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Supporting Information for

Constraining Southern Ocean CO_2 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.

CO_2 flux calculations

CO_2 flux is calculated using:

$$CO_2 \text{ flux} = k \times K_o \times \Delta pCO_2$$

where k is the gas transfer velocity as a function of wind speed (Wanninkhof, 2014), K_o is the solubility coefficient for CO_2 as a function of SST and SSS (Weiss, 1974; Weiss et al., 1982), and ΔpCO_2 is seawater pCO_2 – air pCO_2.

The $ASVCO_2$ provides directly-measured seawater and air pCO_2. For the floats, seawater pCO_2 is calculated using measured pH and estimated total alkalinity as described by Williams et al. (2017) and atmospheric pCO_2 is calculated from air *x*CO2 observations from the NOAA Greenhouse Gas Marine Boundary Layer Reference product (Dlugokencky et al., 2019) converted to pCO_2 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 CO_2 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.

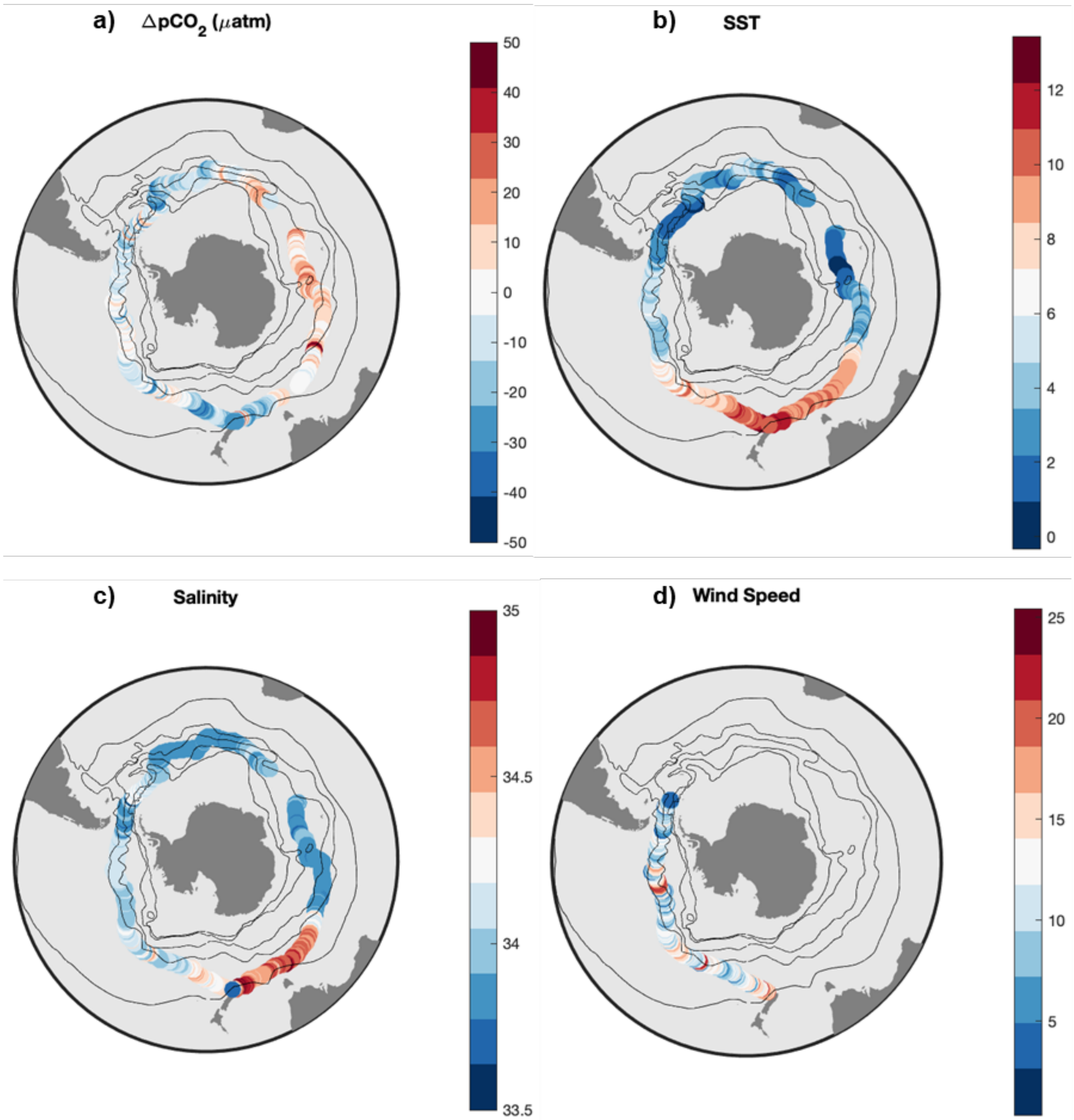

Figure S1. Saildrone USV-measured a) ΔpCO_2 (µatm), b) SST (^oC), c) SSS, and d) wind speed (m s^{-1}) during the mission along with black lines indicating climatological locations of the major fronts from Orsi et al. (1995). Zones moving from Antarctica north are: Seasonal Ice Zone, Antarctic-Southern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

