Global Biogeochemical Cycles

Supporting Information for

Quantifying net community production and calcification at Station ALOHA near Hawai'i: Insights and limitations from a dual tracer carbon budget approach

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Introduction

This supporting information contains further details on methodologies used for the gas exchange term in Method A (Text S1) and a description of all alternative methods listed in Table 1 of the main text for sensitivity checks (Text S2).

Supplemental figures can be consulted to further illustrate mixed layer (Figure S1, Movie S1-2) and horizontal transport dynamics (Figure S3), and for results of the sensitivity checks (Figures S4-6).

Text S1. Gas exchange term: Detailed calculation

1.1. Data:

pCO_2sw and pCO_2air, SST, SSS (3-hourly) and wind speed data (hourly average) are all taken from WHOTS mooring sensors. pCO_2sw is normalized to a salinity of 35.

1.2. Wind speed:

The speed at 10m above sea level (U10) calculation is done using z=3.4m (an average of deployments) for measurement height, and a rolling 3-hour mean of hourly measurements to match pCO_2 temporal resolution.

$$U10 = (10/z)^{1/7}$$

1.3. CO_2 solubility:

CO_2 solubility (α) in mol/L atm is calculated from Weiss, (1974), with SST in K

$$\alpha = e^{90.5069*\left(\frac{100}{SST}\right)-58.0931+22.2940*\log\left(\frac{SST}{100}\right)+SSS*\left(0.027766-0.025888*\left(\left(\frac{SST}{100}\right)+0.0050578*\left(\left(\frac{SST}{100}\right)*\left(\frac{SST}{100}\right)\right)\right)\right)}$$

1.4. Schmidt Number:

The Schmidt number (Sc) calculation is taken from Wanninkhof et al. (1992), with SST in°C

$$Sc = 2073.1 - 125.62 * SST + 3.6276 * SST^2 - 0.043219 * SST^3$$

1.5. Piston velocity:

Piston velocity (k) in cm/hr is calculated from Ho et al. (2006) as

$$k = (0.266 * U10^2) * \left(\frac{Sc}{660}\right)^{-0.5}$$

1.6. CO_2 flux & DIC flux:

CO_2 flux is calculated in cm mol µatm hr^{-1} L^{-1} atm^{-1}; then converted to mol C m^{-2} hr^{-1}

$$F = \left((\alpha * k * \Delta pCO_2)/10^6\right) * 10$$

Then, units are further adjusted to get from *moles of C per hour* to *monthly change in µmol/kg DIC*:

1. Daily mean value of mol C/m^2hr; multiplied by 24 hr/day → mol C/m^2day
2. Monthly mean value of mol C/m^2day; multiplied by days/month for each month → mol C/m^2 month
3. Multiplied by monthly MLD values to convert m^2 to m^3; convert mol to µmol and include density in kg/m^3:

$$F_{DIC}(\mu mol/kg) = F_{mol\ C}(mol/m^2) * 10^6(\mu mol/mol)/\left(MLD(m) * \rho(kg/m^3)\right)$$

Text S2. Alternative methods/sensitivity analysis

2.1 Seasonality in current speeds and gradients

AVISO long-term (1993-present) climatology (mean ± SD) of meridional (a) and zonal (b) current speeds is plotted in Figure S4, showing that there is no significant seasonal component in current speed variability. Climatologies of meridional and zonal TA and DIC gradients at ALOHA from Broullón et al. (2019, 2020) are also shown in Figure S4 for DIC (c) and TA (d). The larger meridional gradients are reduced to about 30% when normalizing to salinity (Figure S4 e, f), while zonal gradients of sDIC & sTA are of the same order of magnitude as DIC & TA.

