*AGU Advances*

Supporting Information for

# Subantarctic Mode Water Biogeochemical Formation Properties and Interannual Variability

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## Introduction

Included in the Supporting Information are figures to supplement those in the main text and a table that indicates float observations identified as bad.

## Text S1. Float biogeochemical observations

Only float data flagged as "good" were used for this analysis. Observations in the upper 20 m for each float were assessed to identify large anomalous changes in individual biogeochemical tracers that do not correspond to observed changes in temperature, salinity, or other biogeochemical parameters. Obvious outliers were removed from the analysis dataset (Table S1). Note that these are profiles removed from the entire float dataset prior to filtering for data that fall in the relevant SAMW formation areas. Most of the removed data therefore do not impact this study but are included to allow reproducibility of the original dataset considered.

The relationship between density and wintertime mixed layer properties is similar between the Pacific and Indian Oceans (Fig S1). This indicates that the differences in mean properties between SAMW that forms in each region are due to the different densities of the waters that form in these regions.

Differences between Biogeochemical Southern Ocean State Estimate (BSOSE) properties output sampled at float locations and actual float measurements or derived quantities are shown in Fig. S2. Differences are shown for the upper 200 m, using data from August and September float profiles when float calculated MLD is at least 200 m. Averages from the upper 200 m only were used to avoid the impact of differing BSOSE and float MLDs on the comparisons as profile differences are at a maximum at the high tracer gradients just below the MLD.

**Text S2. Calculation of $\Delta p\mathrm{CO_2}$**

$\Delta p\mathrm{CO_2}$ (μatm) values were calculated using the atmospheric $\mathrm{CO_2}$ mole fraction ($\mathrm{xCO_2}$ (μmol/mol), NOAA Greenhouse Gas Marine Boundary Layer Reference; Dlugokencky et al. 2019) matched to the nearest latitude:

$$p\mathrm{CO_{2,atm}} = \mathrm{xCO_2}\left(\frac{\mathrm{SLP}}{1013.25} - p\mathrm{H_2O}\right) \quad (1)$$

$$\Delta p\mathrm{CO_2} = p\mathrm{CO_{2,surf}} - p\mathrm{CO_{2,atm}} \quad (2)$$

where $p\mathrm{CO_{2,surf}}$ is the seawater $p\mathrm{CO_2}$, $p\mathrm{CO_{2,atm}}$ is the atmospheric partial pressure of $\mathrm{CO_2}$ adjusted for local climatological sea level pressure (SLP, (mbar)) and water vapor pressure ($p\mathrm{H_2O}$ (atm), calculated from sea surface temperature (SST) and sea surface salinity (SSS); Zeebe and Wolf-Gladrow 2001). The average $p\mathrm{H_2O}$ for the wintertime float data used in this study was 0.01 atm (~ 4 μatm impact on $p\mathrm{CO_2}$).

In order to compare $\Delta p\mathrm{CO_2}$ between different years we calculated a 10-year climatology of sea level pressure from National Centers for Environmental Prediction (NCEP; Kalnay et al., 1996) reanalysis sea level pressure at the location of each observation. We fit a seasonal harmonic to the 2011 to 2020 SLP and used each observation's day of year to determine SLP for the $\Delta p\mathrm{CO_2}$ calculation (equations 1 and 2). We used this approach to avoid the impact of short-term variations in pressure, such as storms, that might not be equally distributed between float and shipboard datasets. The mean ± 1 SD correction to SLP was -0.7 ± 13.9 mbar (in situ SLP minus climatological SLP), which equated to a $\Delta p\mathrm{CO_2}$ correction of -0.8 ± 5.3 μatm ($\Delta p\mathrm{CO_2}$ calculated using in situ SLP minus $\Delta pCO_2$ using climatological SLP). While the average correction is small, this ensures that there are no large differences in $\Delta pCO_2$ due to short-term pressure variations.

