Figure S1. The three-dimensional model skill score array of all the experiment ensembles tested in this study.
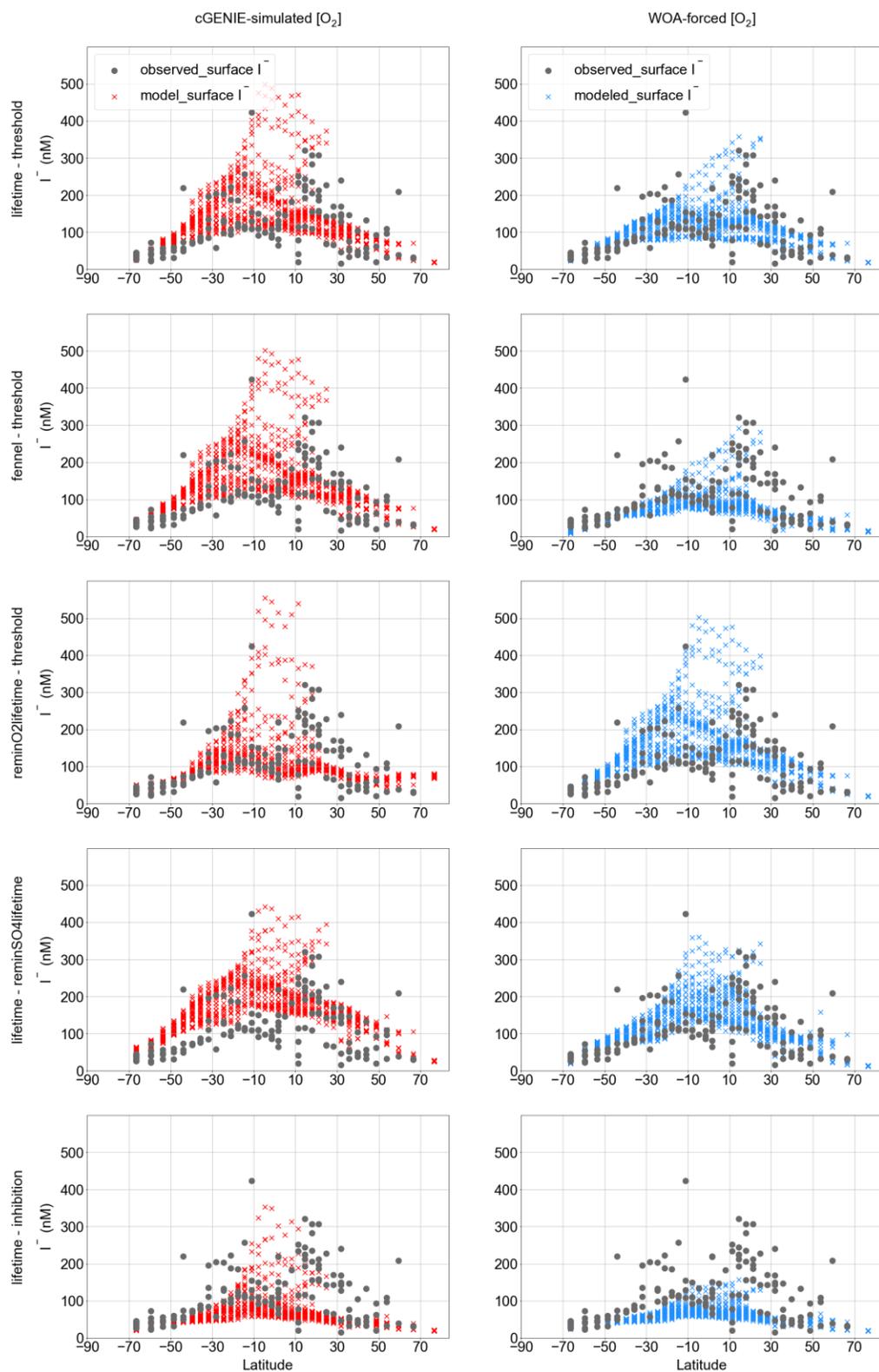
Figure S2. Modeled latitudinal surface iodide distribution compared with observation with the cGENIE simulated [O₂] and the WOA-[O₂] restoring forcing.
