 2019 (yellow) subsampled at the Saildrone locations and 314 times and averaged over 10 days; and from Bushinsky et al. (2019) using the same methods of 315 the SOM-FFN v2020 ship-based climatology for the years 2014–2017 but incorporating 316 seawater pCO_2 estimated from both ships and SOCCOM biogeochemical-float observations 317 (light blue), and using only SOCCOM biogeochemical float observations (dark blue) for the 318 years 2014–2017. The shaded area represents the interannual variability in the SOCCOM-only 319 product over 2014–2017. b) Antarctic Zone monthly-averaged USV fluxes (red) plotted with 320 monthly mean SOCCOM float-based CO₂ flux from 2015–2019 in that zone (gray). The shaded 321 area is 1 σ of monthly mean SOCCOM CO₂ flux. 322

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Analysis of the Saildrone USV observations reveal several potential sources of bias and error in USV-, ship-, and float-based CO_2 flux (Tables S1 and 1). Given the significant fine-scale temporal and spatial variability observed during 2019, the 10-day sampling routine of floats may introduce a bias (more outgassing/less uptake in this case), which could account for some of the difference between float- and ship-based CO_2 flux reported previously (Bushinsky et al., 2019; Gray et al., 2018). It is also critical to better constrain how shifts in SAM conditions play a role

- in Southern Ocean CO₂ flux. The larger differences between the ship-based climatology and 330
- float-based flux during prolonged positive SAM conditions in 2015–2016 suggests an influence 331
- of measurement bias during those years or the possibility that the ship-based climatology does 332
- 333 not constrain increased upwelling of CO₂-rich water in higher latitudes. Sustained observations
- are needed to better constrain interannual variability like the anomalous strong winter outgassing 334
- observed by floats in 2015–2016 relative to 2017–2019. Better coverage of ships, USVs, and 335 floats are needed to resolve these uncertainties in measurements and variability in the Southern
- 336
- Ocean. 337

4 Conclusions 338

Climate change is predicted to reduce ocean CO₂ uptake under climate model scenarios 339 that show intensification of winds and acceleration of the overturning circulation in the Southern 340 Ocean (Le Quéré et al., 2007). Over the next century models also predict reductions in sea-ice 341 342 cover and surface ocean warming, freshening, and stratification, which are all expected to impact the carbon sink. How these processes impact the overall balance of CO₂ outgassing and uptake in 343 the Southern Ocean is uncertain. Better representation of these processes in models is necessary 344 to predict the Southern Ocean's role in a future climate. 345

- Our results indicate that the strong wintertime outgassing observed by floats in 2015 and 346 2016 was not prevalent in 2019. The change may be linked to a decline in the SAM index in the 347 later years leading to a reduction in upwelling of CO₂ rich waters to the surface. More sustained 348 observations are needed to constrain interannual variability and the impact on both Southern 349 350 Ocean and global ocean CO₂ uptake estimates. The first circumnavigation of the Southern Ocean by a USV described here has shown the capability to collect high quality data that can be used to 351 constrain multi-platform measurement uncertainties and interrogate how variability from the 352 scale of hours to years may impact CO₂ flux estimates. 353
- A multi-platform observing network consisting of USVs directly surveying air-sea 354 interactions, floats measuring full water column biogeochemistry even under ice, and the ship-355 based measurements for ground-truthing autonomous sensors would, in combination, best track 356 changes in ocean carbon uptake and better constrain variability. USVs fill a unique niche with 357 the ability to survey regions for extended periods where ships do not routinely operate, opening 358 up new opportunities for filling persistent gaps in the ocean observing system with high-quality 359 pCO_2 and meteorological observations. 360

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Geophysical Research Letters

Supporting Information for

Constraining Southern Ocean CO₂ Flux Uncertainty Using Uncrewed Surface Vehicle Observations

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Introduction

Additional figures and tables of 2019 Southern Ocean Saildrone USV observations and intercomparisons as well as a summary of CO_2 flux calculations are included here as supporting information.

CO₂ flux calculations

CO₂ flux is calculated using:

 CO_2 flux = $k \times K_0 \times \Delta p CO_2$

where *k* is the gas transfer velocity as a function of wind speed (Wanninkhof, 2014), K_0 is the solubility coefficient for CO₂ as a function of SST and SSS (Weiss, 1974; Weiss et al., 1982), and Δp CO₂ is seawater pCO₂ – air pCO₂.