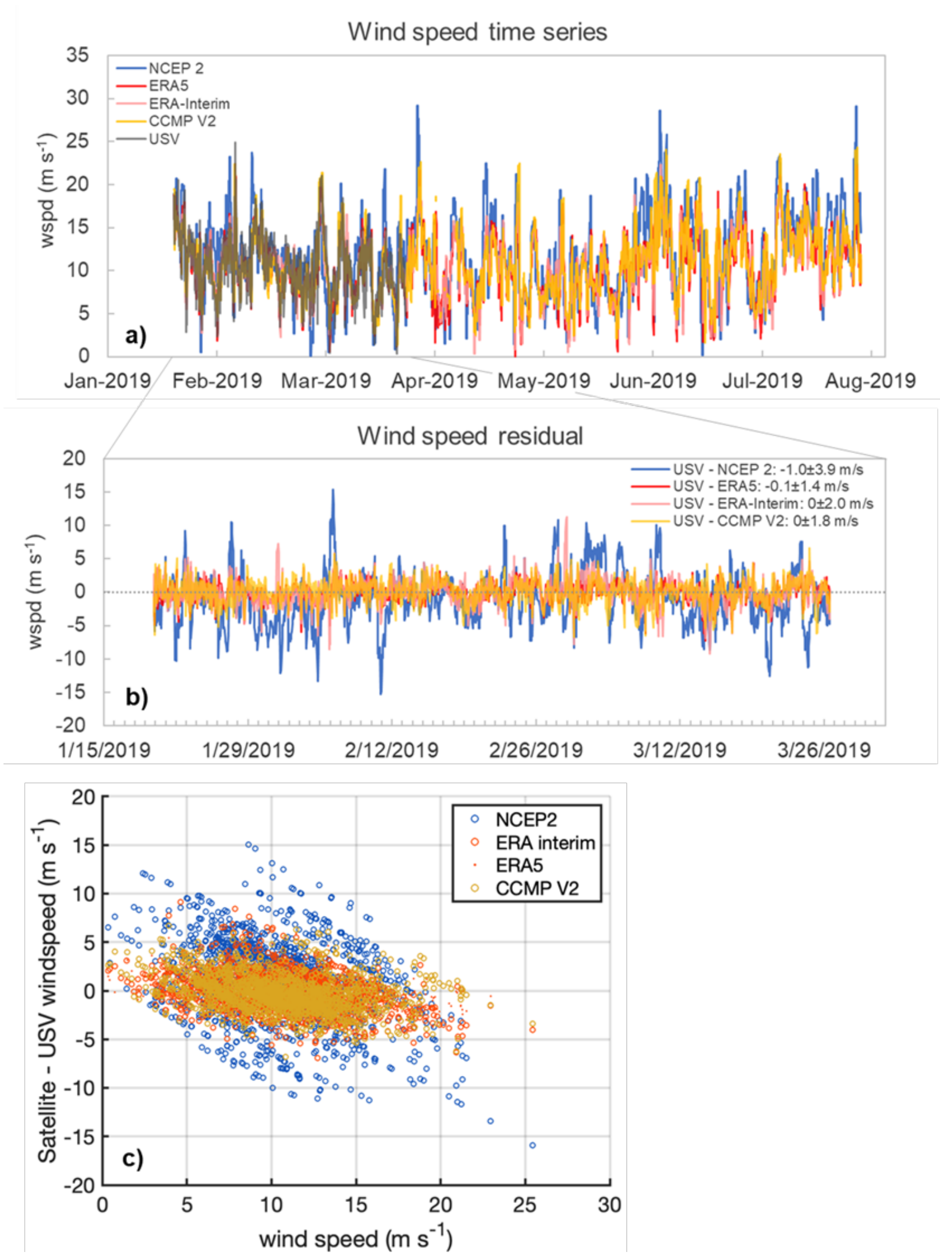

Figure S2. a) Wind speed time series from January to August 2019 from directly-measured Saildrone USV anemometer (gray) and the following satellite-based products: NCEP 2 (dark blue), ERA-Interim Reanalysis (red), ERA5 (pink), and CCMP V2 (yellow). b) Residual between Saildrone-measured wind speed and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

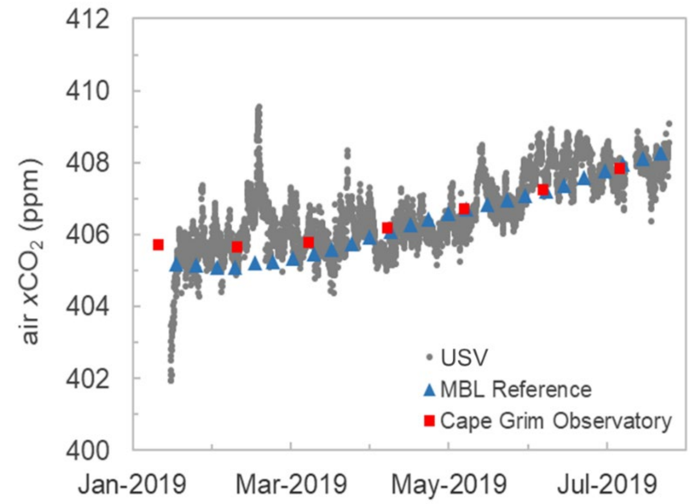

Figure S3. Comparison of directly-measured air xCO_2 (gray), a fixed time series