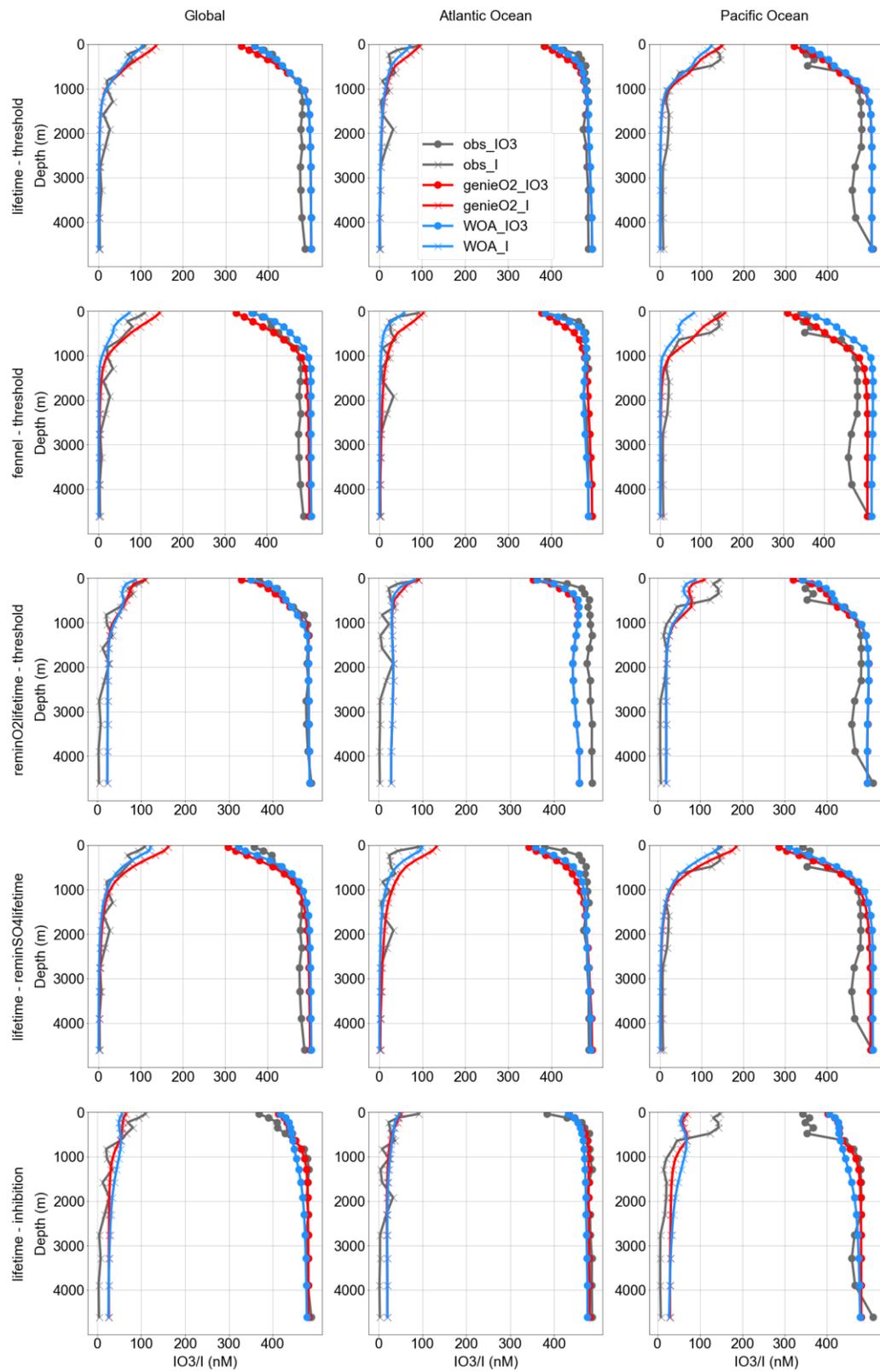
Figure S3. Modeled averaged iodine (including iodate and iodide) depth profile among global ocean, the Pacific, the Atlantic compared with observation.