2.2 Eddy diffusivity: Heat budget

Following Cronin et al. (2015), a heat budget for the mixed layer can be written as:

$$\rho_0 C_p h \frac{\partial T}{\partial t} = Q_0 - Q_{pen}\Big|_{z=-h} - \rho_0 C_p h \boldsymbol{u} \cdot \nabla T - \rho_0 C_p \left(w_{-h} + \frac{dh}{dt}\right)(T - T_{-h}) - \rho_0 C_p \overline{w'T'}\Big|_{z=-h}$$

Where $\rho_0 C_p$ is the volumetric heat capacity of seawater, 4.088 x 10^6 J °C^{-1} m^{-3}, h is the mixed layer depth, T is the temperature averaged over the mixed layer, Q_0 is the net downward surface heat flux in W m^{-2} and Q_{pen} is the radiative flux through the base of the mixed layer (in W m^{-2}), $\boldsymbol{u}$ is the current speed averaged over the mixed layer, ∇T is the horizontal temperature field, w_{-h} is the vertical (upward) current speed at the base of the mixed layer, T_{-h} is the temperature at the base of the mixed layer, and $\overline{w'T'}\Big|_{z=-h}$ is the diffusive heat flux across bottom of the mixed layer. The equation can be rearranged to solve for the diffusive heat flux to yield:

$$\overline{w'T'}\Big|_{-h} = \frac{Q_0 - Q_{pen}\Big|_{z=-h}}{\rho_0 C_p} - h\boldsymbol{u} \cdot \nabla T - \left(w_{-h} + \frac{dh}{dt}\right)(T - T_{-h}) - h\frac{\partial T}{\partial t}$$

Terms 1-3 describe surface heat flux, horizontal advection, and vertical transport, respectively. To appropriately resolve the physical reality of the processes in question that is relatively short-term and small-scale (on the order of days for Ekman pumping and eddies, and on the order of ≤ 100km for eddies), but attain the desired monthly-frequency data and avoid the high-frequency up-and-downs of mixed layer depth at that time scale, temporal averaging is executed as follows.

For term 1, $\frac{Q_0 - Q_{pen}\big|_{z=-h}}{\rho_0 C_p}$, Q_0 is averaged monthly, and then Q_{pen} is calculated monthly. For term 2, $h\boldsymbol{u} \cdot \nabla T$, $\boldsymbol{u} \cdot \nabla T$ is evaluated daily, then averaged monthly and multiplied by h. For term 3, $\left(w_{-h} + \frac{dh}{dt}\right)(T - T_{-h})$, w_{-h} is calculated daily, then averaged monthly and the whole term evaluated monthly. $-h\frac{\partial T}{\partial t}$ is evaluated monthly. Input data for the heat budget are listed in Table S1.

2.2.1 Term 1: Surface heat flux

Q_0 is available at daily resolution from the WHOI UOP group (http://uop.whoi.edu/ReferenceDataSets/whotsreference.html)and averaged monthly. Q_{pen} is taken to be 0.38 x $Q_{shortwave}$ x $e^{(2\lambda)}$, with λ = 20m, and is a very small term (Cronin et al., 2015).

2.2.2 Term 2: Horizontal advection

Zonal and meridional current speeds, $\boldsymbol{u}$, are calculated from depth-interpolated current data from WHOTS mooring ADCPs, averaged over the mixed layer. Data gaps are filled in with WHOTS mooring VMCMs at 10m and 30m. The meridional and zonal mixed layer temperature gradient, ∇T is approximated as the SST gradient, and evaluated daily from a high resolution (9km) Optimally-Interpolated SST (from microwave and infrared) satellite product from Remote Sensing Systems[1]. Maximum current speeds are up to 50 km day^{-1} zonally and meridionally, so the satellite SST field was averaged to a 0.25° spatial resolution. $\boldsymbol{u} \cdot \nabla T$ was calculated daily and then averaged monthly, and then multiplied by the monthly mean MLD (h).

2.2.3 Term 3: Vertical transport

Vertical velocity at the base of the mixed layer, w_{-h}, was approximated as the Ekman pumping velocity, calculated from the curl of the wind stress field, ignoring geostrophic convergence and divergence in the mixed layer (due to the multi-year time scale at which the Sverdrup balance holds true):

$w_{-h} \approx \frac{\nabla \times \left(\frac{\tau}{f}\right)}{\rho}$, where τ is wind stress, f is the Coriolis parameter, and ρ is density. Daily ASCAT wind stress data was downloaded from APDRC[2]. Since this product is only available starting March 2007, 2004-2007 were added from the NCEI Blended Sea Winds product[3]. Wind stress is reported in Pa on a daily, 0.25° grid. The velocity was evaluated daily at the grid point nearest Station ALOHA (22.75°N, -158°W) and then averaged monthly. The temperature gradient within the mixed layer was defined as the temperature at the mixed layer base subtracted from average mixed layer temperature.

