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Global Biogeochemical Cycles

Supporting Information for

Calculating surface ocean pCO₂ from biogeochemical Argo floats equipped with pH: an uncertainty analysis

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Text S1.

Equation for SOCCOM-specific TA algorithm (see Table S1 for coefficients):

 $TA = \beta_0 + \beta_1 \sigma_\theta + \beta_2 O_2 + \beta_3 S + \beta_4 T + \beta_5 P + \beta_6 gpan$

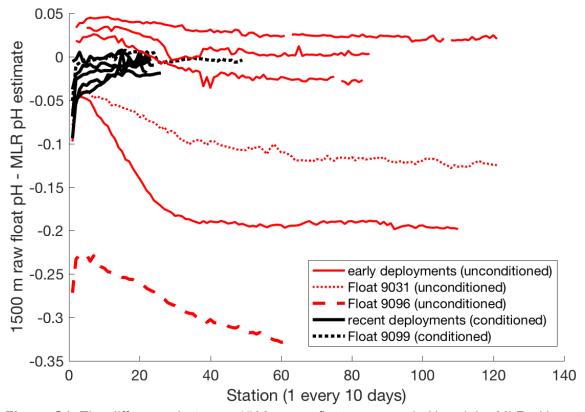


Figure S1. The difference between 1500 m raw float-measured pH and the MLR pH estimate (this difference is roughly equivalent to the cumulative offset column in Table 1) for unconditioned pH sensors from early deployments (red) and conditioned pH sensors from more recent deployments (black). The three of the four floats used in this study are differentiated by dashed or dotted lines.

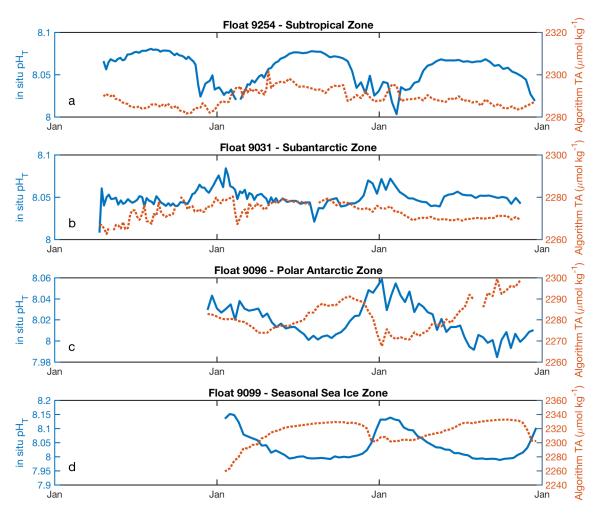


Figure S2. In situ pH (blue lines) and algorithm TA (red dashed lines) for SOCCOM floats 9254 (a), 9031 (b), 9096 (c), and 9099 (d).

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parameter	coefficient	value	\mathbb{R}^2	RMSE
constant	β_0	734.72		
$\sigma_{ heta}$	β_1	-15.478		
$O_2 \ (\mu mol \ kg^{-1})$	β_2	-0.11149		
S	β_3	59.752	0.981	4.3
T (°C)	β_4	-2.7905		
Р	β_5	0.013460		
gpan ^b (dynamic m)	β_6	-37.121		

Table S1. SOCCOM-specific TA MLR algorithm coefficients^a

^a fit using S4P 2011, P16S 2014, P18S 2007 south of 45 °S between 0-2100 m ^bgeopotential anomaly (at 50 m referenced to 1000 m) is a proxy for location relative to Antarctic Circumpolar Current fronts

 Table S2. Uncertainty in carbonate system equilibrium constants

K_0^{b}	$\mathbf{K_1}^{\mathbf{c}}$	K_2^{c}
-0.99	-0.99	-0.21
0.002	0.0075	0.015
0.50%	1.73%	3.45%
0.50%	1.71%	0.72%
	1.92%	
	-0.99 0.002 0.50%	-0.99 -0.99 0.002 0.0075 0.50% 1.73% 0.50% 1.71%

^a from Dickson and Riley [1978]

^busing K₀ from Weiss [1974]

°using K_1 and K_2 from Lueker et al. [2000]