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Exploring the role of different data types and timescales in the quality of marine biogeochemical model calibration

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Table S1. As Table 2, but including results of an optimisation S4-DOP that is similar to S4-SO, but includes all phytoplankton data including the Southern Ocean.

	S6*-All	S6-All	S6-DOP	S4-DOP	S4-SO	S4-Org	L4-SO	ECCO*
L	140	138	349	64	87	115	39	-
J_{RMSE}	6.030	6.052	6.082	6.045	6.046	6.874	6.125	7.072
Optimal parameters:								
I_{c}	34.44	33.98	31.57	28.46	28.84	38.38	22.11	9.65
	[31.4- 37.4]	[31.5- 35.0]	[28.3- 34.7]	[26.4- 32.5]	[26.0- 31.8]	[32.4- 39.9]	[17.2- 25.2]	
μ_{ZOO}	2.801	2.594	2.895	2.967	2.807	1.021	2.369	1.893
	[2.63- 2.87]	[2.45- 2.72]	[2.63- 3.00]	[2.68- 3.00]	[2.44- 3.00]	[1.00- 1.33]	[2.10- 2.79]	
$R_{-\mathrm{O2:P}}$	187.8	188.3	200.0	199.5	200.0	189.5	169.3	151.1
	[185.9- 193.6]	[181.3- 190.4]	[194.0- 200.0]	[185.4- 200.0]	[184.9- 200.0]	[180.0- 190.6]	[161.8- 175.9]	
b	0.803	1.000	1.000	1.000	1.000	1.800	1.024	1.461
	[0.77- 0.83]	[1.00- 1.02]	[1.00- 1.04]	[1.00- 1.03]	[1.00- 1.03]	[1.78- 1.80]	[1.00- 1.09]	
σ_{DOP}	0.028	0.000	0.049	*0.000*	*0.000*	*0.000*	*0.000*	0.150
	[0.02- 0.07]	[0.00- 0.00]	[0.00- 0.07]					
λ_{DOP}	0.238	0.184	0.168	*0.184*	*0.184*	*0.184*	*0.184*	0.170
	[0.20- 0.34]	[0.15- 0.22]	[0.12- 0.24]					

Table S2. Surface J_{RMSE} (Equation 1 and bias of optimised models after 10 years of simulation. For all tracers we present the value for ECCO* and the minimum and maximum value of S6*-All to L4-SO. Bias is in mmol m^{-3} for nutrients and oxygen, and in μmol P m^{-3} for other components.

	PO_4	NO_3	O_2	Phy	Zoo	POP	DOP
			J_{RMSE}, 10 year spin-up				
ECCO*	0.492	0.615	0.077	0.826	1.830	1.665	1.567
Minimum	0.254	0.303	0.058	0.756	1.720	1.678	1.172
% of ECCO*	51.7	49.3	75.3	91.6	94.0	100.7	74.8
Maximum	0.310	0.355	0.062	1.332	1.854	1.765	1.304
% of ECCO*	63.0	57.6	80.1	161.3	101.3	106.0	83.2
			J_{RMSE}, 3000 year spin-up				
ECCO*	0.579	0.612	0.069	0.855	1.878	1.674	2.292
Minimum	0.319	0.362	0.060	0.754	1.694	1.691	1.183
% of ECCO*	55.0	59.1	86.8	88.2	90.2	101.0	51.6
Maximum	0.490	0.453	0.080	1.515	1.942	1.834	1.767
% of ECCO*	84.5	74.1	116.4	177.2	103.4	109.5	77.1
			Bias, 10 year spin-up				
ECCO*	0.229	2.599	4.616	2.960	2.100	13.490	170.850
Minimum	0.044	0.083	0.434	0.120	0.020	9.210	4.690
% of ECCO*	19.3	3.2	9.4	4.1	1.0	68.3	2.7
Maximum	0.106	0.809	2.086	14.620	0.660	16.430	94.850
% of ECCO*	46.2	31.1	45.2	493.9	31.4	121.8	55.5
			Bias, 3000 year spin-up				
ECCO*	0.274	2.359	2.579	4.880	2.910	12.740	348.160
Minimum	0.063	0.322	0.064	0.070	0.200	6.680	5.790
% of ECCO*	23.0	13.7	2.5	1.4	6.9	52.4	1.7
Maximum	0.214	1.315	4.967	18.980	1.360	17.720	229.930
% of ECCO*	78.3	55.7	192.6	388.9	46.7	139.1	66.0

Table S3. Correlation coefficient r, RMSE, standard deviation bias normalised by observed standard deviation ($\sigma_{\mathrm{m}}/\sigma_{\mathrm{o}}$), bias and relative bias (normalised by observed mean) of model simulations after a spin up of 3000 years in comparison to metrics reported by Ilyina et al. (2013, Table 5; range over two different circulations, surface and 100m), Seferian et al. (2013, Table 3; range over three different circulations) and Kwiatkowski et al. (2014, Table 3; range over six biogeochemical models). Note that all metrics of the present study have been calculated from volume-weighted properties in the upper 100 m, whereas the other studies mostly report "surface" data, or discrete levels in the upper 100m. Also, the method for metric computation (area- or volume weighting; data sets used from comparison) might differ in the other studies. *: Value for S4-Org.