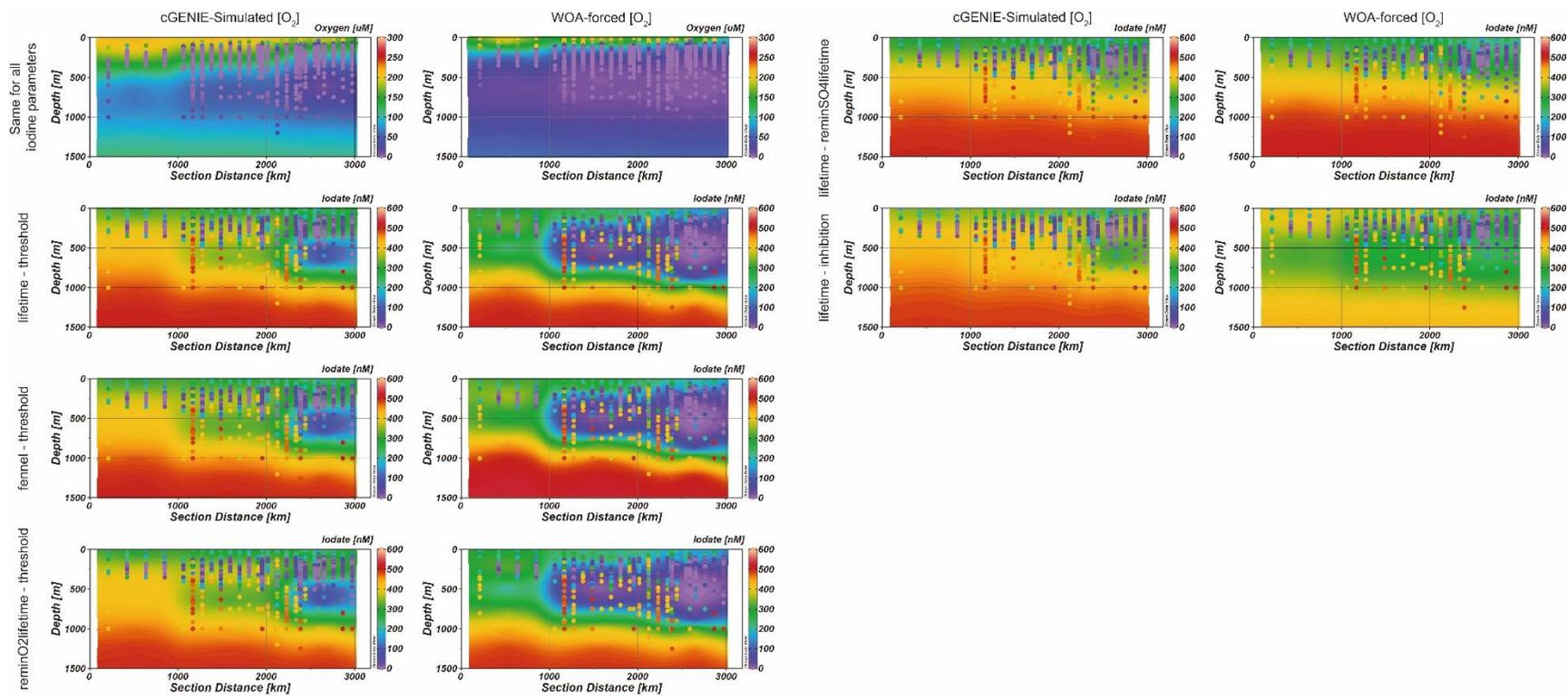
Figure S4. Modeled (contour) and observed (colored dots) transects of IO₃⁻ in the ETNP.
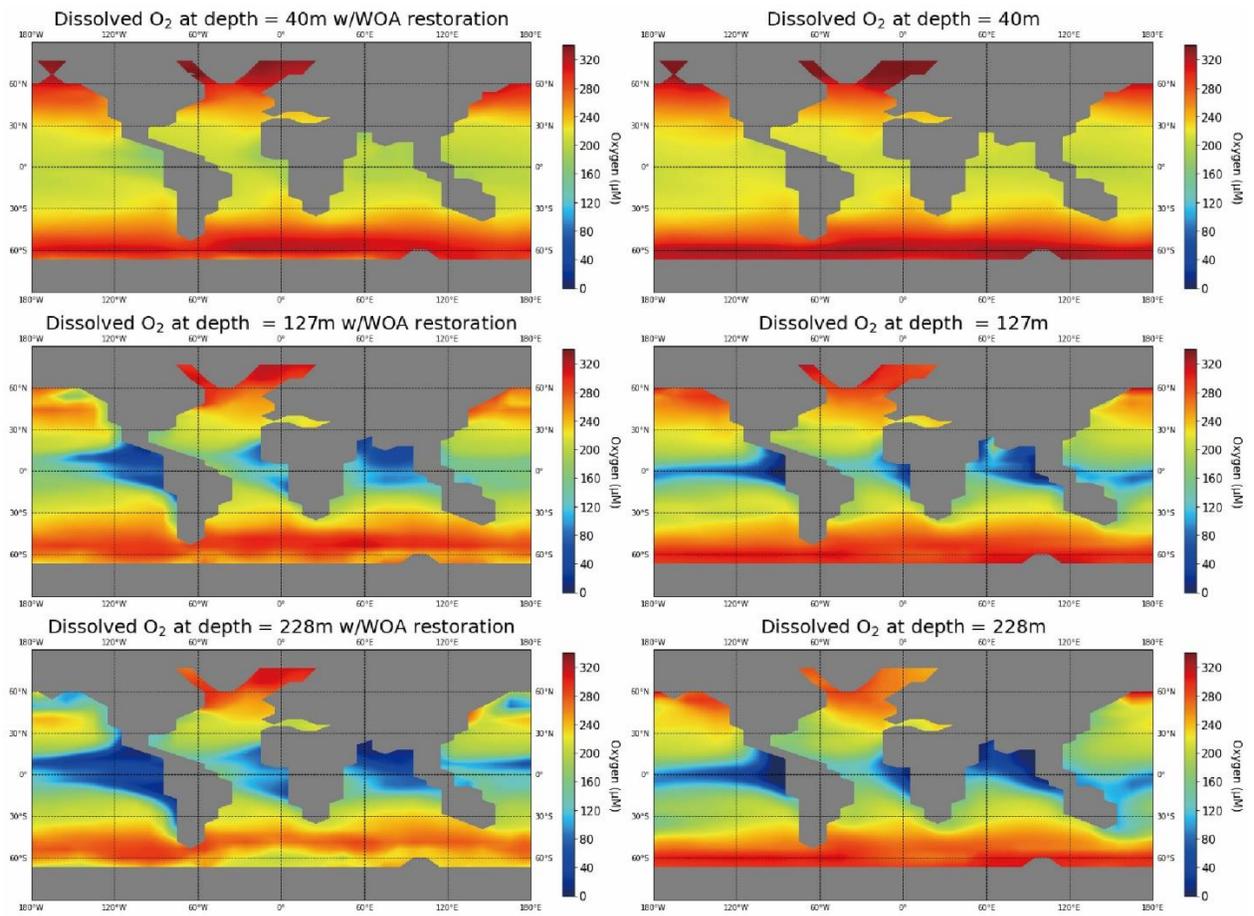
Figure S5. The modeled O₂ distribution in the surface and subsurface with [O₂] forced to restore the WOA observation and without forcing.
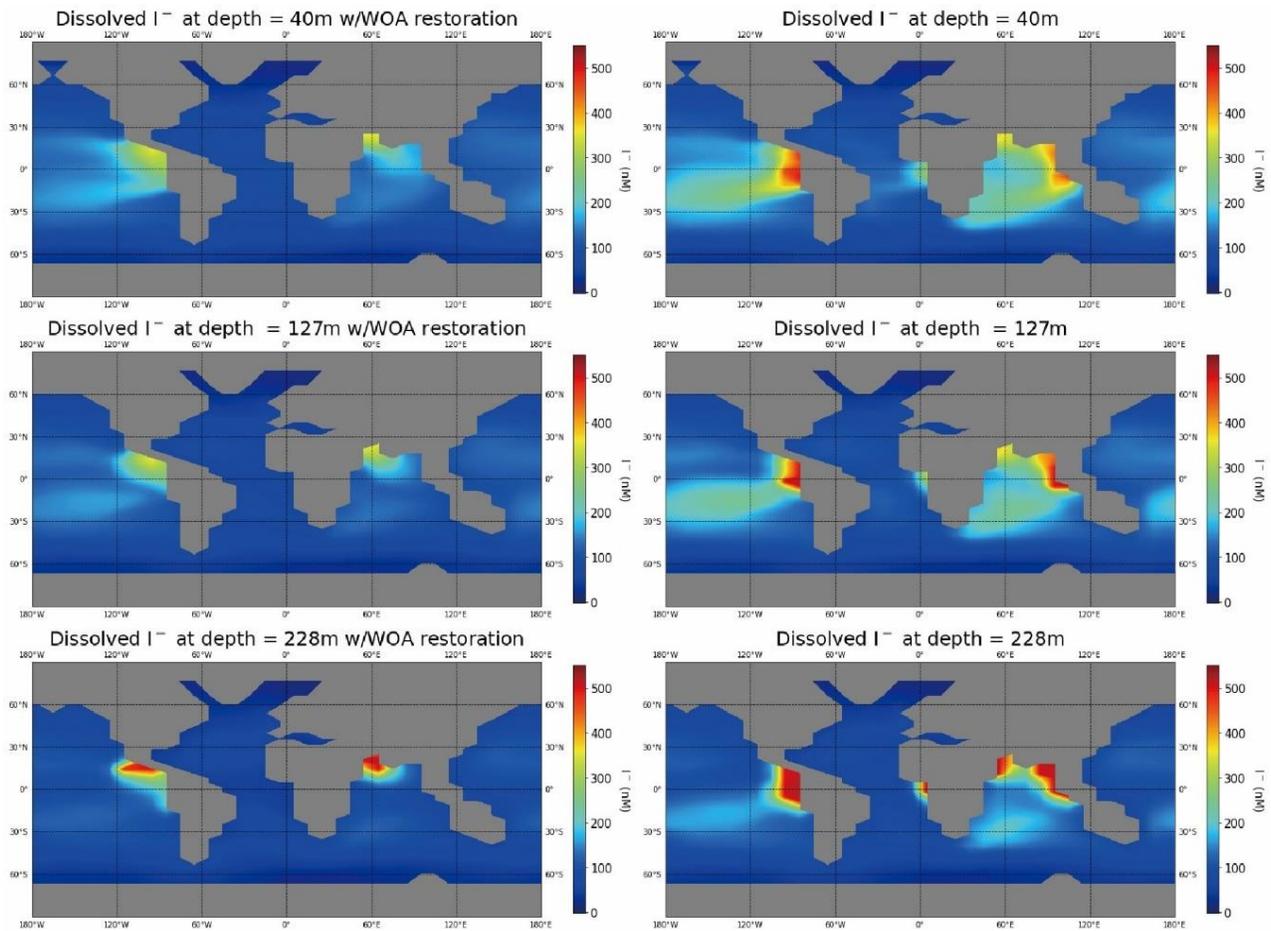
Figure S6. The modeled I⁻ distribution in the surface and subsurface with [O₂] forced to restore the WOA observation and without forcing. Associated iodine cycling parameters: "lifetime" = 50 yrs; "threshold" = 10×10⁻⁶ mol; I:C ratio = 1.5×10⁻⁴ mol/mol. This is an example of cGENIE overestimating surface I⁻ when the overall model performance is tuned to the best.