at the Cape Grim Baseline Air Pollution Station (red; data from the Australian Bureau of Meteorology and CSIRO Oceans & Atmosphere), and the NOAA Greenhouse Gas Marine Boundary Layer Reference product (blue; Dlugokencky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

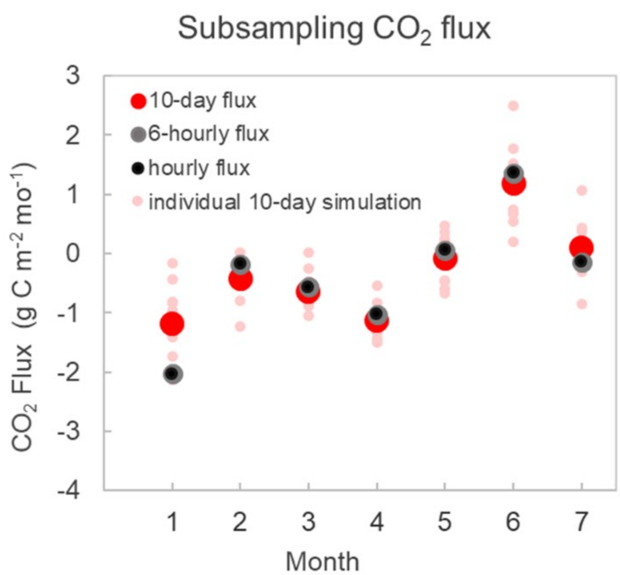

Figure S4. Comparison of calculated monthly mean CO_2 flux using hourly (black), 6-hourly (gray), and 10-day (red) sampling frequencies with each realization of the 10-day subsampling shown in pink.

