



Supplement of

The Ocean Carbon States Database: a proof-of-concept application of cluster analysis in the ocean carbon cycle

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S3. Methodology

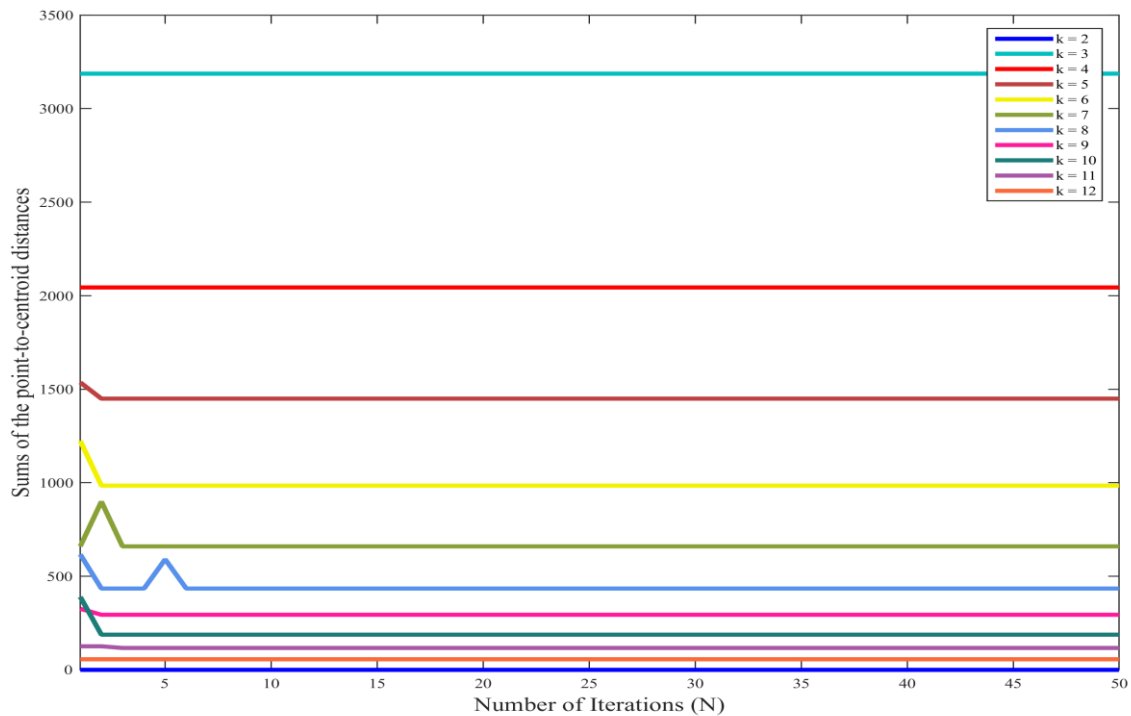


Fig. S1: Convergence test that shows the number of iterations needed so that clusters are unchanged. Each clustering analysis is performed for a different number of predetermined clusters (k) and is deemed as converging when the sum of the distances between each member 2D histogram from the cluster centroid is no longer changing. Convergence is tested for different number of predetermined clusters, k=1, k=2, ..., k=12. We find that less than 10 iterations are needed to obtain convergence.

S4. Results

S4.1 The North Atlantic Ocean Carbon States

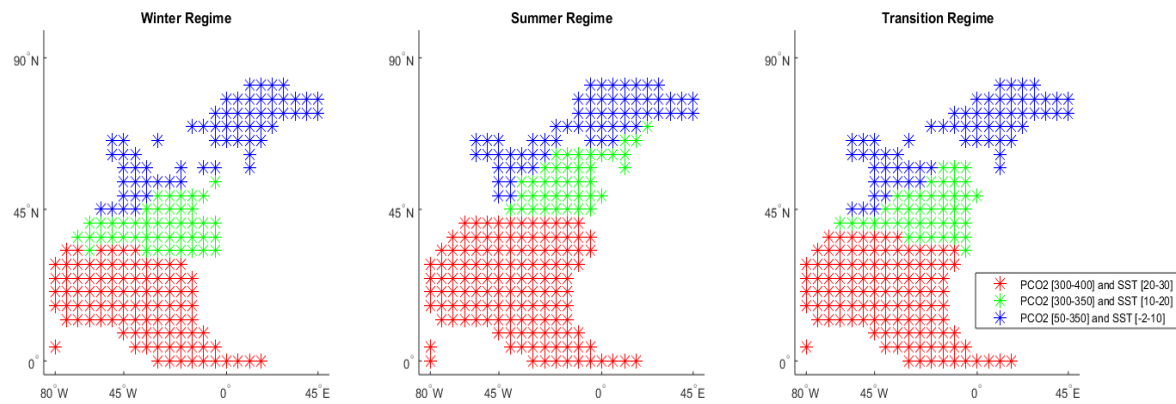
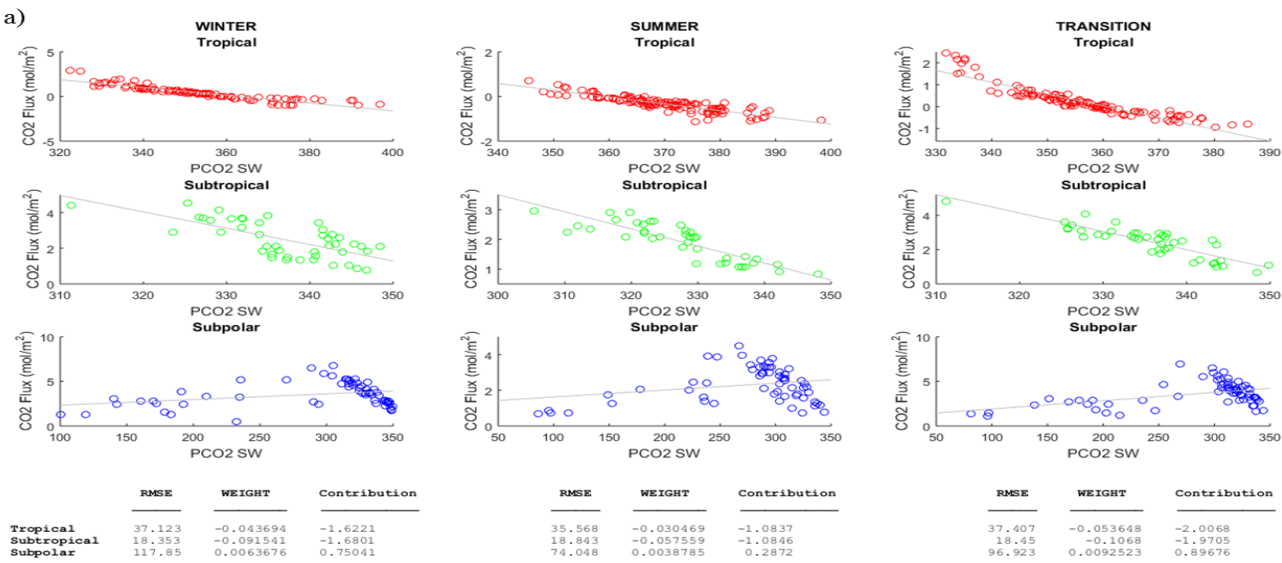
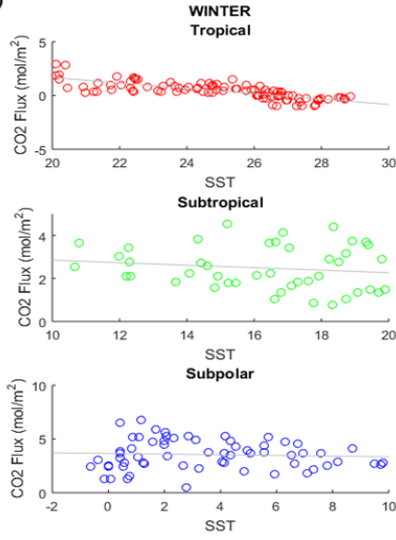