The ASVCO₂ provides directly-measured seawater and air pCO₂. For the floats, seawater pCO₂ is calculated using measured pH and estimated total alkalinity as described by Williams et al. (2017) and atmospheric pCO₂ is calculated from air xCO₂ observations from the NOAA Greenhouse Gas Marine Boundary Layer Reference product (Dlugokencky et al., 2019) converted to pCO₂ using NCEP 2 sea level atmospheric pressure. As noted in the main text, the float fluxes were not extrapolated over time as was done by Gray et al. (2018). This means that the monthly averages presented here are averages of the instantaneous flux at the time of the float surfacing.

Gradients in seawater pCO_2 are assumed insignificant between the Saildrone measurements depth at about 0.5 m and the float measurements depth at 5–7 m in the well-mixed surface waters of the Southern Ocean. These measurements are also well below the surface boundary layer where skin temperature effects could impact the flux comparison between the different measurement approaches (Watson et al., 2020).

Several sources of wind speed have been used in previous studies to calculate CO₂ flux: Cross-Calibrated Multi-Platform Near Real Time V2.0 (CCMP V2) (Mears et al., 2019), NCEP-DOE AMIP-II Reanalysis 2 (NCEP 2) (Kanamitsu et al., 2002), ERA-Interim Reanalysis (Dee et al., 2011), and ERA5 (Hersbach et al., 2020). All wind speed data assessed here are 6-hourly except for ERA5 and USV-measured wind speed, which are hourly resolution. All satellite-based winds used here are at 10 m, with USV wind speed measured at 3.8 m corrected to a height of 10 m using parameterizations of Large and Pond (1981) as described in Sutton et al. (2017).

CCMP V2 wind speed is used to calculate both USV and 2015–2019 SOCCOM biogeochemical float fluxes. For the other two comparison data sets, Landschützer et al. (2020) uses ERA5 wind speed with *k* scaled for ERA5 wind data, and Bushinsky et al. (2019) uses ERA-Interim using *k* of Wanninkhof (2014), which is scaled for CCMP wind data.

Given the USV provides hourly in situ air-sea pCO_2 and wind speed observations, the 2019 USV data set is used to estimate potential bias and error in satellite-based wind speed and sea level pressure, different sources of air xCO_2 , and the effect of different sampling periods. In Table S1, bias is the mean difference between the USV measurements and these other sources. Error is one standard deviation (σ) of the differences.

The effect of the 10-day sampling period used by biogeochemical floats on monthly flux is estimated by subsampling hourly USV air and seawater pCO_2 , SST, and SSS every 10 days at noon (UTC) and linearly interpolating the values in between. These values are then combined with high-frequency wind speed to estimate CO_2 flux. To obtain as many realizations of the mean as possible, this is repeated ten times by shifting the starting time by a day. Resulting bias is the mean difference between the monthly USV flux and monthly mean flux from all realizations of the 10-day subsampling, averaged for each month from January through July.

We also use direct measurements of air-sea pCO_2 and wind speed from the USV, which are rare in the Southern Ocean, as the baseline for interrogating how potential bias in other products and interpolated observations impact calculated CO_2 flux. We estimate this by applying the mean bias in Table S1 directly to the USV wind speed, sea level pressure, seawater pCO_2 , and, in the case of sampling frequency, calculated CO_2 flux in the 7-month USV data set. For example, in the case of USV-derived CO_2 flux (first entry in Table 1), the wind speed bias of +0.2 m s⁻¹ is applied to the data set, then CO_2 flux is re-calculated. The resulting mean difference between the original USV CO_2

flux and flux with biases applied is reported for each approach in Table 1. This technique of using the 2019 Southern Ocean USV data to estimate calculated CO_2 flux bias is specific to the conditions observed during this mission and may not apply to the bias in these approaches in other applications.