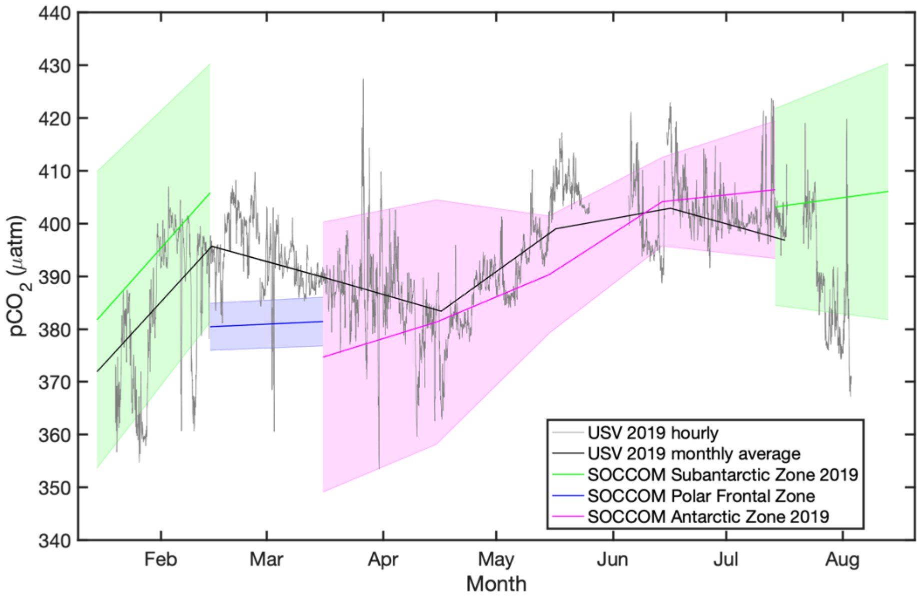

Figure S5. Comparison of hourly and monthly-averaged Saildrone USV directly-measured seawater pCO_2 compared to float-based calculated seawater pCO_2 in the three major Southern Ocean zones sampled during the 2019 Saildrone USV mission. Shaded areas represent 1 σ of monthly mean float-based pCO_2.

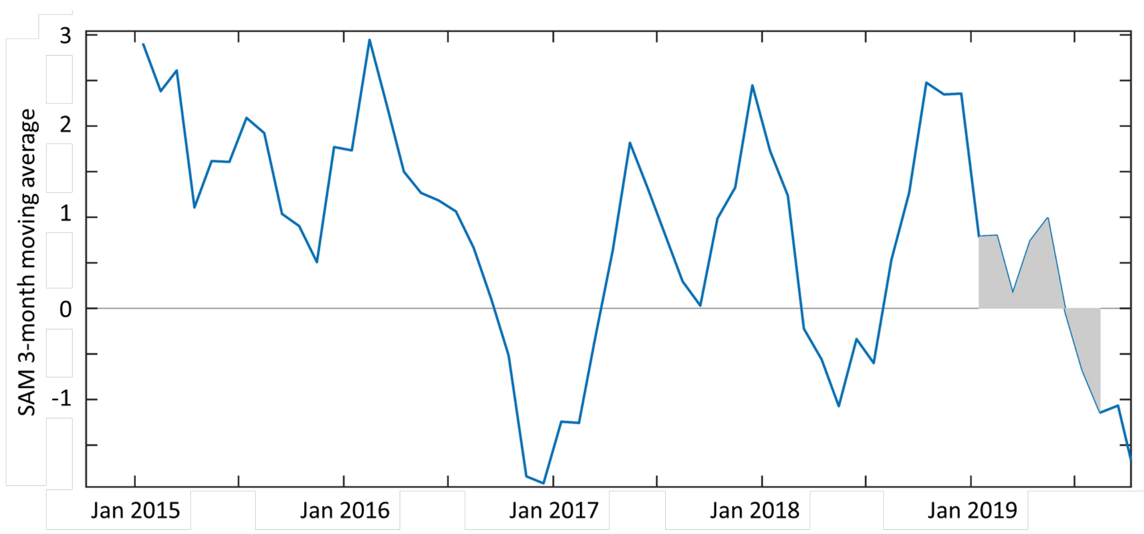

Figure S6. 3-month moving average of the SAM Index based on Marshall (2003). Shaded area is the deployment time for the 2019 Saildrone USV mission.

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 CO_2 flux from various sources. USV wind speed errors are from Zhang et al (2019). Seawater pCO_2 errors are from previous studies: Pierrot et al. (2009) for ship-based pCO_2, Sabine et al. (2020) for USV-based pCO_2, and Williams et al. (2017) for float-based pCO_2. 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
ΔpCO_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.