Source:		Ilyina et al. (2013)	Seferian et al. (2013)	Kwiatkowski et al. (2014)		This study
Experiments:		2 circulations	3 circulations	6 BGC models	ECCO*	1 circulation, 6 optimisations
Spin up length (y):		O(1000)	O(1000)	O(100)	3000	3000
Metric	Tracer					
r	PO_4	0.91-0.95	0.85-0.91	-	0.91	0.93-0.95*
	NO_3	0.87-0.93	0.87-0.94	0.79-0.94	0.92	0.95-0.96*
	Chl	-	0.38-0.43	0.04-0.50	0.28	0.31*-0.38
RMSE	PO_4	0.29-0.43	0.19-0.33	-	0.37	0.20*-0.31
	NO_3	0.33-0.68	1.64-5.50	-	4.25	2.49*-3.13
	Chl	-	0.16-0.18	-	0.16	0.14-0.28*
$\sigma_{\mathrm{m}}/\sigma_{\mathrm{o}}$	PO_4	0.75-0.94	-	-	0.87	1.00-1.05
	NO_3	0.78-0.94	-	0.95-1.21	0.85	0.97*-1.03
	Chl	-	-	0.40-2.65	0.53	0.43-0.91*
Bias	PO_4	-	-0.32-(-0.03)	-	-0.27	-0.21-0.06*
	NO_3	-	-1.3-4.9	-	-2.35	-1.29-0.33*
	Chl	-	-0.12-(-0.07)	-	0.06	-0.01-0.23*
Bias (rel.)	PO_4	-27.2-(-5.1)	-	-	-42.2	-32.9-10.1*
	NO_3	-3.0-8.5	-	-	-33.7	-18.6-4.8*

Table S4. Global average oxygen (mmol $O_2 m^{-3}$), global OMZ volume ($\times 10^6 km^3$; OMZ defined by $O_2 \leq 50$mmol m^{-3}) and global biogeochemical fluxes (Pg C y^{-1}) of this study (range optimised), of ECCO*, from observed estimates, and selected global model publications. Observations: Garcia et al. (2006b, O_2 and OMZ volume), Carr et al. (2006, primary production), Steinberg and Landry (2017, grazing by micro- and mesozooplankton, assuming one trophic level between both), Henson et al. (2012, min. export production and max. flux in 2000m), Dunne et al. (2007, max. export production and min. flux in 2000m).

	ave. O_2	OMZ Vol.	Prim. Prod.	Grazing	Export ($\approx$ 100m)	Flux (2000m)	No. of experiments
Observations	174	56.7	40-60	37.3-42.5	4.0-9.6	0.20-0.66	
Range optimised.	161-198	39.3-87.1	24.1-50.0	14.8-30.3	6.0-6.9	0.19-0.77	6
ECCO*	174	33.4	44.7	28.6	7.3	0.29	1
Keller et al. (2012)			52-54		7.0-7.1	0.35-0.36	2
Bopp et al. (2013)	136-231	12.5-225	30.9-78.7		4.9-8.1		10
Dunne et al. (2013)			68-82		5.4-8.0		2
Ilyina et al. (2013)			55.8-61.6		8.2-9.1		3
Moore et al. (2013)			55.6		8.1		1
Seferian et al. (2013)			25.3-34.0		4.9-7.9		3
Yool et al. (2013)			41.6				1
Lima et al. (2014)					6.0	0.21	1
Stock et al. (2014)			51.9	37.4	6.3		1
Aumont et al. (2015)			44.3	39.8	7.3		1
Kvale et al. (2015)			61.8-64.2		7.1-7.8	0.26-0.36	2
Le Quere et al. (2016)			42.6		7.6		1
Schwinger et al. (2016)			28.4-30.4		4.0-5.6	0.16-0.69	4
Aumont et al. (2017)			41-52		8.1-9.0	0.56-0.81	2
Seferian et al. (2020)			15.1-81.9		2.4-11.9		CMIP5
Seferian et al. (2020)			21.6-57.3		4.9-10.4		CMIP6
Stock et al. (2020)			51.1		6.3.	0.43	1

Table S5. Range of different global model diagnostics of inter-model spread due to model parameter set (after 10 and 3000 years of simulation; Δ Parameter) and between 10 and 3000 years (Δ Time), with range of other global models (Δ GCMs; see Table S4) and observations (Δ Obs; see Table S4). Values in parentheses show range when setup S4-Org is omitted from the analysis. All ranges are expressed as percent of the mean over the respective axis (i.e. mean over all model set-ups or over the two time slices).