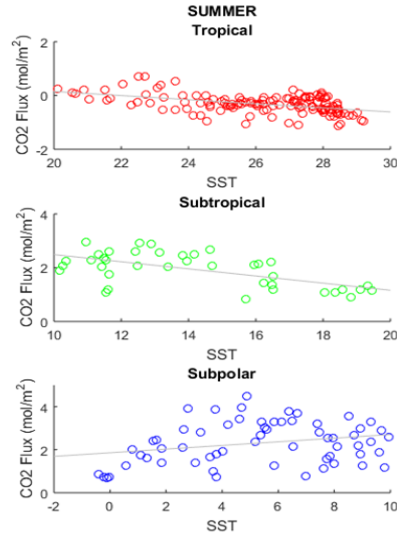
Fig. S2: Demarcated regions within the North Atlantic basin defined by ranges of $\text{pCO}_{2\text{SW}}$ and SST values in the observed ocean carbon states.



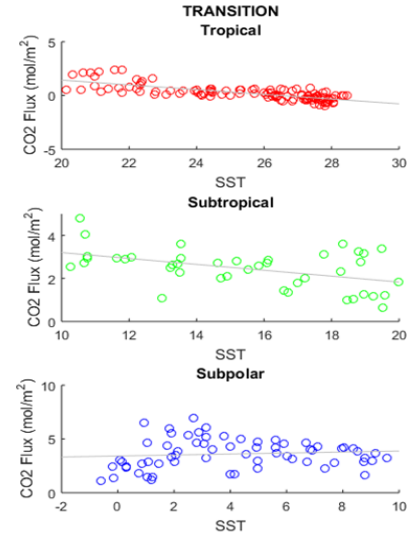
b)



	RMSE	WEIGHT	Contribution
Tropical	1.0468	-0.25058	-0.26232
Subtropical	1.1045	-0.058524	-0.064639
Subpolar	2.8934	-0.030098	-0.087086

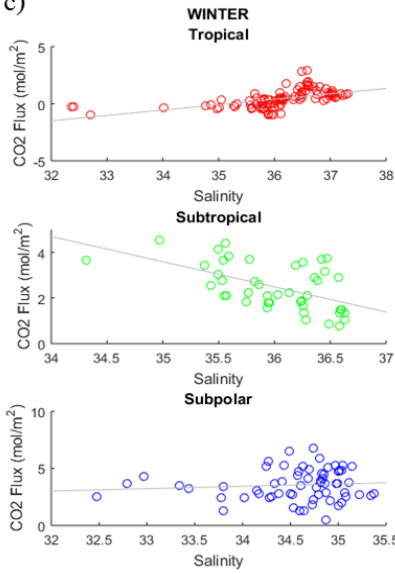


	RMSE	WEIGHT	Contribution
Tropical	1.4495	-0.076231	-0.1105
Subtropical	1.4735	-0.13263	-0.19542
Subpolar	3.4485	0.084806	0.29245

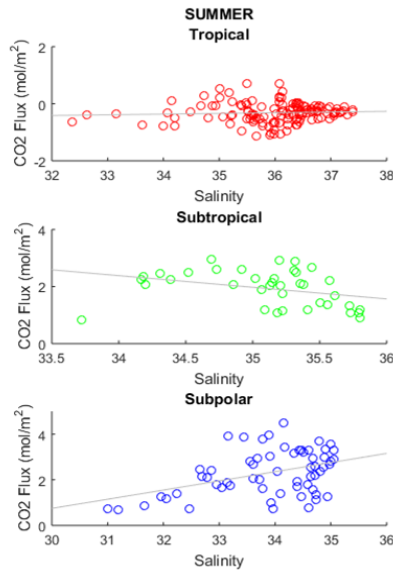


	RMSE	WEIGHT	Contribution
Tropical	1.0793	-0.22019	-0.23765
Subtropical	1.1242	-0.13694	-0.15395
Subpolar	2.9089	0.046045	0.13394

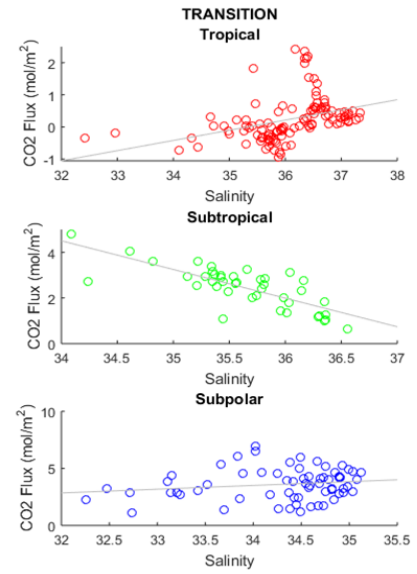
c)



	RMSE	WEIGHT	Contribution
Tropical	0.5883	0.47181	0.27757
Subtropical	0.40244	-1.1026	-0.44372
Subpolar	1.3832	0.20802	0.28773



	RMSE	WEIGHT	Contribution
Tropical	0.59543	0.024209	0.014415
Subtropical	0.44111	-0.40821	-0.18007
Subpolar	1.9603	0.40142	0.78691



	RMSE	WEIGHT	Contribution
Tropical	0.49914	0.31722	0.15834
Subtropical	0.49651	-1.2557	-0.62347
Subpolar	1.5649	0.32974	0.51601