**Text S3. Crossover comparison between SOCAT and float $pCO_2$.**

Prior studies comparing shipboard $pCO_2$ from the SOCAT dataset and float pH-derived $pCO_2$ found that SOCCOM float $pCO_2$ estimates might be high by approximately 4 μatm (Williams et al. 2017; Fay et al. 2018; Gray et al. 2018). Here we perform an updated crossover comparison between the May 2021 SOCCOM snapshot and the Surface Ocean $CO_2$ Atlas v2021 (SOCAT; Bakker et al. (2016)). Crossovers were determined by finding float profiles and SOCAT measurements within ± 1 day and ± 25 km (n=87). Only crossover comparisons with a density difference less than 0.03 kg $m^{-3}$ were used for this analysis (Fig. S3, n=52). $pCO_2$ values were recalculated using CO2SYS (van Heuven et al. 2011) to account for any temperature difference between matched observations. The mean difference between SOCAT and SOCCOM $pCO_2$ was -1.86 ± 15.8 μatm (SOCAT minus SOCCOM).

**Text S4. Biogeochemical Southern Ocean State Estimate**

Interannual variability of biogeochemical properties in the Pacific and central and southeast Pacific sub-regions was assessed using BSOSE. BSOSE mean winter (August and September) ML oxygen concentrations of SAMW formation areas in all regions maintained a fairly consistent negative (undersaturated) $\Delta[O_2]$ of ~11 μmol $kg^{-1}$ with an $[O_2]$ range of 285-301 μmol $kg^{-1}$ (Fig. S4). Comparable annual averages from float observations display a similar $\Delta[O_2]$, though with a lower range in $[O_2]$ of 273-295 μmol $kg^{-1}$. $[O_2]_{saturation}$ as a function of temperature (constant S=34.2) is plotted with no correction for sea level pressure (black dashed line) and with a correction for mean winter SLP at the float profile locations (gray dot-dashed line, calculated from NCEP pressure reanalysis as described in Text S2).

BSOSE Pacific biogeochemical averages were determined from 3-D fields at locations where August or September MLD estimates are deeper than 150 m. This threshold was chosen to exclude shallower mixed layers that are not associated with SAMW formation, but at the same time to ensure we consider a continuous band of deep wintertime mixed layers. Anomalies of meridional averages reveal west to east propagation (Fig. S5). Together with local forcing, this advective signal plays an important role in governing both overall Pacific and east-west differences in interannual variability.