Diagnostic	Δ Parameters				Δ Time		Δ GCMs	Δ Obs
	at t=10		at t=3000		|t=3000 - t=10|			
J_{RMSE}	13.6	(1.6)	24.0	(2.6)	3.1 - 12.9	(3.1 - 5.1)		
PP	46.3	(20.4)	81.9	(22.3)	0.4 - 18.1	(0.4 - 11.4)	141.0	40.0
Grazing	35.5	(23.0)	78.7	(24.8)	1.8 - 22.2	(1.8 - 14.7)		13.0
EP	26.7	(20.9)	14.0	(13.2)	0.6 - 19.0	(0.6 - 12.0)	135.0	94.0
F2000	140.5	(56.2)	106.1	(32.5)	2.5 - 60.3	(2.5 - 14.6)	147.0	113.0
average O_2	0.6	(0.2)	21.8	(7.6)	1.1 - 11.9	(1.1 - 8.5)	53.4	
OMZ volume	11.9	(4.0)	79.2	(76.6)	2.1 - 48.0	(2.1 - 48.0)	239.0	

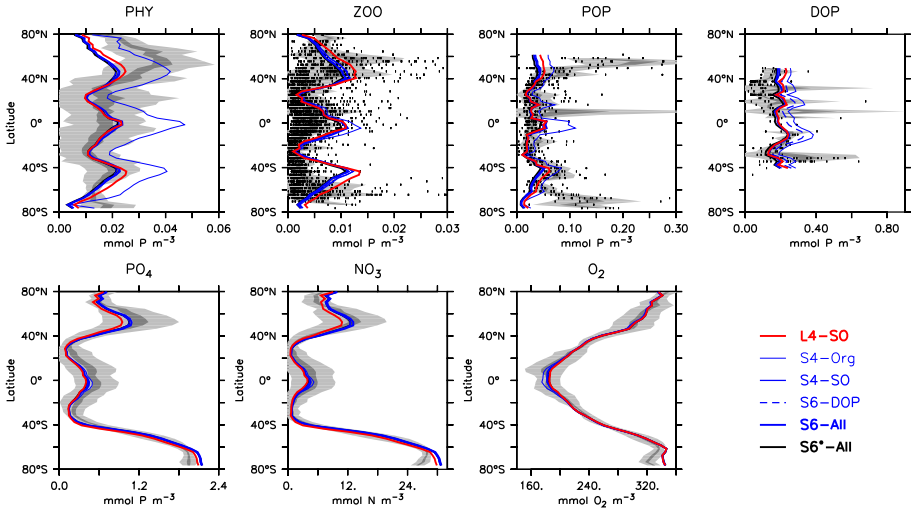

Figure S1. Zonally averaged tracer distributions of model simulations after spin up of 10 years (coloured lines, see legend on the lower right) and observations (light and dark grey shaded areas: one and 1/5 standard deviation around the mean, black symbols: individual data points). All concentrations have been averaged over the upper 100 m, except for phytoplankton (upper 10 m).

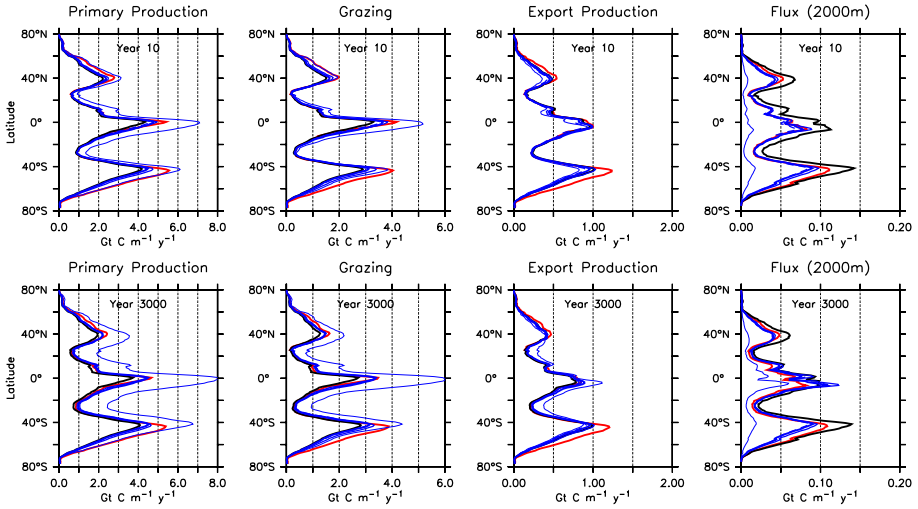

Figure S2. Zonally integrated fluxes of primary production, grazing, export production and particle flux in 2000 m after spin up of 10 years (top panels) and 3000 years (bottom panels). Line colours as in Figure S1.