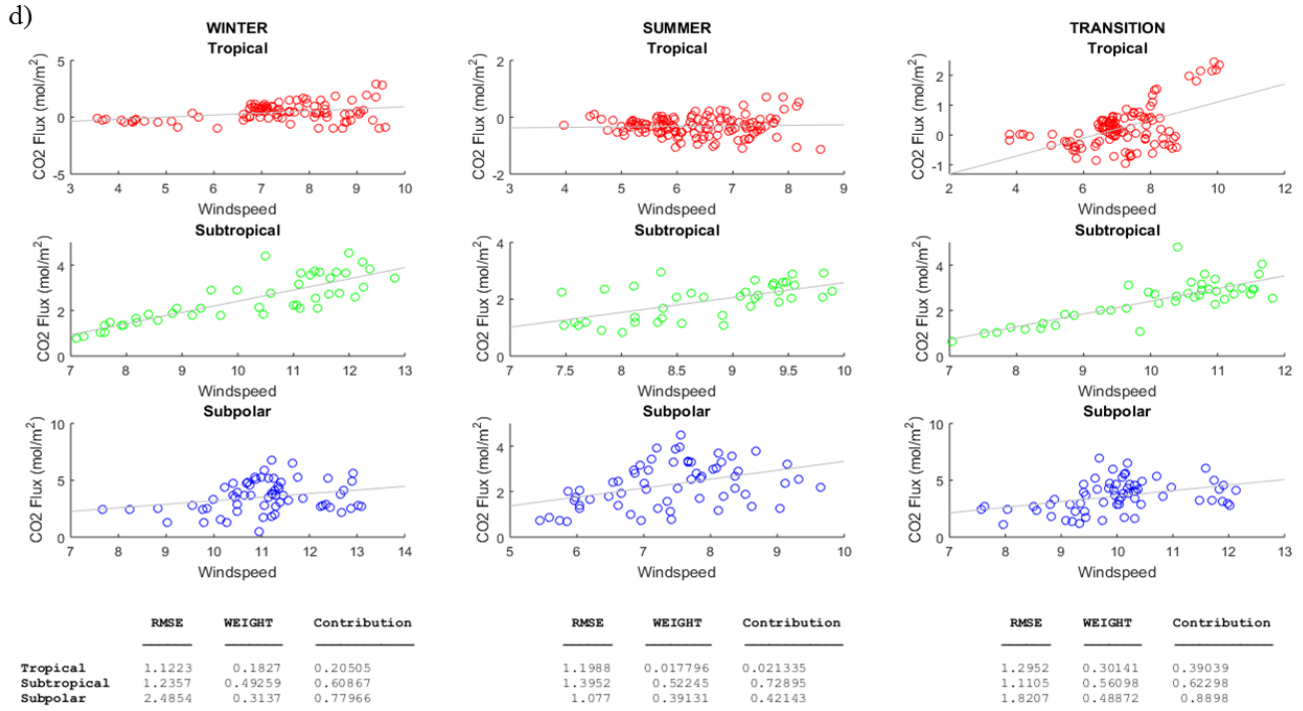
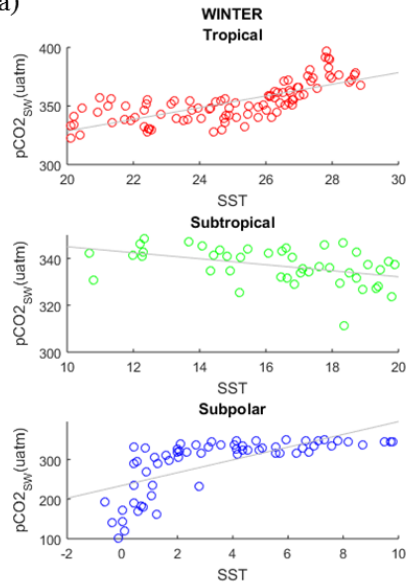
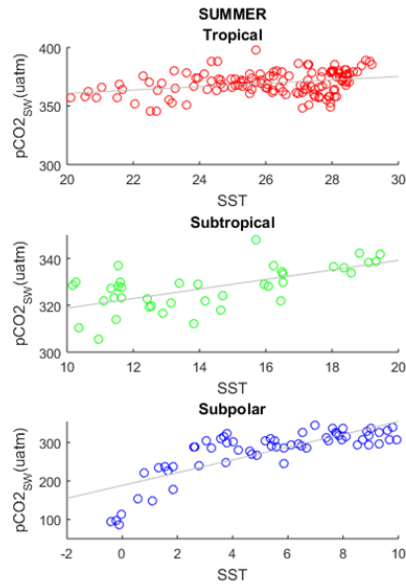


Fig. S3: Scatter diagrams and linear fits of the air-sea flux of CO₂ with a) pCO_{2sw}, b) SST, c) salinity, and d) wind speed in each of the North Atlantic regions that is represented in each regime. The regions are also shown in Fig. S2. The RMSE terms are the bias terms denoted as Δq and the weight terms are the $\frac{\partial F}{\partial q}$ terms in Eq. (5). The contribution terms are the products of each bias*weight terms in Eq. (5).

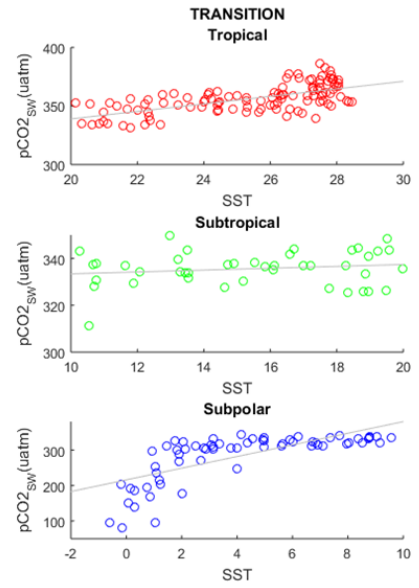
a)



	RMSE	WEIGHT	Contribution
Tropical	1.0468	4.9894	5.223
Subtropical	1.1045	-1.2823	-1.4162
Subpolar	2.8934	16.13	46.67

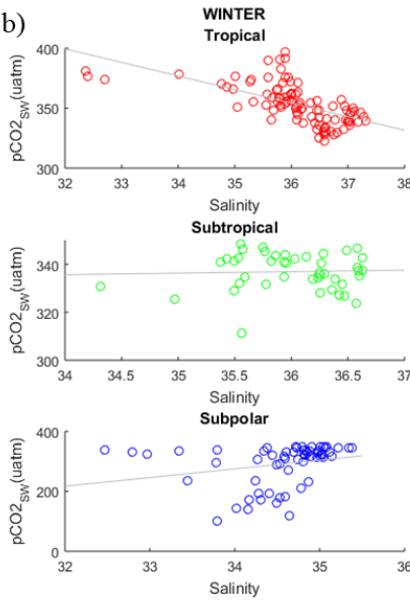


	RMSE	WEIGHT	Contribution
Tropical	1.4495	1.4411	2.0889
Subtropical	1.4735	2.0355	2.9992
Subpolar	3.4485	16.581	57.18

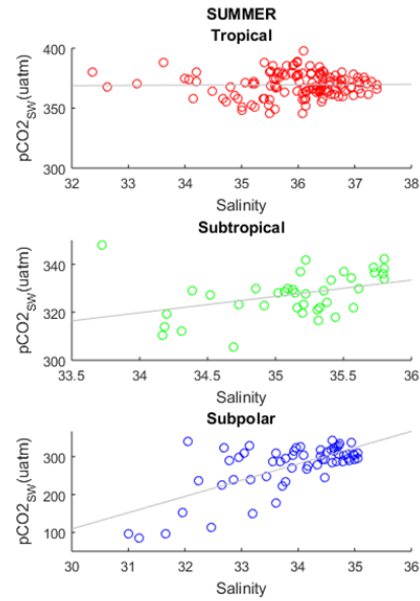


	RMSE	WEIGHT	Contribution
Tropical	1.0793	3.2127	3.4675
Subtropical	1.1242	0.39731	0.44666
Subpolar	2.9089	16.442	47.828