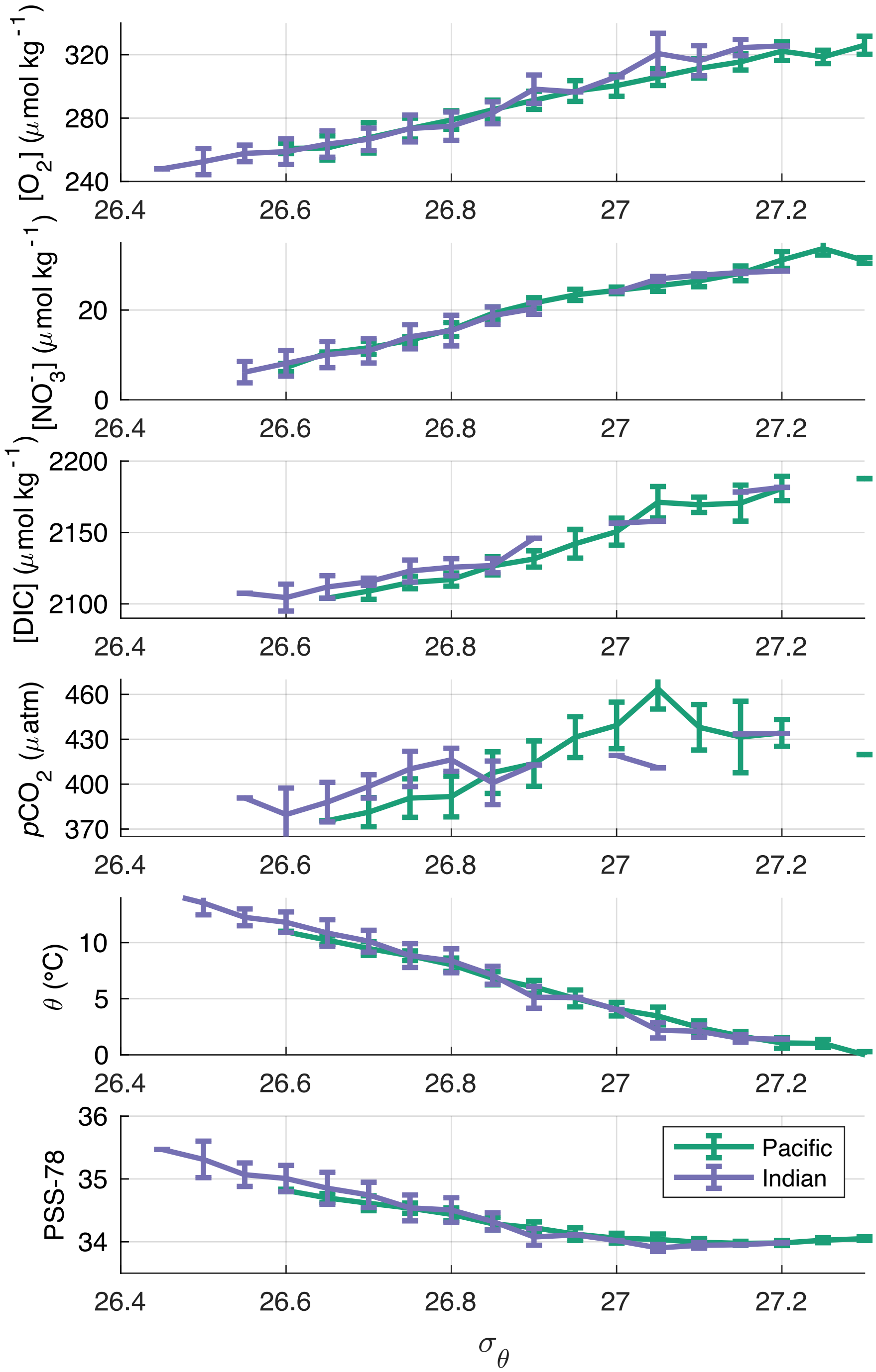


**Figure S1. Overlaid wintertime property vs. density relationships for the Pacific and Indian Ocean sectors.** Properties are August and September mixed layer averages, gridded by density. Only mixed layers deeper than 200 m are included.