2.2.4 Residual term and diffusivity

The residual of the heat budget, $\overline{w'T'}\big|_{-h}$ contains diffusive fluxes, as well as unconstrained processes and errors. κ is estimated as $\kappa = \frac{-\overline{w'T'}\big|_{-h}}{\frac{\partial T}{\partial z}\big|_{z=-h}}$ (Cronin et al., 2015). Since diffusive fluxes are usually downgradient, diffusivity should be positive, and the negative values are due to the uncertainty in the calculation. However, just removing any negative values would bias the result, so the negative values are included. A seasonal climatology of κ from the heat budget calculation is shown in Figure S5.

2.3. Evaporation–Precipitation: Explicit calculation vs. salinity normalization

2.3.1. Explicit calculation

$$\Delta DIC_t|_{E-P} = DIC_{t-1} \times \frac{(E-P)_t}{h_{t-1}}$$

Evaporation (E) and precipitation (P) are estimated from WHOTS mooring ASIMET meteorological sensors[4].

Evaporation is calculated as

$$E = \frac{Q_H}{Lv}$$

[1] http://data.remss.com/SST/daily/mw_ir/v05.0/netcdf/

[2] http://apdrc.soest.hawaii.edu/erddap/griddap/hawaii_soest_a6ab_91f7_b38f.html

[3] https://www.ncdc.noaa.gov/data-access/marineocean-data/blended-global/blended-sea-winds

[4] From http://uop.whoi.edu/currentprojects/WHOTS/whots.html

Where Q_H is the latent heat flux, and Lv is the latent heat of vaporization, 2.26 * 10^6 J/kg. Latent heat flux and precipitation are reported hourly and available from IFREMER[5].

2.3.2. Salinity normalization

For this approach, each term of the carbon budget is normalized to a salinity of 35:

$$DIC_n = \frac{DIC}{Sal} \times 35$$

[5] http://tds0.ifremer.fr/thredds/catalog/CORIOLIS-OCEANSITES-GDAC-OBS/DATA_GRIDDED/WHOTS/catalog.html

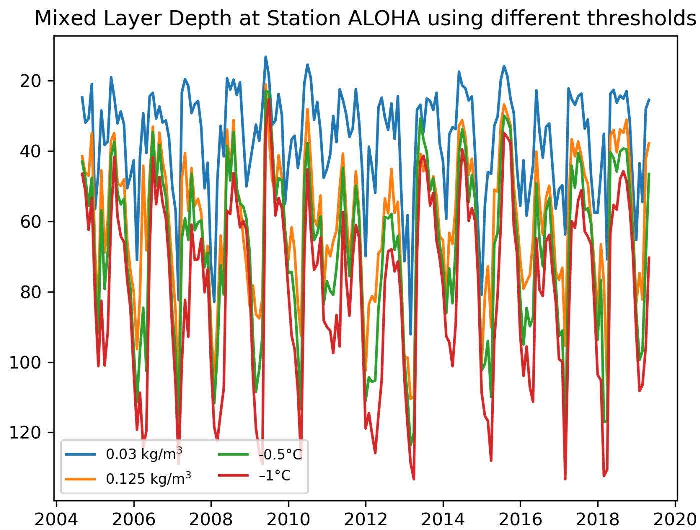


Figure S1. Mixed layer depth estimated from different criteria.