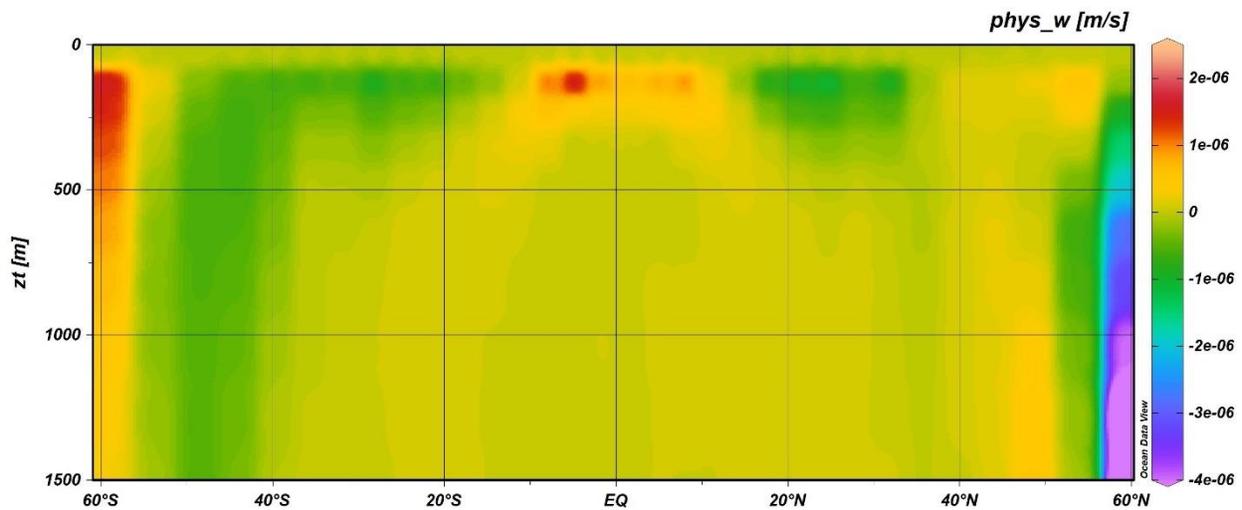
Figure S7. The averaged latitudinal distribution of vertical circulation (phys_w) simulated by cGENIE.