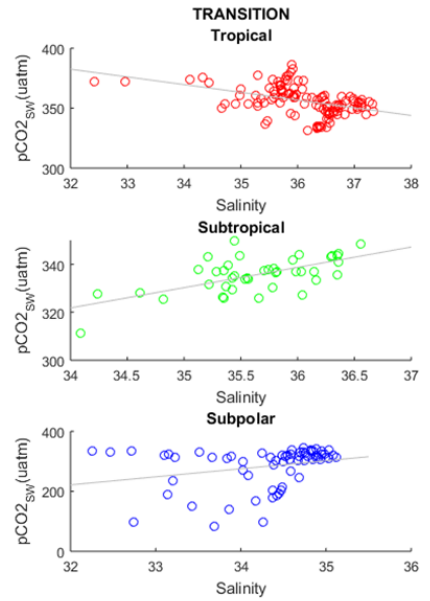
b)



	RMSE	WEIGHT	Contribution
Tropical	0.5883	-11.311	-6.6541
Subtropical	0.40244	0.62911	0.25318
Subpolar	1.3832	28.93	40.015



	RMSE	WEIGHT	Contribution
Tropical	0.59543	0.17952	0.10689
Subtropical	0.44111	6.7983	2.9988
Subpolar	1.9603	43.005	84.304



	RMSE	WEIGHT	Contribution
Tropical	0.49914	-6.4285	-3.2088
Subtropical	0.49651	8.4545	4.1977
Subpolar	1.5649	26.782	41.911

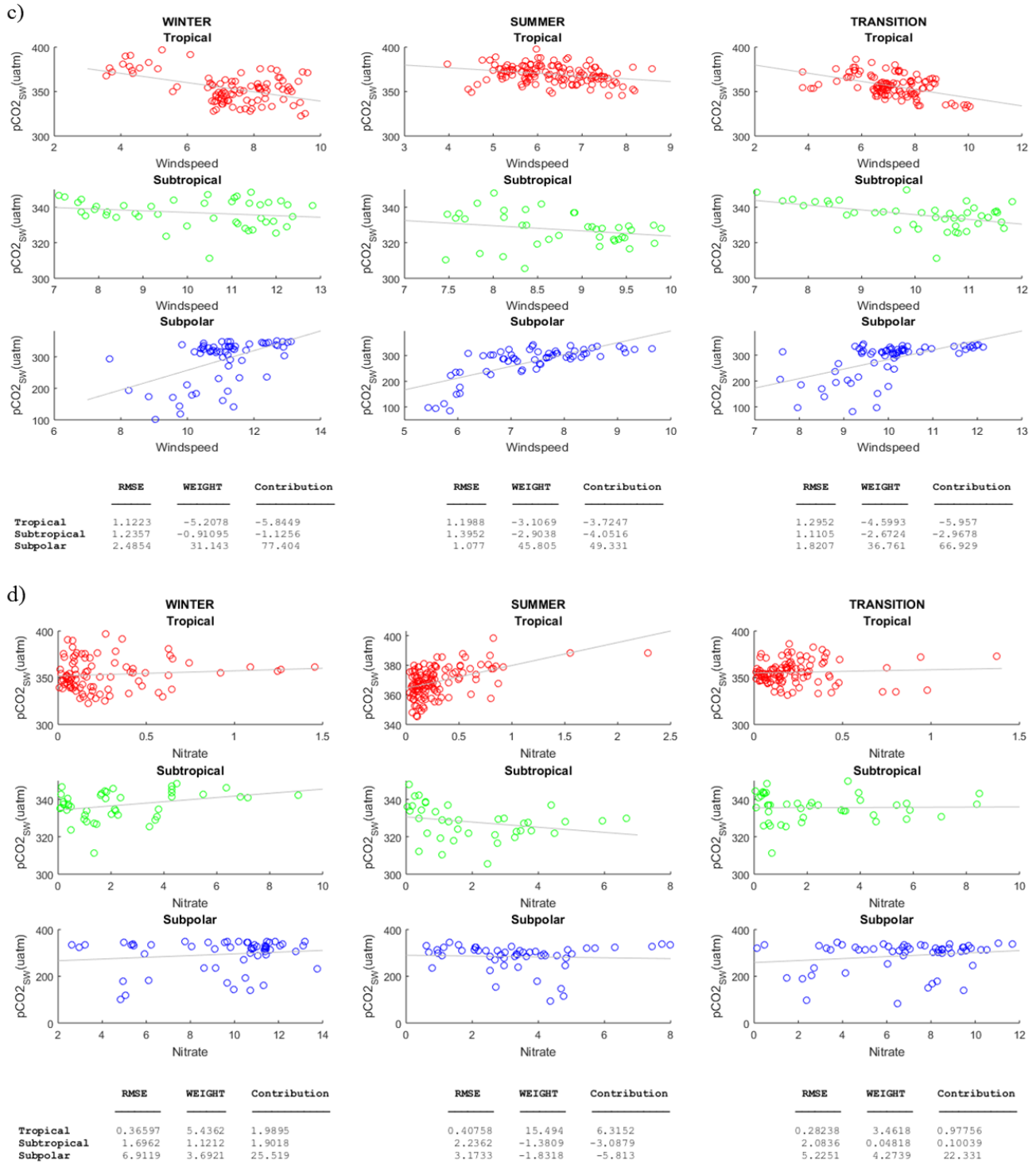


Fig. S4: Scatter diagrams and linear fits of pCO_{2sw} with a) SST, b) salinity, c) wind speed and d) nitrate in each of the North Atlantic regions of each regime.