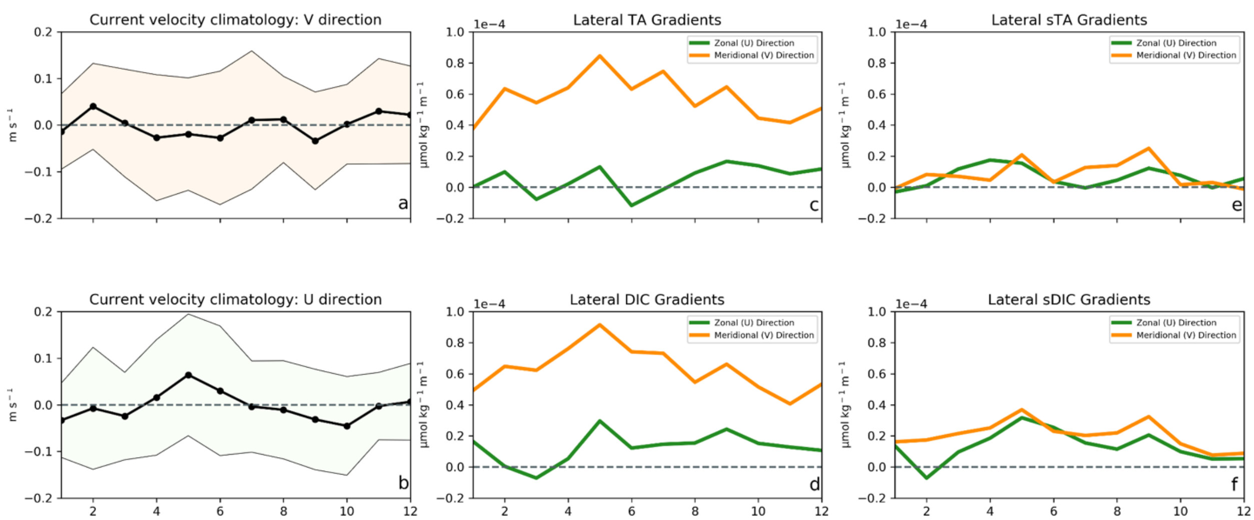


Figure S2. Current velocity climatology ± 1 SD from the WHOTS mooring ADCP (S3a, b), lateral gradients from Broullón et al. (2019, 2020) in DIC and TA (S3c, d), and these same gradients normalized to salinity 35 (S3e, f).