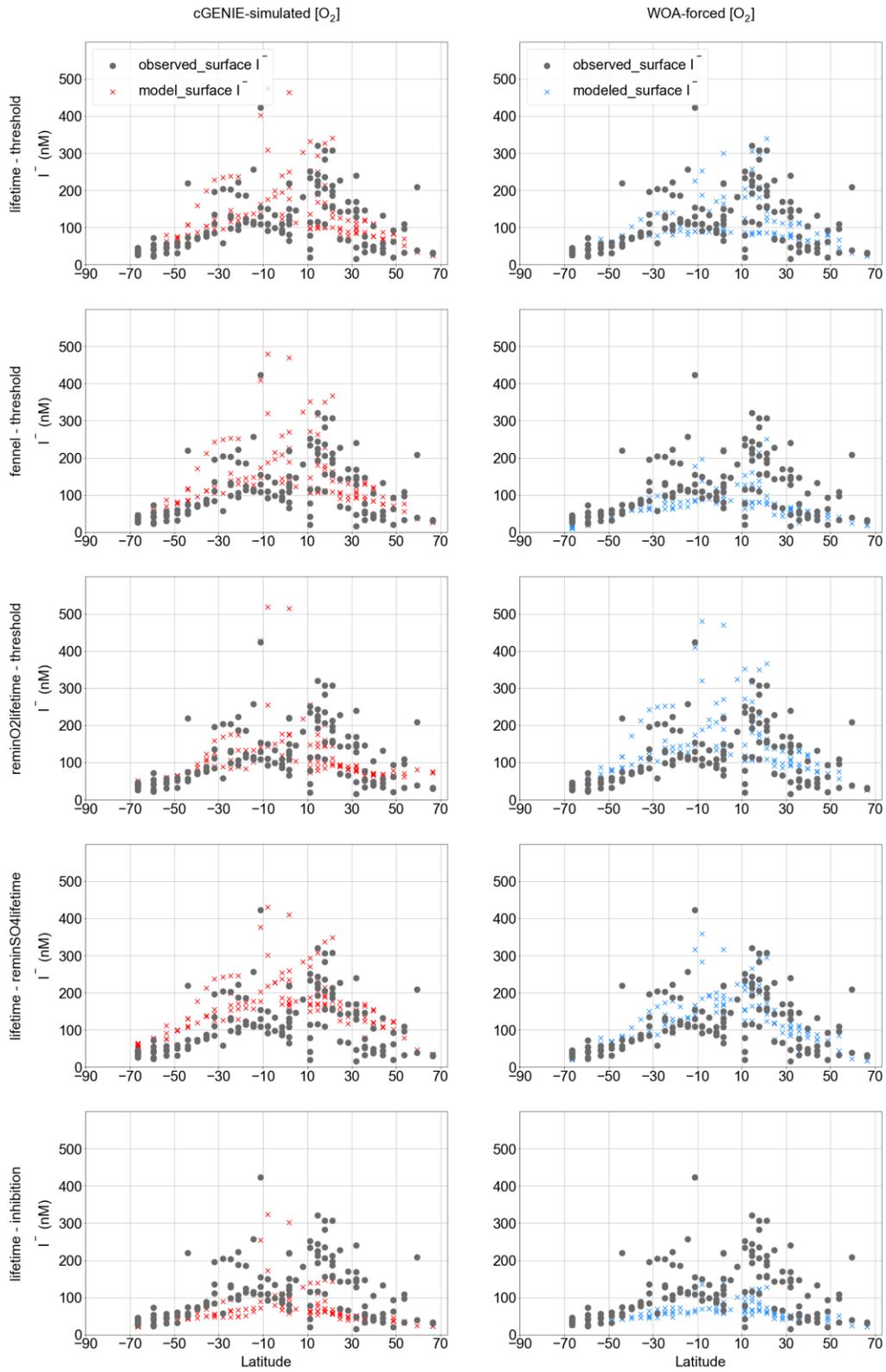
Figure S8. Modeled latitudinal surface iodide distribution compared with observation with the cGENIE simulated [O₂] (masked only include grid points with corresponding observations) and the [O₂] restoring forcing.
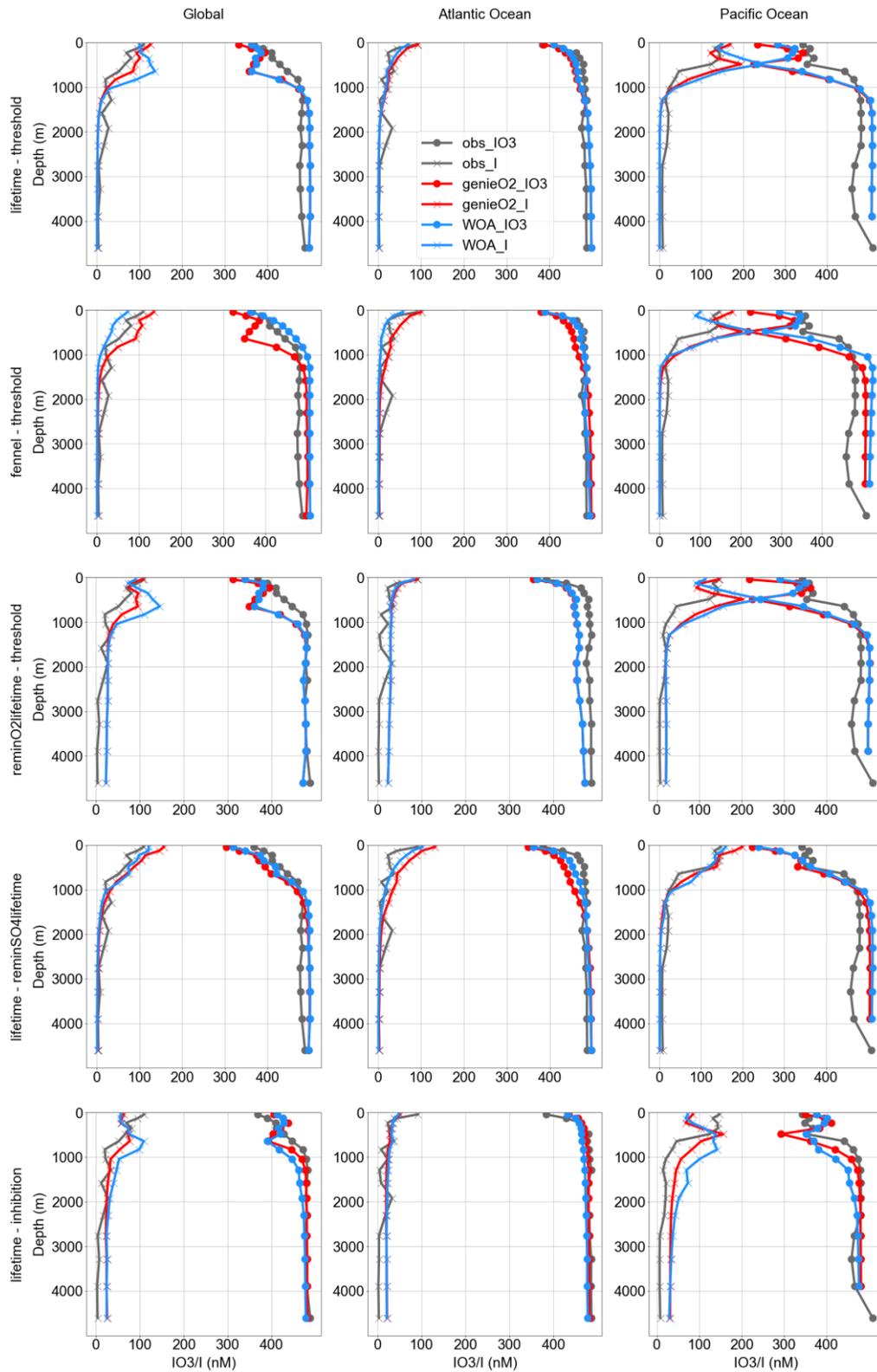
Figure S9. Modeled averaged iodine (including iodate and iodide, and masked only include grid points with corresponding observations) depth profile among global ocean, the Pacific, the Atlantic compared with observation.
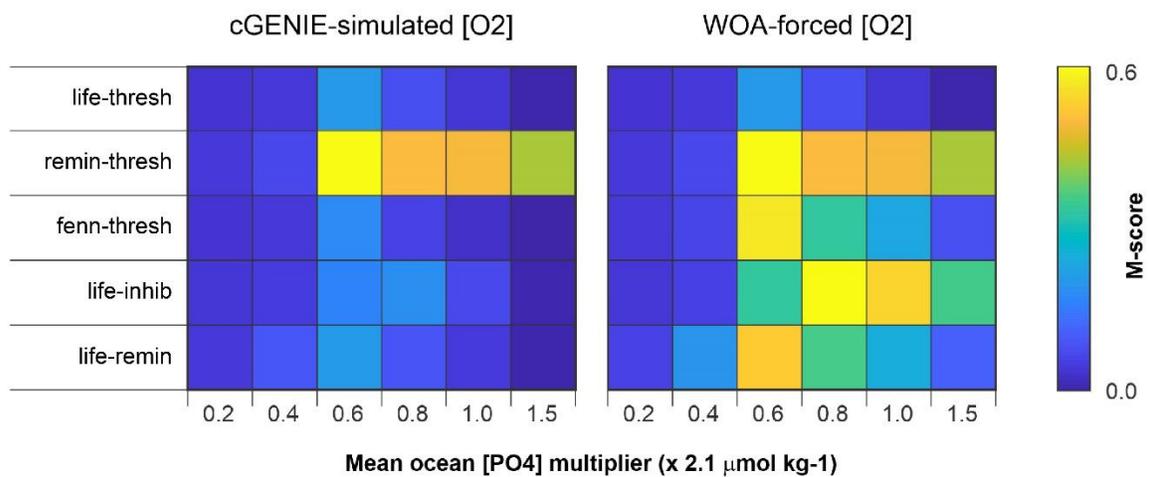
Figure S10. The model skill scores between modeled and measured I:Ca during the pre-OAE2. The iodine cycling parameters are derived from modern simulations with cGENIE-simulated [O_2] and WOA-forced [O_2], respectively. lifetime-thresh = lifetime-threshold; remin-thresh = reminO2lifetime-threshold; fenn-thresh = fennel-threshold; life-inhib = lifetime-inhibition; life-remin = lifetime-reminSO4lifetime

| Parameter description		Iodine oxidation parameters				Iodine reduction parameters			I:C ratio (× 10^{-4} mol/mol)
		'lifetime' (years)	'reminO2lifetime' (× 10^{-5} mol/kg)	'Fennel' (Inhibition µM O_2)	constant/	'threshold' (µM O_2)	'inhibition' (µM/ year^{-1})	'reminSO4lifetime' (× 10^{-6} mol/kg)	
'lifetime'-'threshold'	cGENIE O_2	10-170	\	\		1-110	\	\	0.5-3.5
	WOA	10-170	\	\		1-110	\	\	0.5-3.5
	no excess I$^-$ filtration	10-170	\	\		1-110	\	\	0.5-3.5