Figure S1. Saildrone USV-measured a) ΔpCO_2 (µatm), b) SST (°C), c) SSS, and d) wind speed (m s⁻¹) during the mission along with black lines indicating climatological locations of the major fronts from Orsi et al. (1995). Zones moving from Antarctica north are: Seasonal Ice Zone, Antarctic-Southern Zone, Polar Frontal Zone, Subantarctic Zone, and Subtropical Zone.



Figure S2. a) Wind speed time series from January to August 2019 from directlymeasured Saildrone USV anemometer (gray) and the following satellite-based products: NCEP 2 (dark blue), ERA-Interim Reanalysis (red), ERA5 (pink), and CCMP V2 (yellow). b) Residual between Saildrone-measured wind speed and satellite products (mean residual ± one standard deviation). c) Comparison of wind speed products to USVmeasured wind speed as a function of wind speed.



Figure S3. Comparison of directly-measured air xCO_2 (gray), a fixed time series at the Cape Grim Baseline Air Pollution Station (red; data from the Australian Bureau of Meteorology and CSIRO Oceans & Atmosphere), and the NOAA Greenhouse Gas Marine Boundary Layer Reference product (blue; Dlugokencky et al., 2019).



Figure S4. Comparison of calculated monthly mean CO₂ flux using hourly (black), 6-hourly (gray), and 10-day (red) sampling frequencies with each realization of the 10-day subsampling shown in pink.



Figure S5. Comparison of hourly and monthly-averaged Saildrone USV directlymeasured seawater pCO_2 compared to float-based calculated seawater pCO_2 in the three major Southern Ocean zones sampled during the 2019 Saildrone USV mission. Shaded areas represent 1 σ of monthly mean float-based pCO_2 .



Figure S6. 3-month moving average of the SAM Index based on Marshall (2003). Shaded area is the deployment time for the 2019 Saildrone USV mission.

Source of error	Mean bias	σ
Ship and USV-based pCO ₂ (µatm)	-	0.5%
Float-based seawater pCO_2 (µatm)	-	2.8%
NCEP 2 sea level pressure (hPa)	-0.2	3.6
ERA-Interim sea level pressure (hPa)	+0.2	1.8
ERA5 sea level pressure (hPa)	-0.5	0.9
USV wind speed (m s ⁻¹)	+0.2	1.0
CCMP V2 wind speed (m s ⁻¹)	+0.2	1.8
NCEP 2 wind speed (m s^{-1})	-0.8	3.9
ERA-Interim wind speed (m s ⁻¹)	+0.2	2.0
ERA5 wind speed (m s ⁻¹)	+0.1	1.4
10-day sampling frequency (g C m ⁻² mo ⁻¹)	+0.05	0.43

Table S1. Sources of error in calculating CO₂ flux from various sources. USV wind speed errors are from Zhang et al (2019). Seawater pCO₂ errors are from previous studies: Pierrot et al. (2009) for ship-based pCO₂, Sabine et al. (2020) for USV-based pCO₂, and Williams et al. (2017) for float-based pCO₂. Mean bias and standard deviation (σ) of sea level atmospheric pressure and wind speed are calculated from residuals between USV-measured parameters and each data product. For wind speed, these biases are reported relative to the "true" wind speed by correcting the difference reported in Figure S2(b) for the USV wind speed bias of +0.2 m s⁻¹. Error due to 10-day sampling frequency of float-based measurements is calculated by subsampling the hourly USV data set at all possible 10-day intervals starting at 12:00 UTC.

	Mean	σ	Range	
air xCO ₂ (µmol mol ⁻¹)	407	1	402	410
seawater pCO_2 (µatm)	393	11	354	427
$\Delta p \mathrm{CO}_2$	-4	12	-40	33
SST (°C)	4.8	3.0	-0.3	13.5
SSS	34.04	0.27	32.12	34.95
wind speed (m s^{-1})*	10.2	3.4	0.3	24.9
CCMP-NRT wind speed (m s ⁻¹)	10.8	3.8	1.3	24.3

* USV wind speed statistics represent measurements made from the beginning of the mission until 26 March 2019 due to loss of sensor. CCMP V2 wind speeds for the entire deployment are also included to indicate that mean, variance, and range during January through March were similar to conditions throughout the deployment.

Table S2. Mean, one standard deviation of the mean (σ), and range of observations measured on the Saildrone USV from 19 January to 3 August 2019.