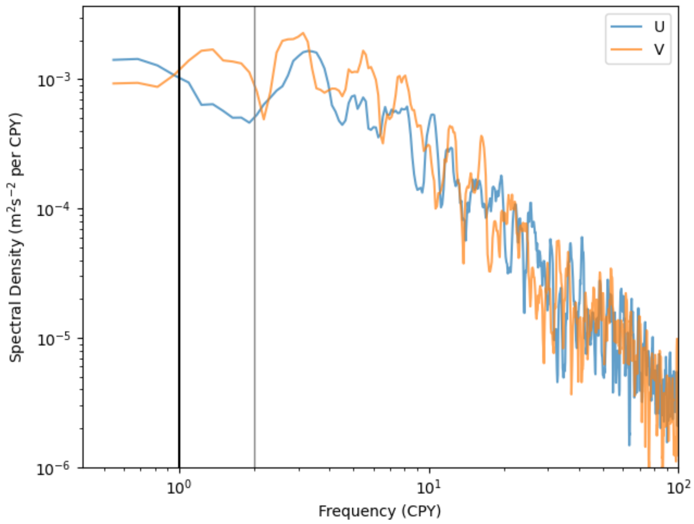
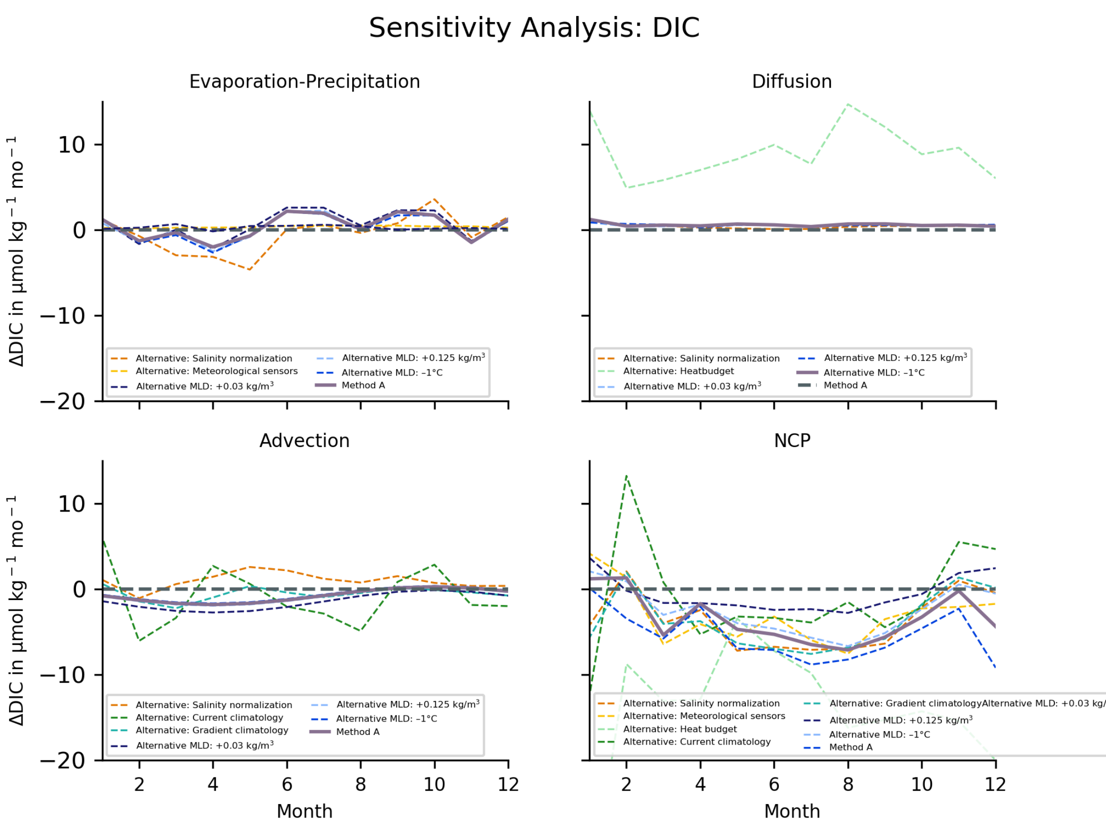


Figure S3. Power spectrum of WHOTS ADCP meridional and zonal current speeds. The black vertical line is at the annual frequency; the lighter vertical line is at the semiannual frequency.



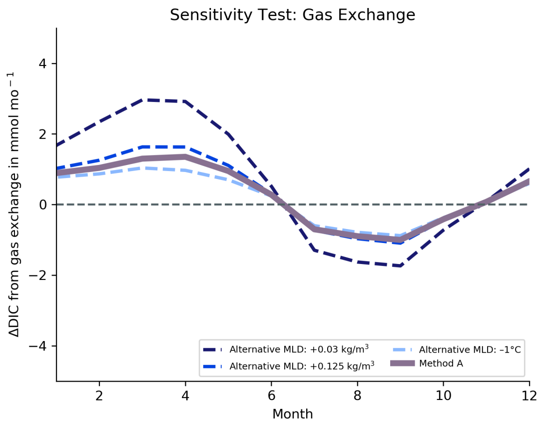


Figure S4a. Sensitivity test for all different methodologies and resulting average rates for model terms of the DIC budget.