	no excess I$^-$ filtration + WOA	10-170	\	\		1-110	\	\	0.5-3.5
'reminO2lifetime'-'threshold'	cGENIE O_2	\	0.01-1	\		1-100	\	\	0.5-3.5
	WOA	\	0.01-1	\		1-100	\	\	0.5-3.5
'Fennel'-'threshold'	cGENIE O_2	10-170 (1/k)	\	20		1-110	\	\	0.5-3.5
	WOA	10-170 (1/k)	\	20		1-110	\	\	0.5-3.5
	WOA(alternative)	10-170 (1/k)	\	20		1-110	\	\	0.5-3.5
'lifetime'-'inhibition'	cGENIE O_2	0.5-50	\	\		\	10/0.1-10	\	0.5-3.5
	WOA	0.5-50	\	\		\	10/1.0-10	\	0.5-3.5
'lifetime'-'reminSO4lifetime'	cGENIE O_2	10-170	\	\		\	\	0.01-1	0.5-3.5
	WOA	10-170	\	\		\	\	0.01-1	0.5-3.5

Table S1. The cGENIE iodine redox options and the associated range of parameters of these options in this research. Only simulations 1-3 are chosen for detailed discussion in the manuscript for higher M scores and reasonably replicating iodine ocean gradients (See Discussion).

Parameter description		Iodine oxidation parameters				Iodine reduction parameters			I:C ratio (× 10^{-4} mol/mol)	Model skill score (global)
		'lifetime' (years)	'reminO2lifetime' (× 10^{-5} mol/kg)	'Fennel' (Inhibition constant/ μM O_2)		'threshold' (μM O_2)	'inhibition' (μM/ year^{-1})	'reminSO4lifetime' (× 10^{-6} mol/kg)		
'lifetime'- 'threshold'	cGENIE O_2	50	\	\		10	\	\	1.5	0.305
	WOA	50	\	\		10	\	\	1.5	0.385
	no excess I$^-$ filtration	50	\	\		10	\	\	2.5	0.316
	no excess I$^-$ filtration + WOA	50	\	\		10	\	\	2.5	0.393
'reminO2lifetime'- 'threshold'	cGENIE O_2	\	0.1	\		10	\	\	3.5	0.266