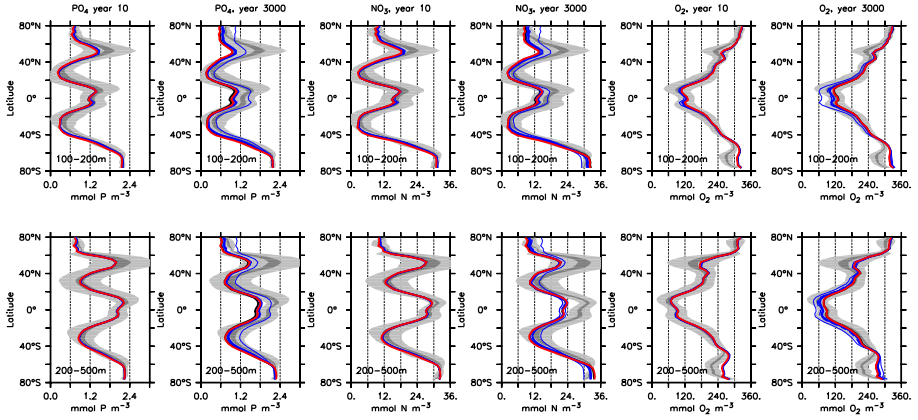

Figure S3. Zonally averaged inorganic tracer distributions of model simulations after spin up of 10 and 3000 years (coloured lines) and observations (light and dark grey shaded areas), averaged over the 100-200 m (upper panels) and 200-500 m (lower panels). Line and shade colours as in Figure S1

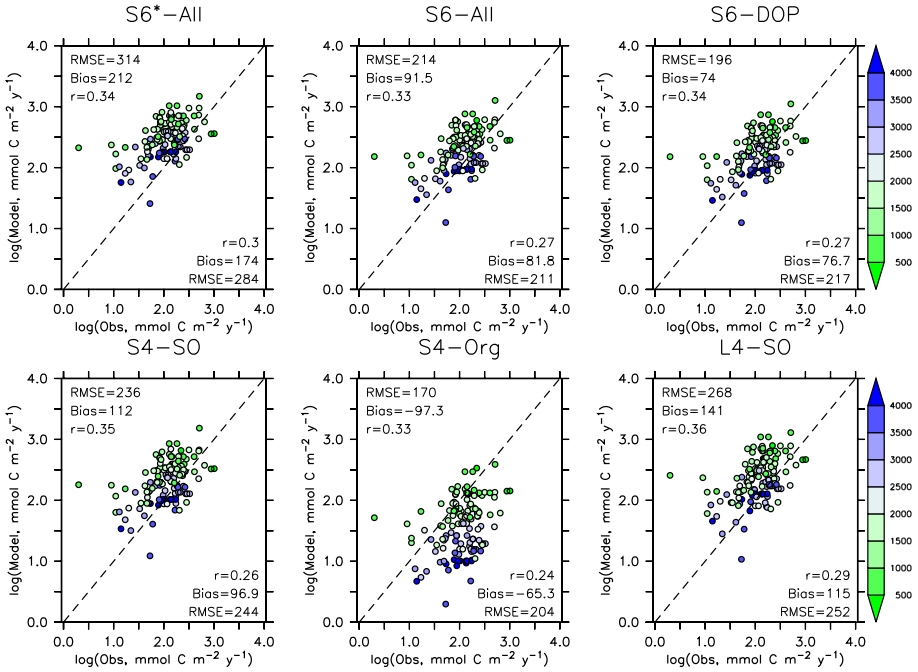

Figure S4. Simulated particle flux after a spin up of 10 years plotted against observations by Honjo et al. (2008). Both model and observations are log-transformed. Colour indicates trap depth. Numbers in upper left corner denote RMSE, bias and correlation coefficient after 10 years, calculated from non-transformed data. Numbers in lower right panels denote metrics after 3000 years.