S4.2 The Southern Ocean Carbon States

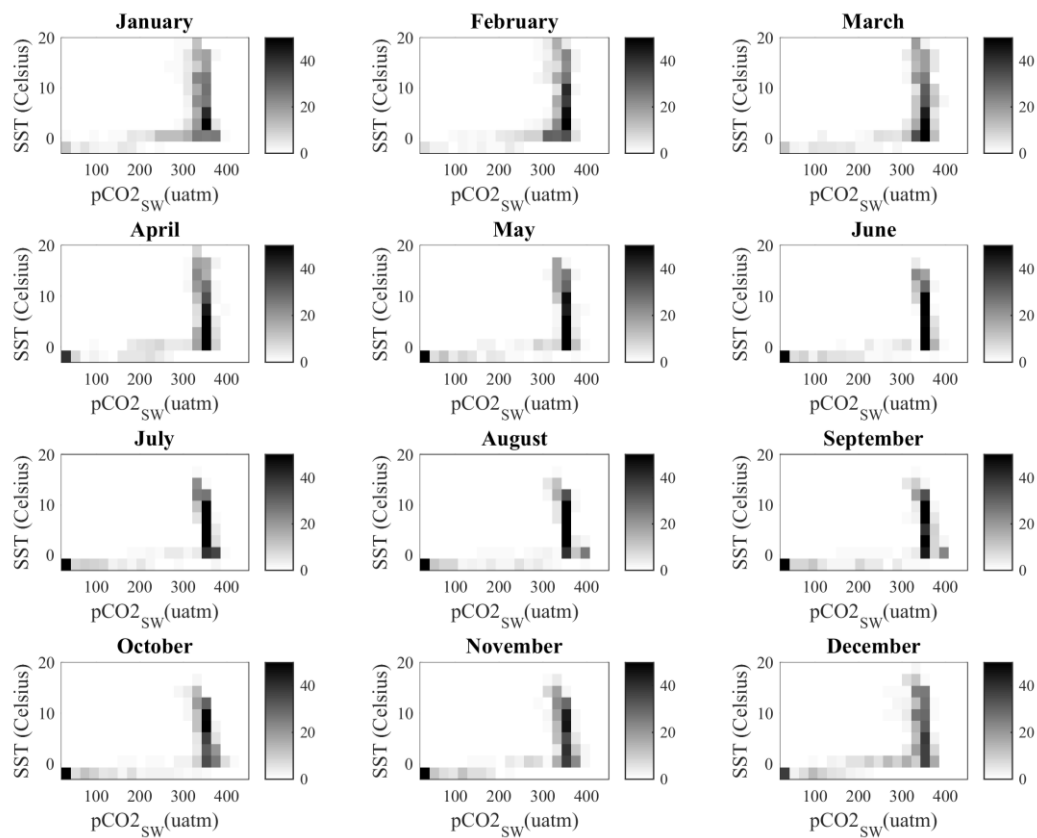


Fig. S5: Monthly 2D histograms of pCO₂ of surface water (pCO₂sw) and SST in the Southern Ocean (defined as 180°W to 180°E, 90°S to 40°S) from the Takahashi observational dataset.

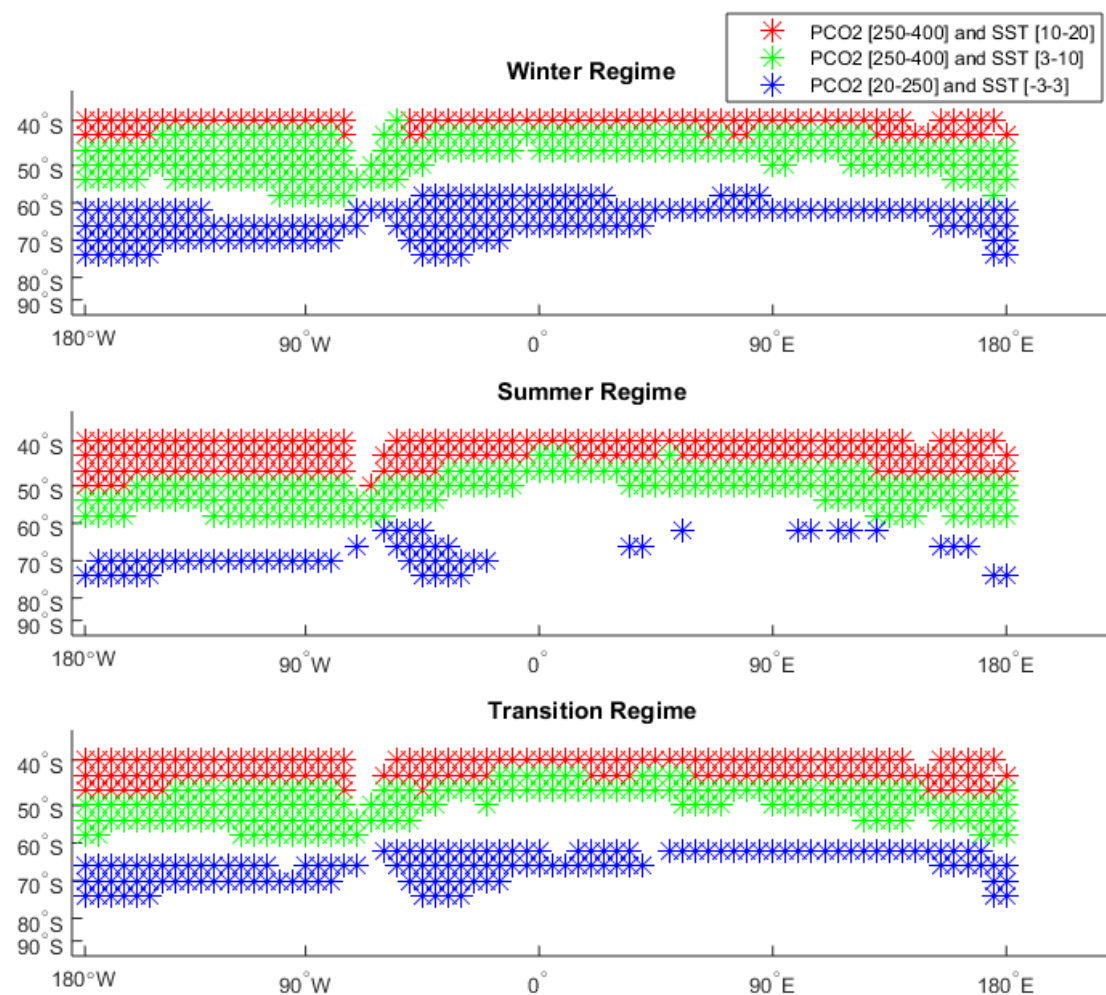


Fig. S6: Demarcated regions within the Southern Ocean basin defined by ranges of $p\text{CO}_{2\text{sw}}$ and SST values. The choice of the regions is based on the dominant bins in each ocean carbon state.