	WOA	\	0.1	\		10	\	\	3.5	0.365
'Fennel'- 'threshold'	cGENIE O_2	50 (1/k)	\	20		10	\	\	1.5	0.308
	WOA	10 (1/k)	\	20		10	\	\	3.5	0.385
	WOA(alternative)	50 (1/k)	\	20		10	\	\	1.5	0.379
'lifetime'- 'inhibition'	cGENIE O_2	50	\	\		\	10/0.1	\	1.5	0.289
	WOA	10	\	\		\	10/1.0	\	1.5	0.289
'lifetime'- 'reminSO4lifetime'	cGENIE O_2	50	\	\		\	\	0.5	1.5	0.307
	WOA	10	\	\		\	\	0.1	2.5	0.363

Table S2. The performance of the cGENIE iodine simulations of all the combinations of parameters in this research and associated parameterization when the model reaches the best global M score.

Section	Site location	Depth	Pre-CIE d13C	CIE d13C	Post-CIE d13C	Pre-CIE I:Ca	CIE I:Ca	Post-CIE I:Ca
Raia del Pedale	Shallow water	Few meters	-0.353	2.013	0.681	0.688	0.837	1.296
Demerara Rise	Low lat. pelagic	Below storm wave base	-27.616 (org)	-23.816 (org)	-26.345 (org)	0.427	0.530	0.153
Tarfaya	Low lat. pelagic	Below storm wave base	-27.019 (org)	-24.841 (org)	-26.729 (org)	0.836	0.494	0.869

South Ferriby	Mid. lat. Pelagic	Below storm wave base	3.200	3.780	3.260	3.656	4.953	3.344
Eastbourne	Mid. lat. Pelagic	Below storm wave base	2.796	4.335	3.803	2.351	3.005	4.241
Newfoundland	Mid. lat. Pelagic	Below storm wave base	2.803	3.064	2.697	2.883	1.552	2.364

Table S3. The Cretaceous OAE2 sections where I:Ca data were measured from for model-data comparison. The d13C from Demerara Rise and Tarfaya are organic data (d13Corg) instead of carbonate data.