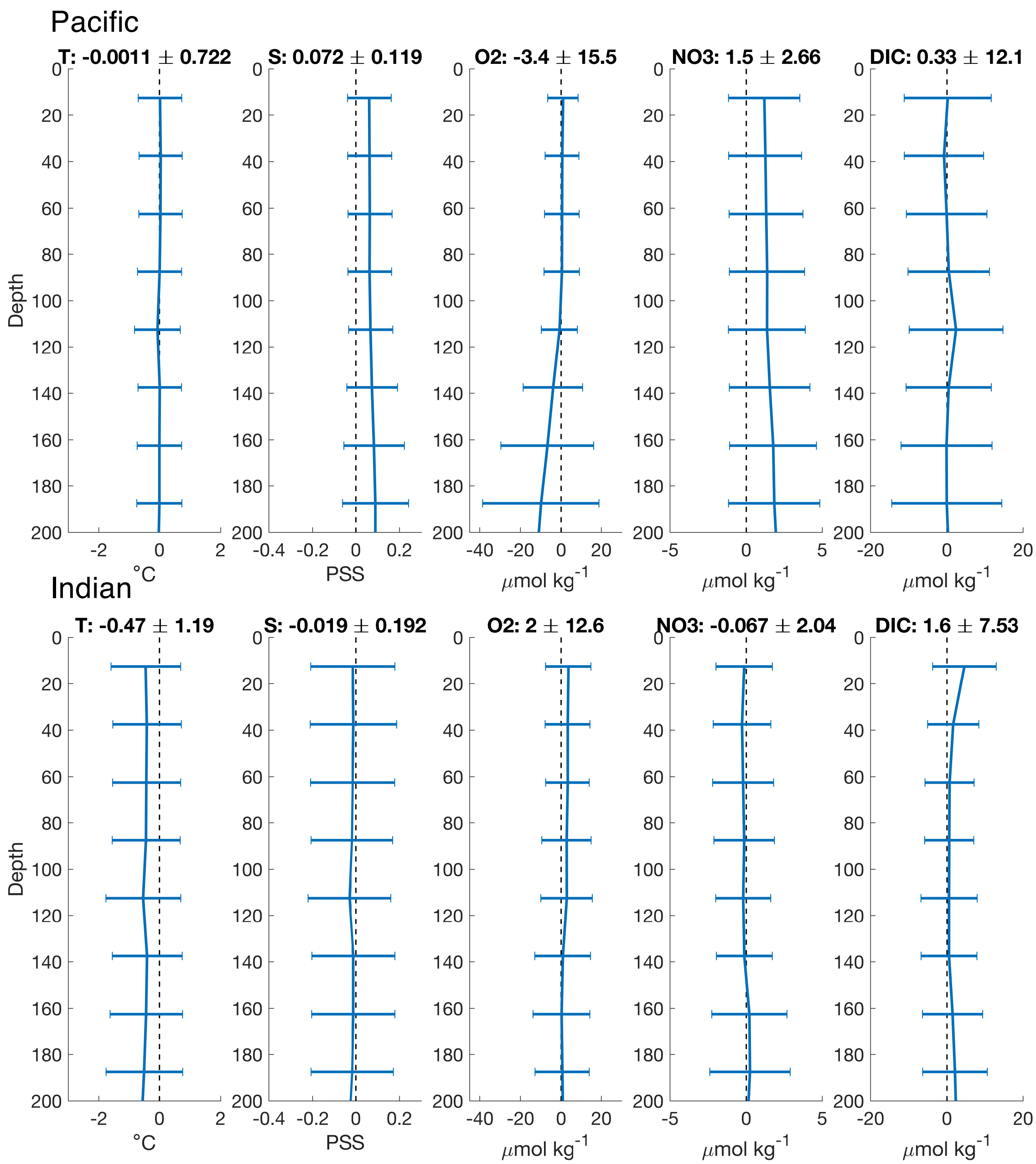


**Figure S2. Mean differences between BSOSE output sampled at float locations and float observations of temperature (T), salinity (S), oxygen (O2), nitrate (NO3), and dissolved inorganic carbon (DIC).** Differences shown are BSOSE minus float, averaged in 25m depth bins with error bars indicating RMSE for each bin. Panel titles contain average mean ± average RMSE for upper 200 m. Data are only shown for August and September profiles when calculated MLD is at least 200 m using the same geographic criteria as described in Section 2. BSOSE comparison data are available at: http://sose.ucsd.edu/SO6/ITER135/PROF/.