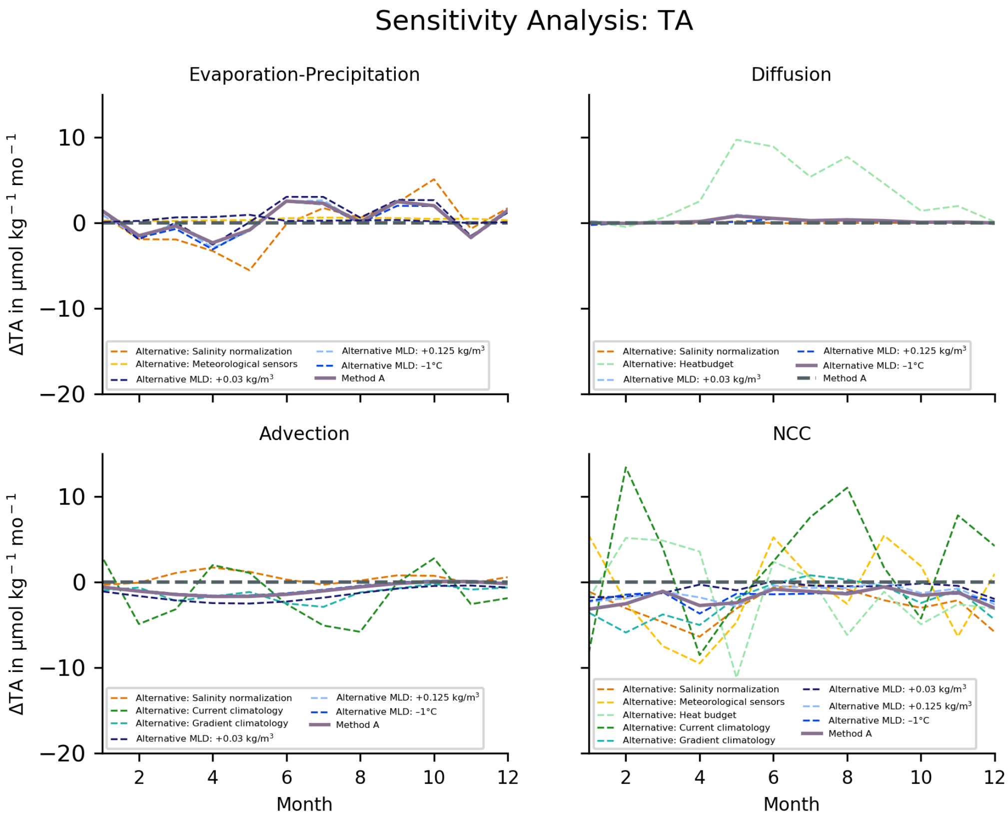


Figure S4b. Sensitivity test for all different methodologies and resulting average rates for model terms of the TA budget.

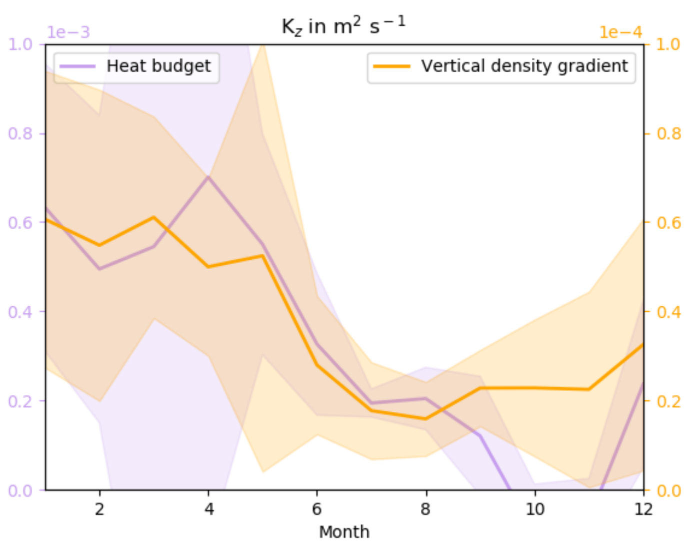


Figure S5. Annual climatology ± 1 SD of eddy diffusivity estimated with a heat budget calculation (from Cronin et al., 2015) or a vertical density gradient (Keeling et al., 2004).