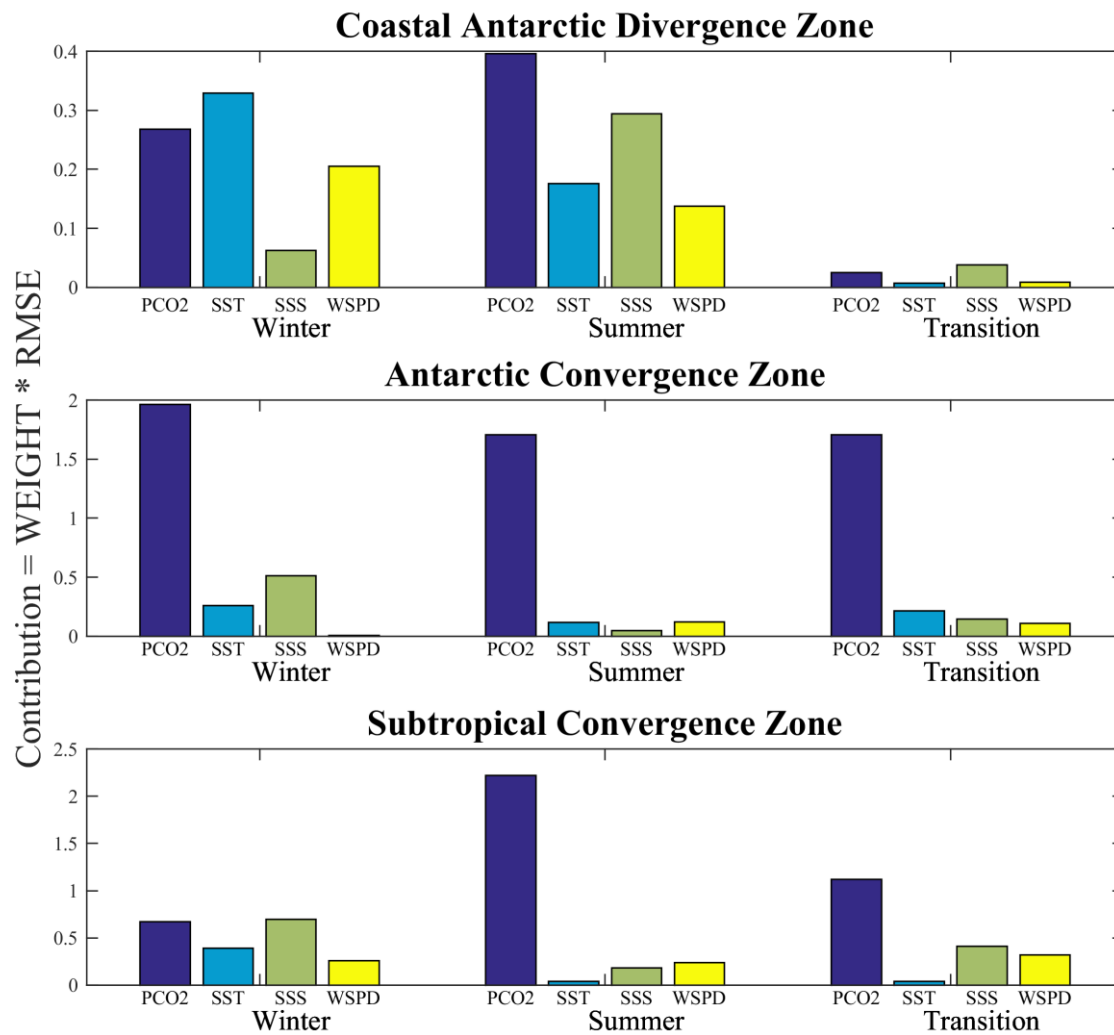
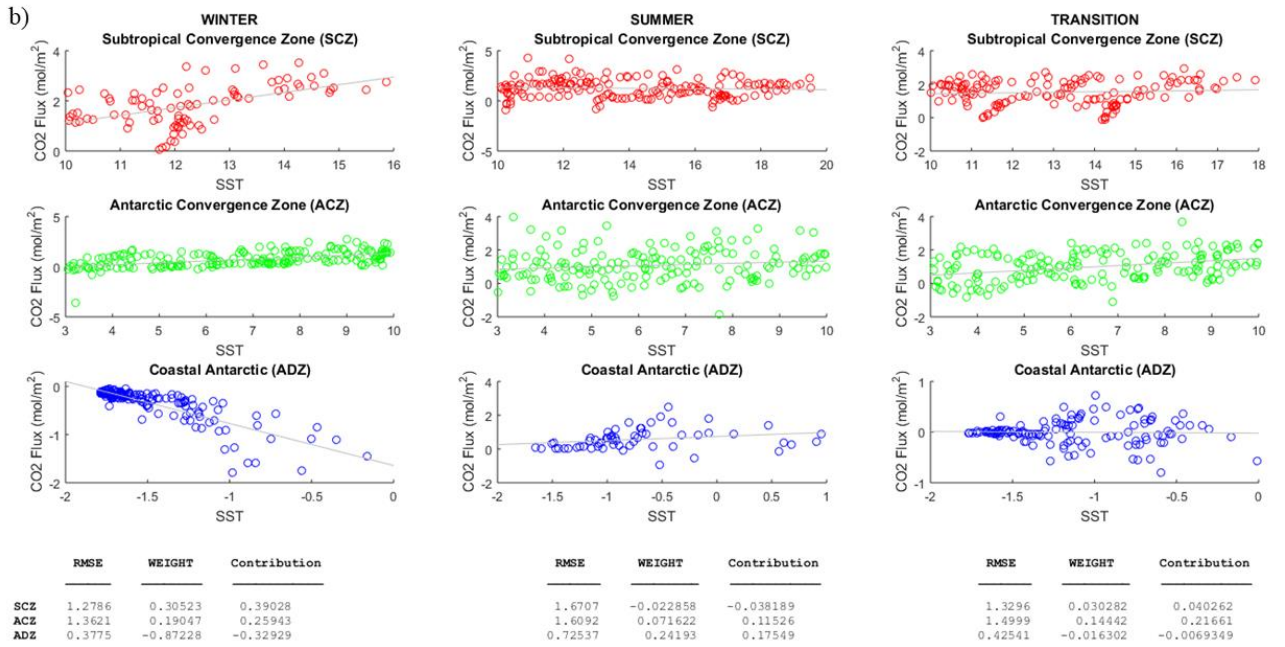
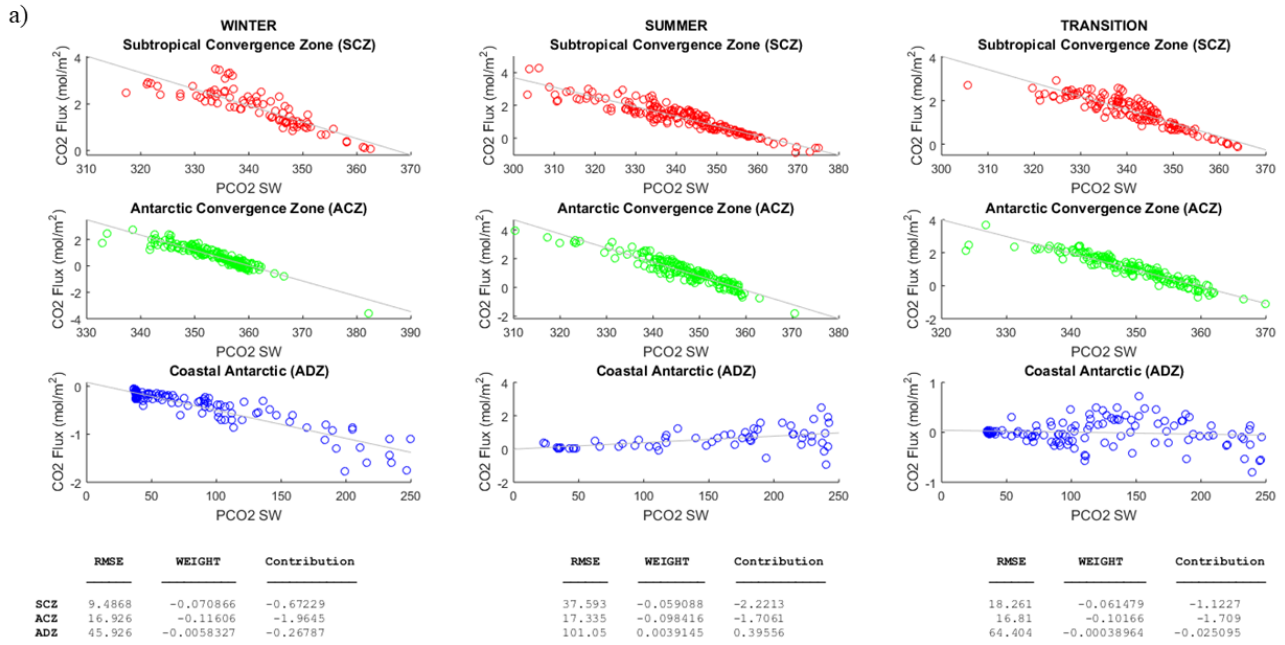


Fig. S7: Bias terms as computed in the Taylor expansion of the model bias for the air-sea flux of CO₂.