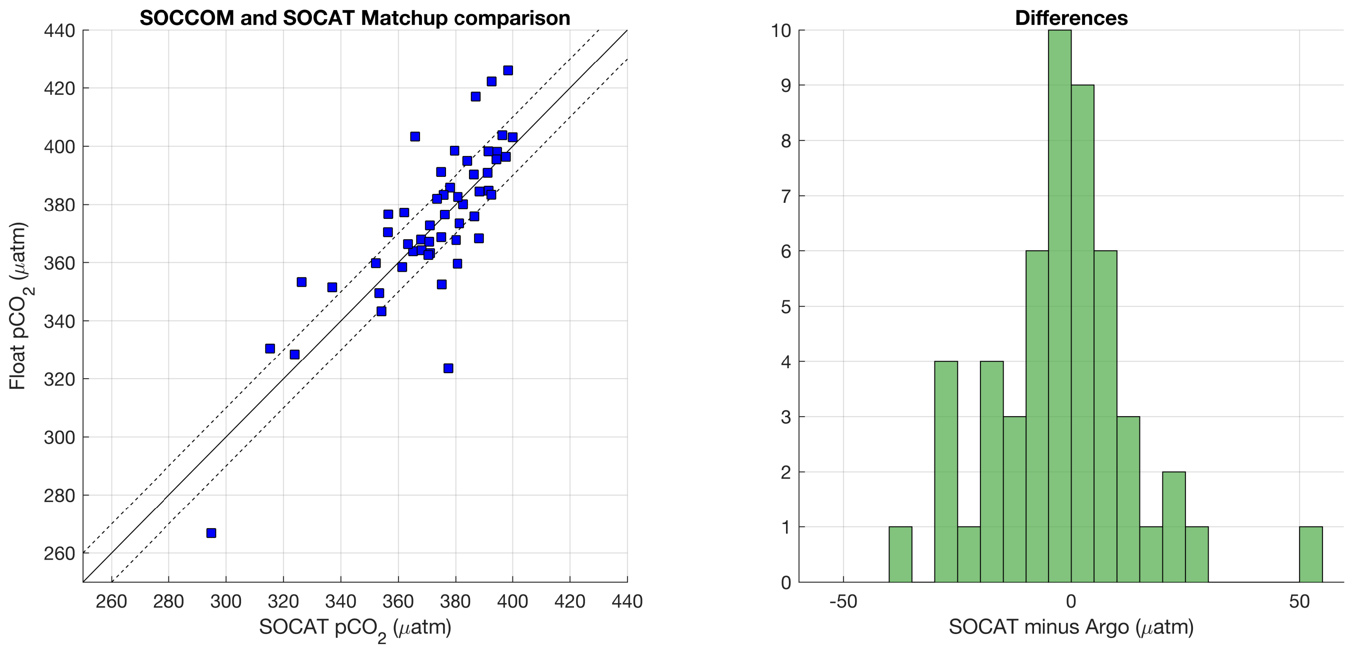


**Figure S3. Crossover comparison of float and SOCAT *p*$CO_2$.** Float and ship crossovers are identified by finding observations within ± 1 day and ± 25 km. Float *p*$CO_2$ estimates are averages of data shallower than 10 db. SOCAT *p*$CO_2$ data are the mean of all measurements within the search criteria. Crossovers with a density different greater than 0.03 kg $m^{-3}$ were removed (original n=87, n=52 after density filtering, left, blue squares). Solid black line is 1:1 line, dashed lines are ± 10 μatm. Mean SOCAT – Argo *p*$CO_2$ is -1.86 ± 15.8 μatm (right).