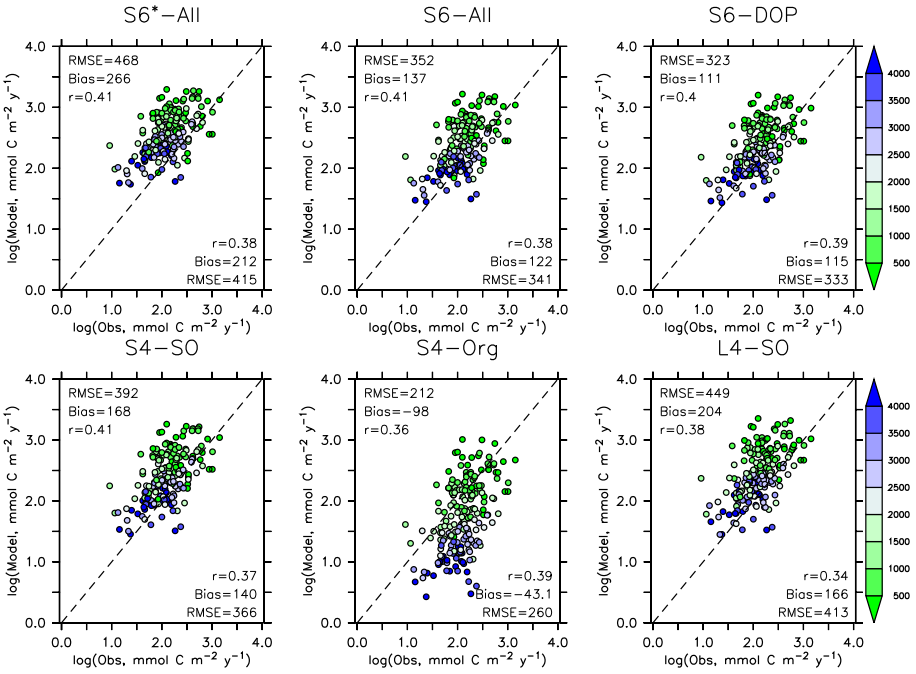

Figure S5. As Figure S4, but for comparison with data set by Lutz et al. (2007).

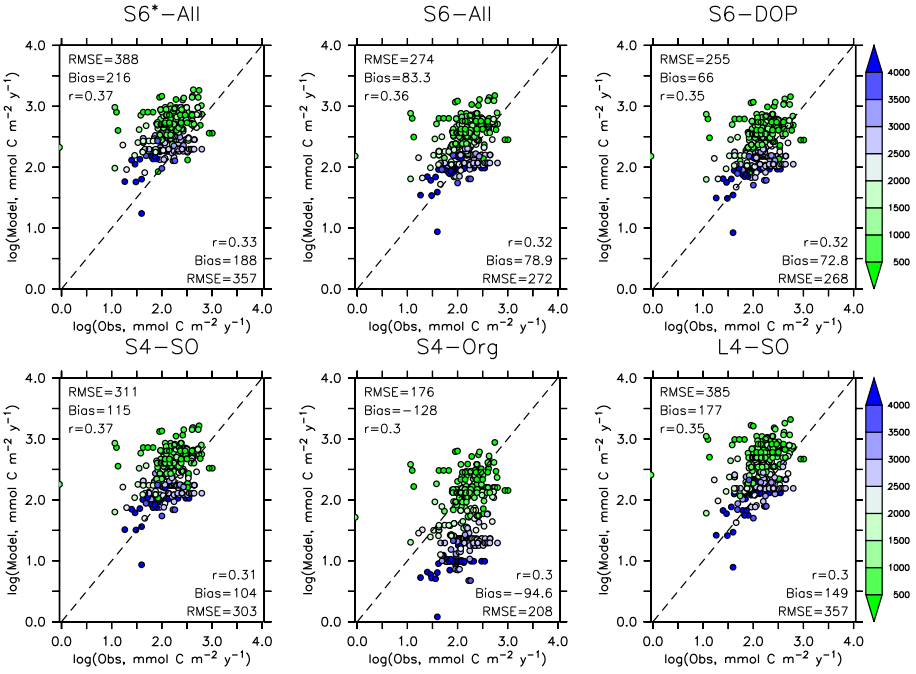

Figure S6. As Figure S4, but for comparison with data set by Mouw et al. (2016).