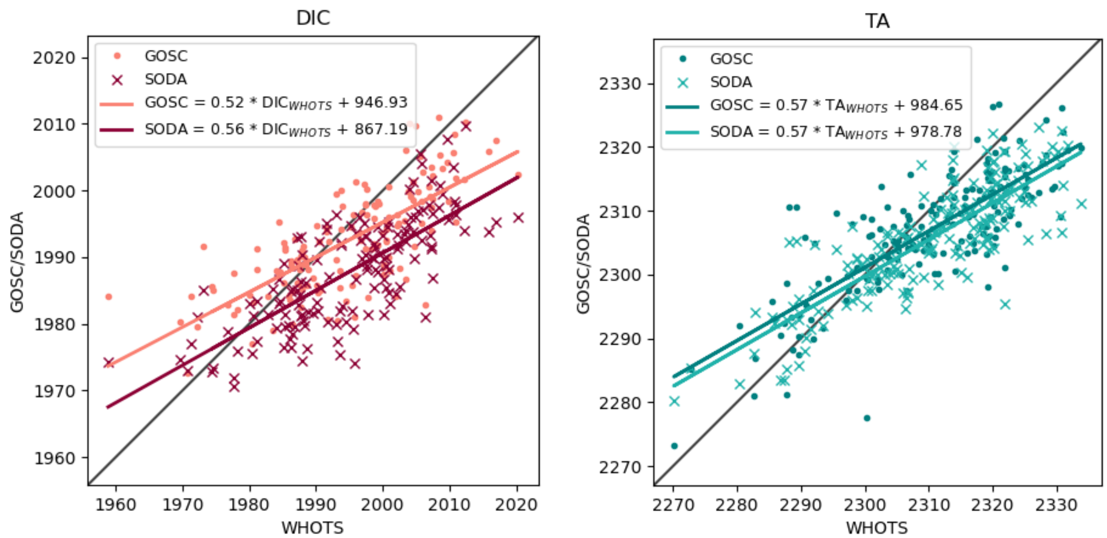


Figure S6. Regression of DIC and TA estimated in this study compared to GOSC (Chau et al., 2022) and Ocean-SODA-ETHZ (Gregory & Gruber, 2021). The black line is the 1:1 line.

Study	**K_z ($m^2\ s^{-1}$)**	**Source/Methodology**	**Timeframe**
Ferrón et al. (2021)	0.5 x 10^{-4}	Quay & Stutsmann (2003)	non-varying
Hamme & Emerson (2006)	0.1 – 1 x 10^{-4}	Range of literature values	
Quay & Stutsmann (2003)	0.5 x 10^{-4}	Inferred from tracer budget	non-varying
Keeling et al. (2004)	0.1 – 0.4 x 10^{-4}	Density gradients after Denmann & Gargett (1983)	Seasonal climatology
This study	0.01 – 0.7 x 10^{-3}	Heat budget after Cronin et al. (2015)	Seasonal climatology

Table S1. Reported estimates of eddy diffusivity.

Symbol	**Quantity**	**Calculation/Source**	**Units**
h	Mixed layer depth	Monthly maximum of MLD calculated as first maximum curvature of density profile, from daily stratification data (WHOTS CTDs) (Lorbacher et al., 2006).	m
T	Temperature (avg. over ML)	WHOTS CTDs (every 15m).	°C
∇T	Horizontal temperature field	Satellite SST field from RSS (daily, 0.25°).	°C/s

$\rho_0 C_p$	Volumetric heat capacity of SW	Taken to be 4.088 x 10^6	J/°C/m^3
Q_0	Downward surface heat flux	WHOTS meteorological instruments. Available on WHOTS UOP website.	W/m^2
Q_{pen}	Radiative flux through base of ML	Taken to be 0.38 x Q_{sw} $e^{(2\lambda)}$; λ = 20m .	W/m^2
u	Current speed (avg. over ML)	Depth-interpolatedWHOTS ADCPs @48 & 115m (gaps filled with VMCMs @10 & 30m).	m/s
w_{-h}	Vertical (upward) current speed @ base of ML	From wind stress curl (ASCAT (2007-2018), NCEI (2004-2007).	m/s
T_{-h}	Temperature @ base of ML	WHOTS CTDs (every 15m) interpolated to h.	°C
w'T'	Residual, diffusive heat flux	Residual term, including all errors.	W/m^2

Table S2. Terms, units and definitions of the heat budget calculation adapted from Cronin et al., (2015).

Movie S1. Interpolated DIC profiles ± measurement uncertainty from HOT samples in the upper 200m and average monthly MLD calculated using a -0.5°C temperature criterion.

Movie S2. Interpolated DIC profiles ± measurement uncertainty from HOT samples in the upper 200m and average monthly MLD calculated using a -0.5°C temperature criterion.