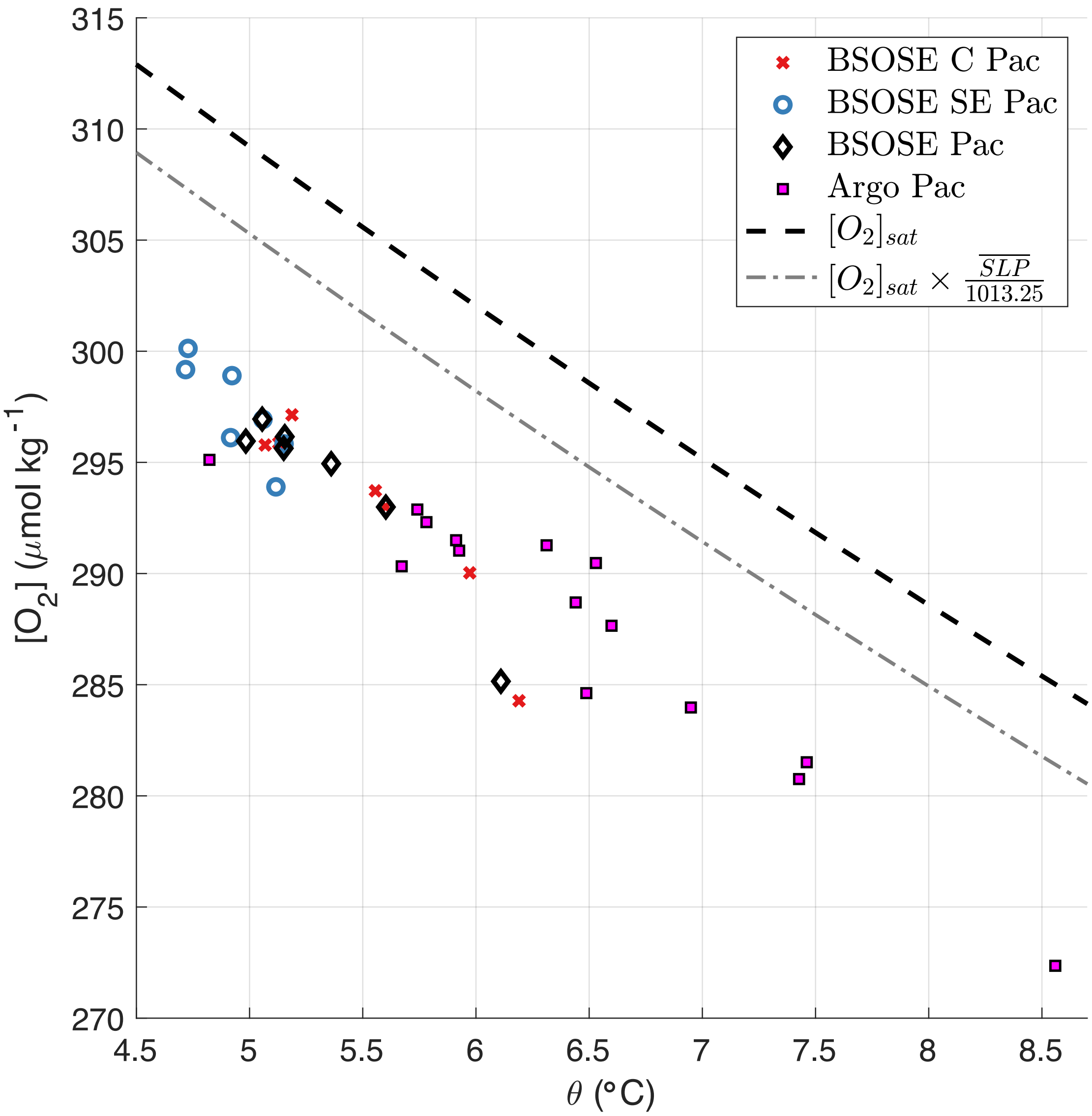


**Figure S4. Winter oxygen concentration vs. potential temperature for Pacific and Pacific sub-region core formation properties.** Yearly BSOSE winter (August and September) mixed layer average oxygen concentrations from the central, southeast, and overall Pacific from the available 2013-2019 output (red "x", blue "o", and black diamond symbols, respectively). Black dashed line is solubility calculated from temperature with a fixed salinity of 34.2 and gray dot-dashed line is the solubility corrected for mean SLP in the wintertime Pacific SAMW formation regions. Magenta squares are averages of float observations for the overall Pacific.