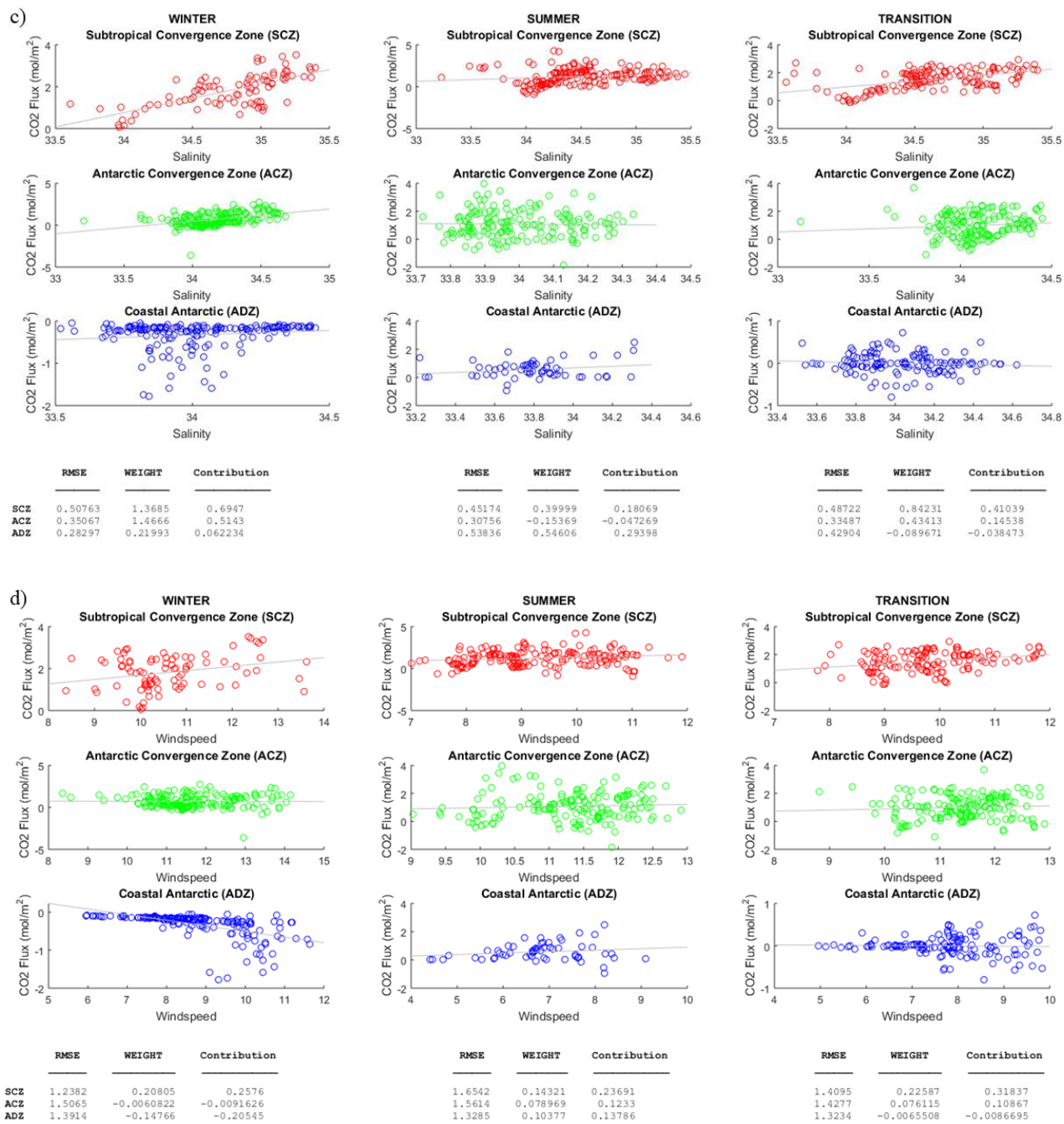
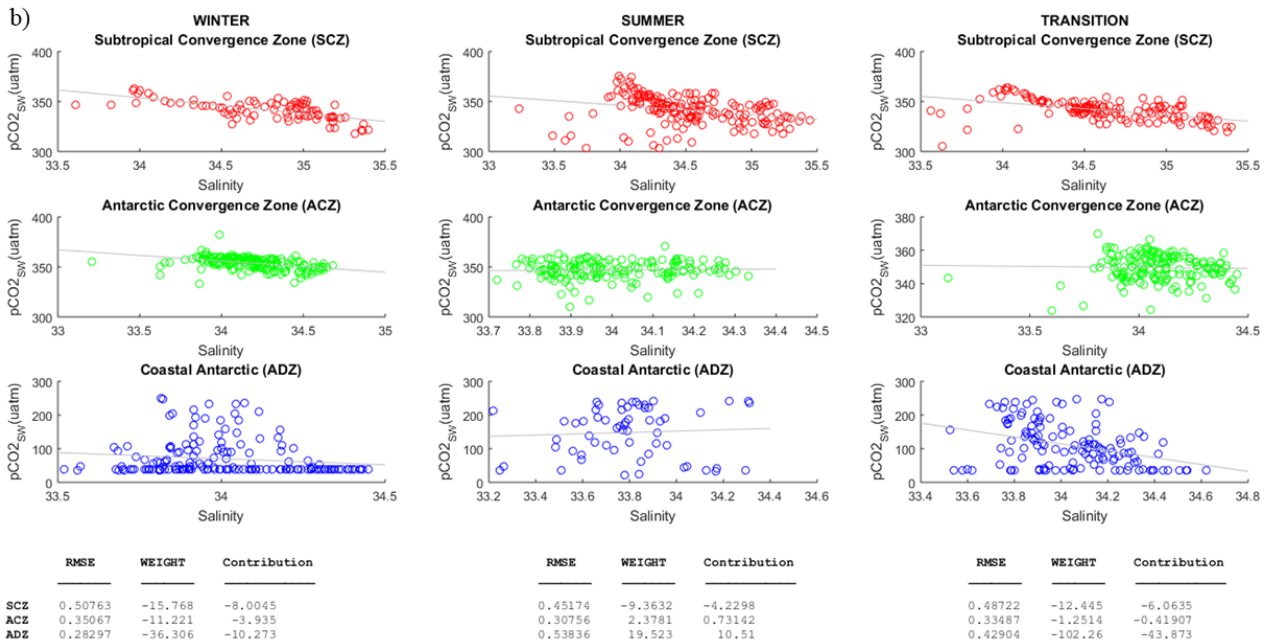
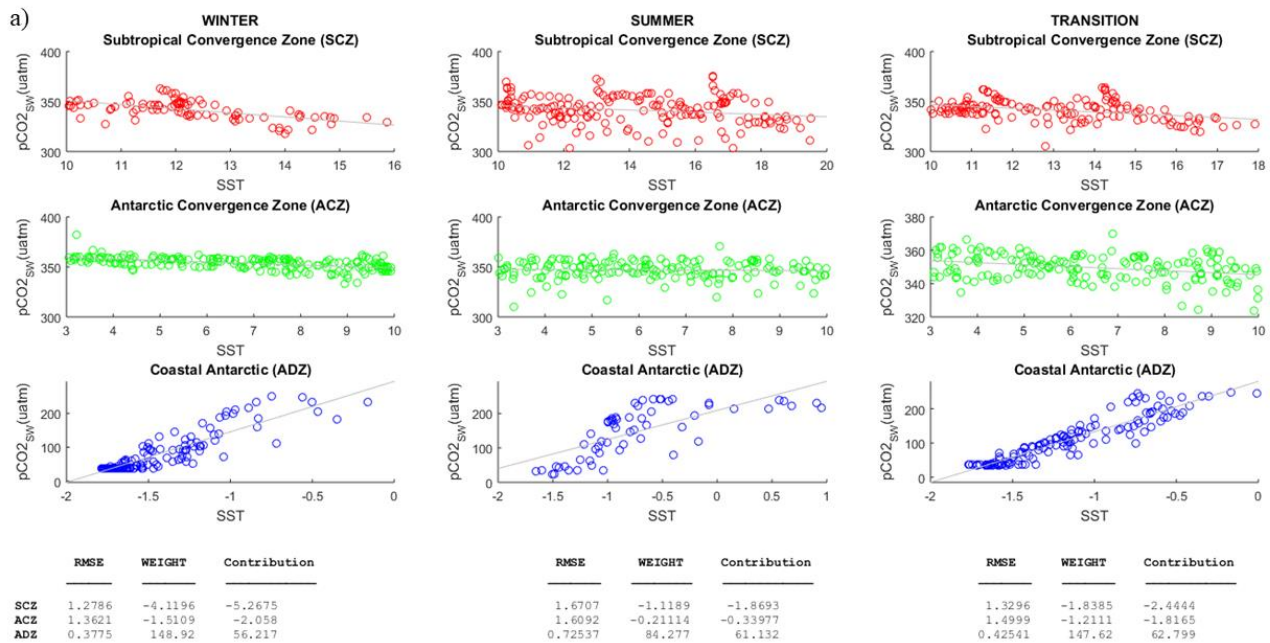