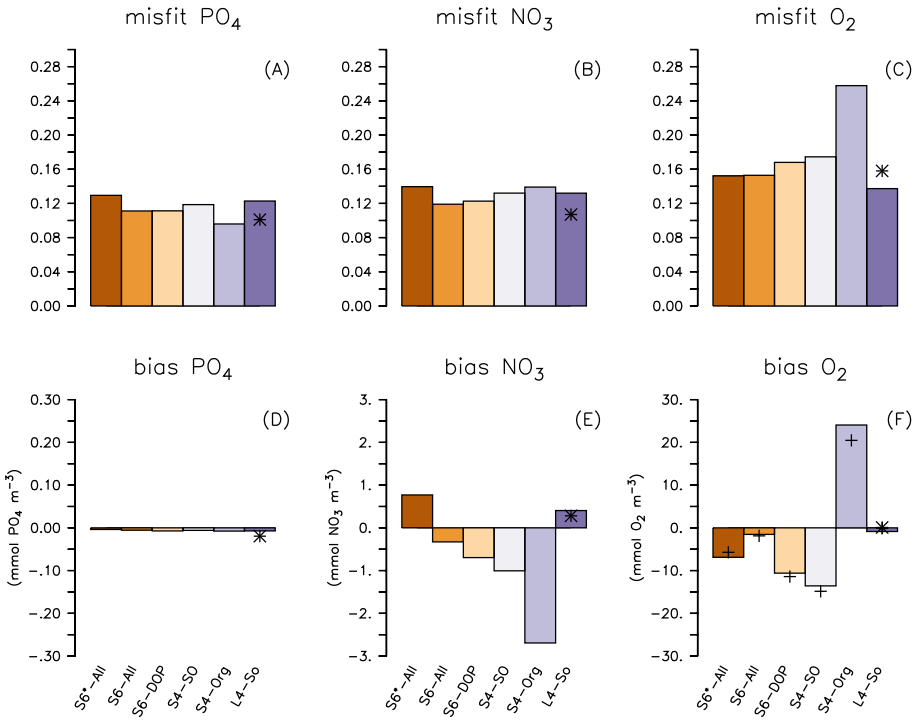

Figure S7. Misfit (panels A-C) and bias (mmol m^{-3}; panels D-F) of phosphate (A, D), nitrate (B, E) and oxygen (C, F), calculated over the entire model domain after a spin up of 3000 years A star indicates the performance of ECCO* by Kriest et al. (2020). Pluses in panel F denote the total oxidant bias for oxic and suboxic remineralisation, calculated from $B_{\mathrm{O2}} + (B_{\mathrm{NO3}} - 16B_{\mathrm{PO4}})\frac{R_{-\mathrm{O2:P}}}{0.8R_{-\mathrm{O2:P}}-16}$, where B_{X} is the bias of the respective tracer and 16 mol N:mol P is the N:P stoichiometry of organic matter.