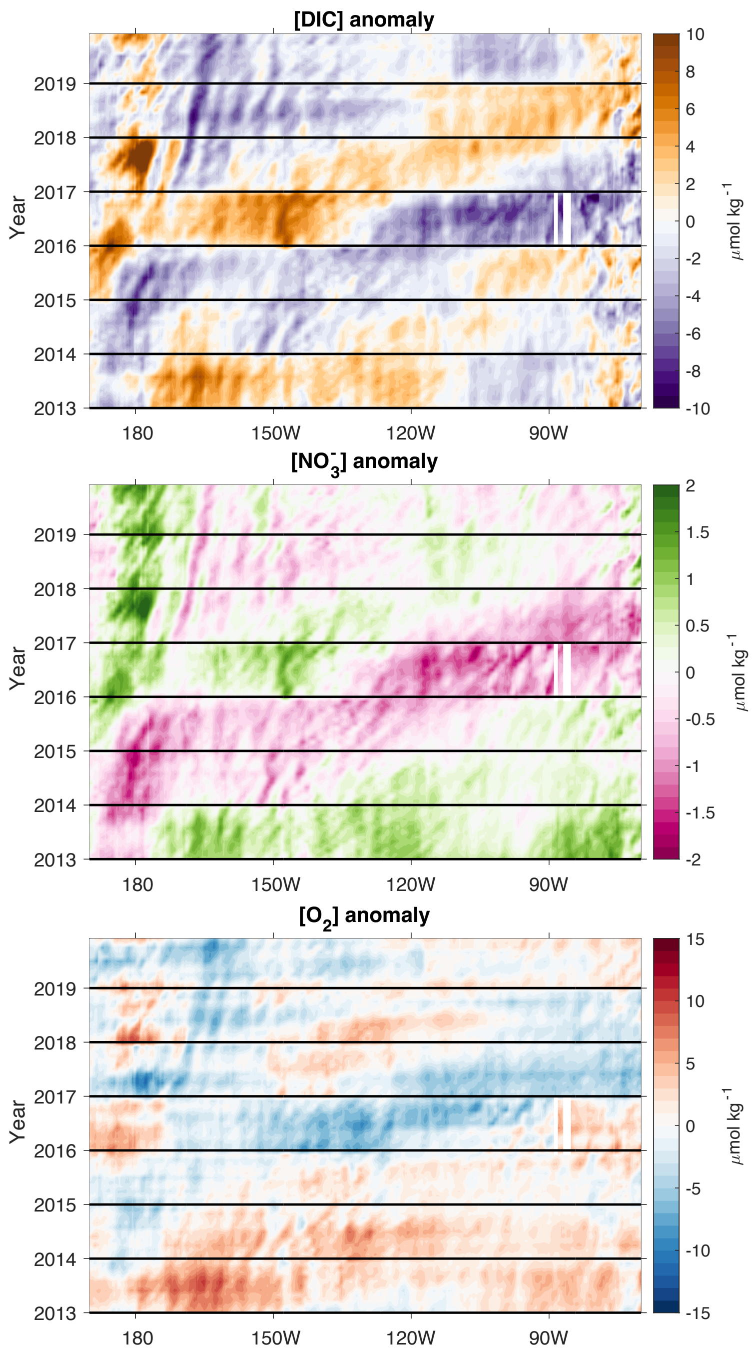


**Figure S5. Hovmöller diagrams of BSOSE Pacific [DIC], [$NO_3^-$], and [$O_2$] anomalies.** Meridional averages were constructed from 3-D fields masked using August-September MLDs when MLs were deeper than 150 m. The slightly shallower ML threshold (relative to the 200 m threshold used for determination of preformed SAMW properties) allowed consideration of a circumpolar band in order to follow the propagating signal. A 200 m. threshold shows a similar pattern but with more data gaps.

**Table S1**

| Float UW SN | WMO # | Profile (sample number)[1] | Parameters affected |
|---|---|---|---|
| 3900345 | 5027 | 162 - end | $O_2$, Salinity |
| 5901043 | 5020 | 109 | $O_2$ |
| 5901046 | 2342 | 177 | $O_2$, Salinity |
| 5901047 | 5004 | 41 | $O_2$ |
| 5901049 | 2343 | 70 | $O_2$ |
| 5901051 | 2344 | 63 - 65 | $O_2$ |
| 5901310 | 5085 | 119 - end | $O_2$, Salinity |
| 5901313 | 5086 | 182 | $O_2$ |
| 5901736 | 5302 | 94 - end | $O_2$, Salinity |
| 5902100 | 5333 | 48 - end | $O_2$, Salinity |
| 5903382 | 6643 | 53 - end | $O_2$ |
| 5904179 | 6091 | 125 | $O_2$ |
| 5904184 | 9091 | 122(3) | pH and derived vars. |
| 5904657 | 9662 | 56, 82 | pH and derived vars. |
| 5904660 | 9652 | 38 | pH and derived vars. |
| 5904679 | 9757 | 83, 102 | pH and derived vars., Salinity |
| 5904686 | 510 | 101 | pH and derived vars. |
| 5904761 | 9660 | 16, 17, 20, 28, 56, 59 | pH and derived vars. |
| 5904844 | 9766 | 21 | pH and derived vars. |
| 5904984 | 569 | 34 | $O_2$ |
| 5905070 | 12537 | 109 | $O_2$ |
| 5906221 | 18796 | 25 | $O_2$ |

[1] Sample number is the float sample relative to the value nearest the surface (1). If no sample number is listed, the entire profile was set to NaN values.