Fig. S8: Scatter diagrams and linear fits of the air-sea flux of CO₂ with a) pCO_{2sw}, b) SST, c) salinity, and d) wind speed in each of the Southern Ocean regions and for each regime.



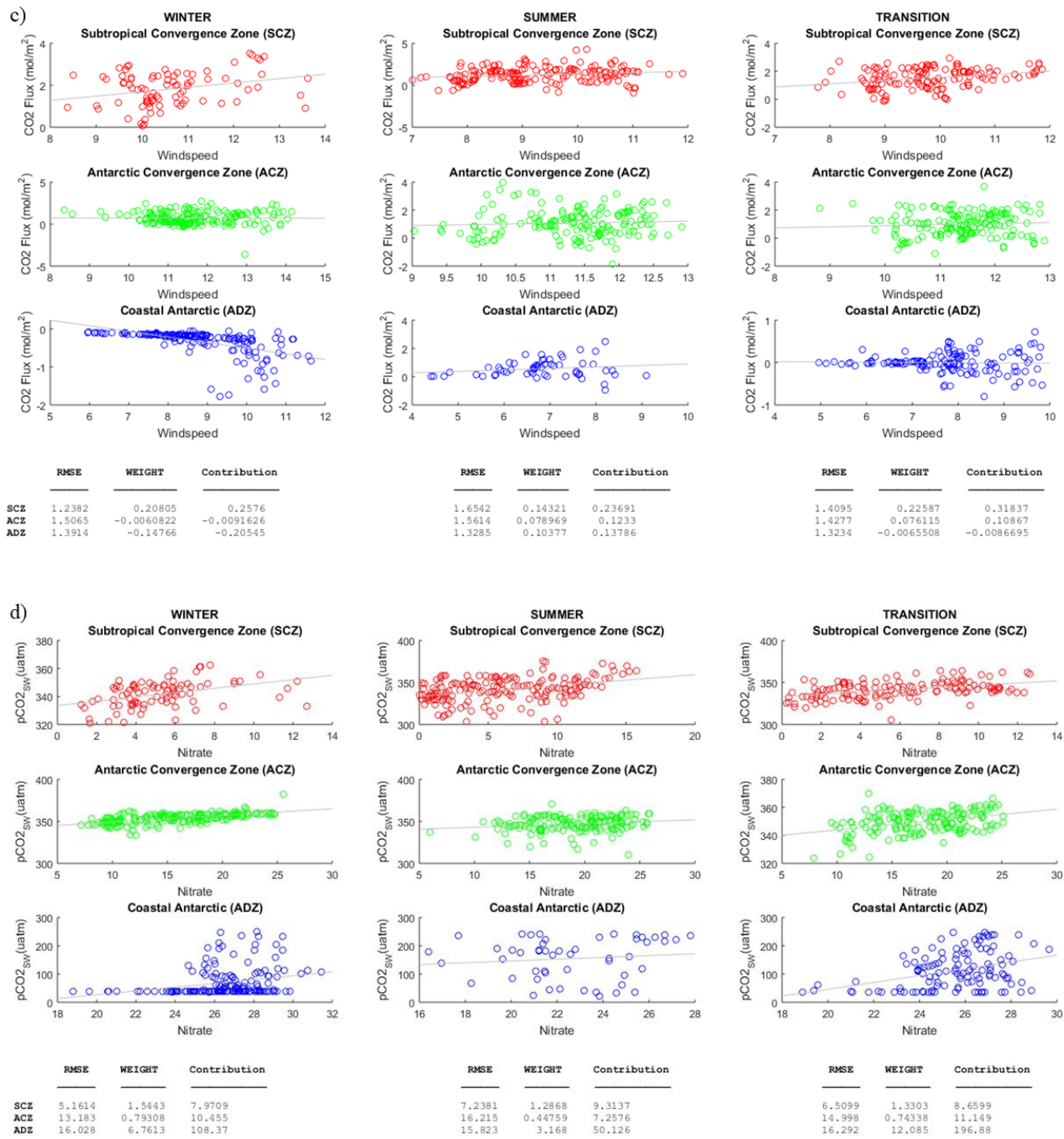


Fig. S9: Scatter diagrams and linear fits of pCO_{2sw} with a) SST, b) salinity, c) wind speed and d) nitrate in each of the Southern Ocean regions and for each regime.