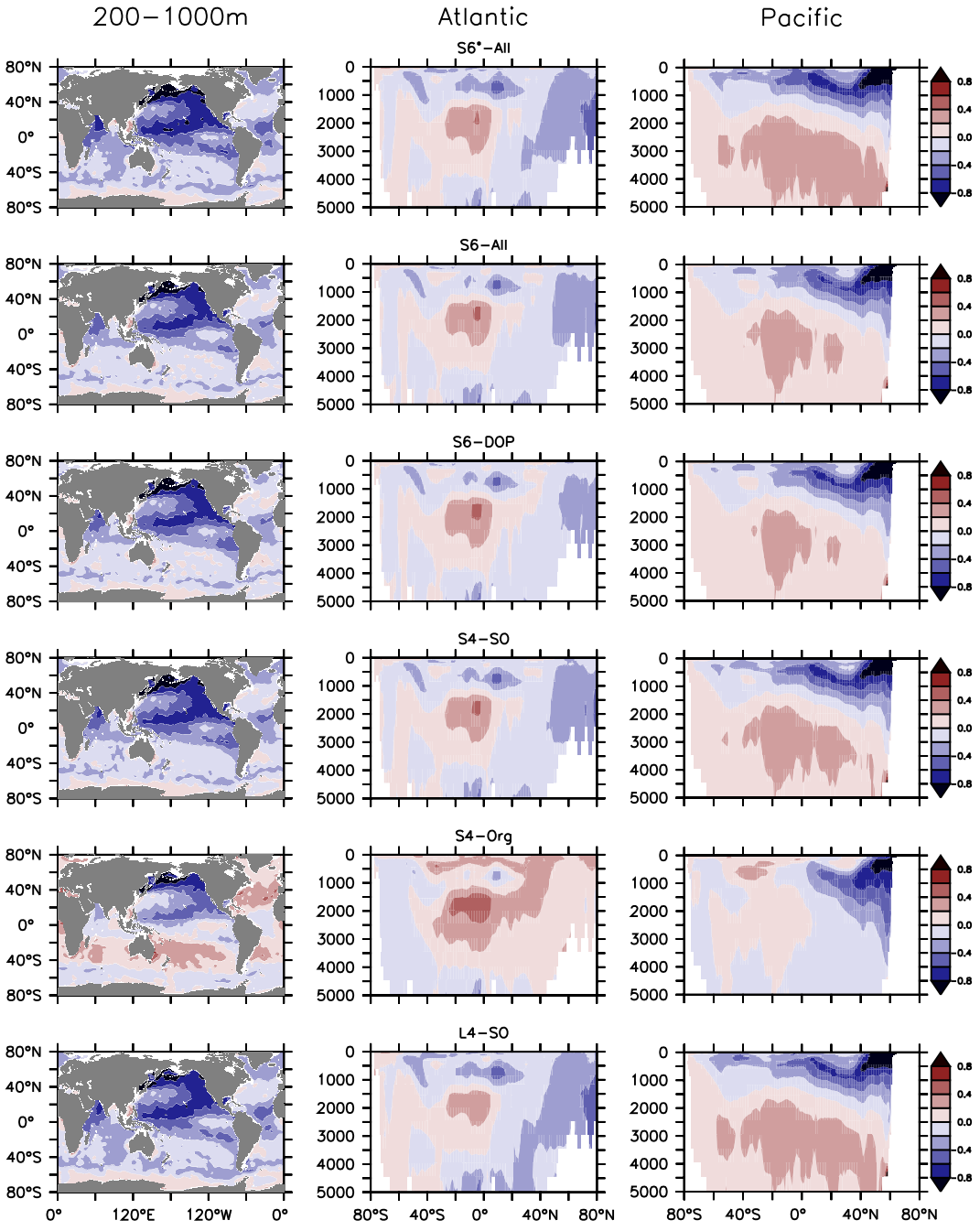

Figure S8. Deviation of model results from observations for phosphate after 3000 years. Left panels: deviations of average between 200 and 1000 m. Middle panels: deviations of Atlantic zonal means. Right panels: deviation of Pacific zonal means.

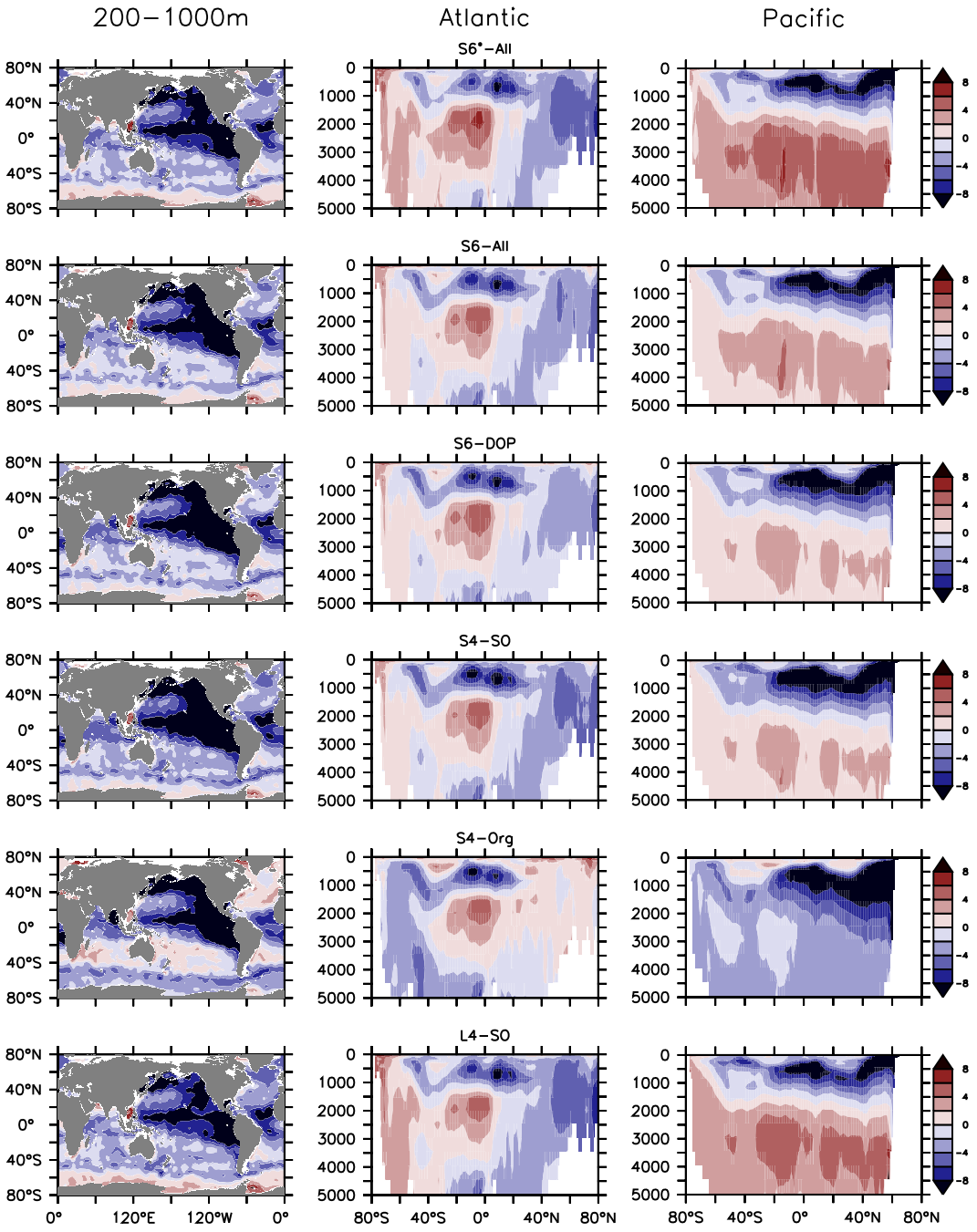

Figure S9. As Figure S8 but for nitrate.

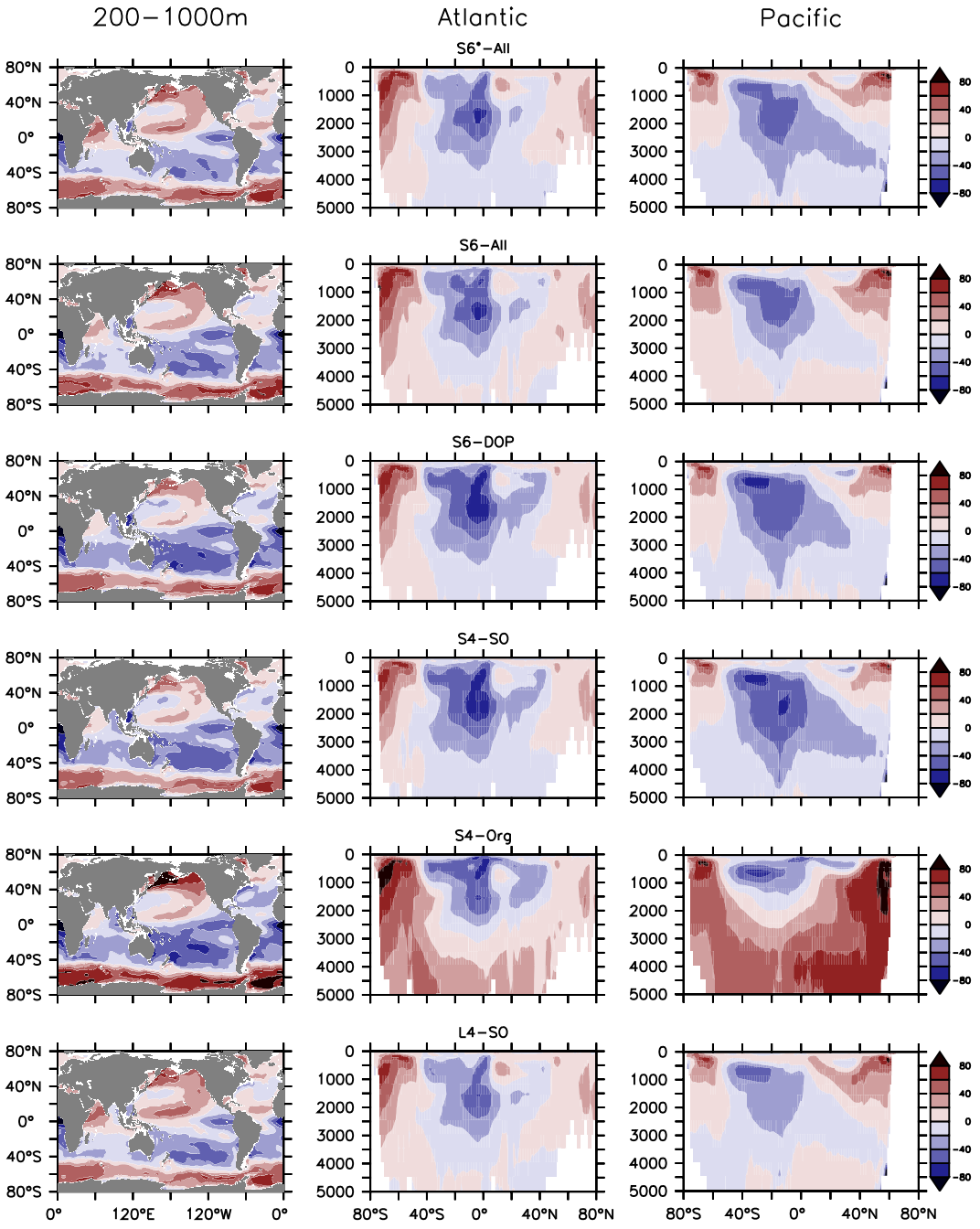

Figure S10. As Figure S8 but for oxygen.

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