

Supplementary Material

Redox-controlled restructuring of marine microbial ecosystems during oceanic anoxic events

Tenga Yokoyama^{1, *}, Eiichi Tajika¹, Yasuto Watanabe^{1, 2}, Kazumi Ozaki^{3, 4}

¹ Department of Earth and Planetary Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113-0033, Japan

² Earth System Division, National Institute for Environmental Studies, 16-2 Onogawa, Tsukuba, Ibaraki, 305-8506, Japan

³ Department of Earth and Planetary Sciences, Institute of Science Tokyo, 2-12-1 Ookayama, Meguro-ku, Tokyo, 152-8551, Japan

⁴ Earth-Life Science Institute, Institute of Science Tokyo, 2-12-1 Ookayama, Meguro-ku, Tokyo, 152-8551, Japan

*Corresponding author. Department of Earth and Planetary Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113-0033, Japan

Email: yokoyama-tenga@g.ecc.u-tokyo.ac.jp

Reproduction of the present-day ocean

We show the reproducibility of the present-day ocean conditions in our model at $\Delta\text{SST} = 0^\circ\text{C}$ (a global mean surface temperature of 15°C). The observed and calculated vertical profiles of some physical and biogeochemical tracers in the open ocean and upwelling regions are shown in Fig. S3. The calculated profiles of potential temperature θ and radiocarbon $\Delta^{14}\text{C}$ as physical tracers fall within the ranges of observational data from GLODAP (Key et al. 2015; Olsen et al. 2016), generally consistent with the averages in the Indian and Pacific oceans. Given the one-dimensional vertical structure, the model does not represent horizontal pattern of deep-water aging from the North Atlantic to the North Pacific, where $\Delta^{14}\text{C}$ values reach approximately -250‰ . Nevertheless, it adequately reproduces the overall aged deep waters, providing a reasonable representation of the ocean biogeochemical structure. The calculated profiles of dissolved O_2 and PO_4 also fall within the ranges of the observational data. In the open ocean, the O_2 concentration reaches a minimum of $\sim 48\ \mu\text{M}$ at a depth of 700 m, which corresponds to OMZ. The overall profiles are similar to those of the Indian and Pacific oceans, but the deep-water O_2 and PO_4 concentrations are $\sim 166\ \mu\text{M}$ and $\sim 1.9\ \mu\text{M}$, respectively, which are relatively close to those of the Atlantic Ocean. This discrepancy may be attributed to the simplified representation of the global conveyor belt in our model, which prevents the deep water from aging sufficiently to form the nutrient-rich, O_2 -poor characteristics of the deep Pacific. Despite

this limitation, our model reproduces the fundamental vertical distribution of oceanic tracers for the present-day ocean.

The simulated global net primary production (NPP) was $54.8 \text{ Gt C yr}^{-1}$, which falls well within the estimated range of $44\text{--}67 \text{ Gt C yr}^{-1}$ (Behrenfeld and Falkowski 1997; Behrenfeld et al. 2005; Carr et al. 2006; Berelson et al. 2007; Johnson and Bif 2021; Ryan-Keogh et al. 2023). Similarly, the export production, the flux of organic matter transported below the euphotic zone, was 9.8 Gt C yr^{-1} , which is consistent with previous estimates of $8.5\text{--}12 \text{ Gt C yr}^{-1}$ (Laws et al. 2000; Sarmiento and Gruber 2006; Dunne et al. 2007; Heinze et al. 2009). The total burial flux of organic carbon was $9.2 \text{ Tmol C yr}^{-1}$, which agrees with the previous estimate of $\sim 10 \text{ Tmol C yr}^{-1}$ (e.g., Berner 1982). The global N_2 fixation rate (NPP of N_2 -fixing cyanobacteria) was 216 Tg N yr^{-1} , which also aligns with the recent estimate of $223 \pm 30 \text{ Tg N yr}^{-1}$ (Shao et al. 2023). The primary production is overwhelmingly dominated by oxygenic photoautotrophs, with only a minor contribution from N_2 -fixing cyanobacteria. The simulated NPP values of oxygenic photoautotrophs and N_2 -fixing cyanobacteria were 13.5 and $0.33 \text{ mol C m}^{-2} \text{ yr}^{-1}$, respectively, in the open ocean. In the coastal upwelling region, these values were 45.8 and $2.1 \text{ mol C m}^{-2} \text{ yr}^{-1}$, respectively. The elevated NPP in the upwelling region agrees with observed values of $\sim 40\text{--}90 \text{ mol C m}^{-2} \text{ yr}^{-1}$ in some eastern boundary upwelling systems (Steinfeldt et al. 2015; Testa et al. 2018). As expected for the fully-oxic present-day ocean, GSB are completely

absent and not active in both regions. Collectively, these results confirm the model's ability to reproduce the present-day marine environment.

Relationship between ΔT and riverine P input

In this study, ΔSST and riverine P input rate J_P^{riv} are taken as independent parameters. However, for reference, the trajectory of the relationship between temperature and chemical weathering shown by the white dotted curve in the parameter spaces (Figs. 6 and 7) is an approximate prediction based on the assumption that warming progresses on a geological timescale. Here, this appendix describes the equations used to derive this trajectory.

First, we assume that ΔSST equals the global mean surface temperature anomaly, ΔT (in $^{\circ}\text{C}$). ΔT is calculated as follows (e.g., Berner and Kothavala 2001):

$$\Delta T = T - T^* = ESS \log_2 R_{\text{CO}_2} - W_s \left(\frac{t}{570} \right), \quad (\text{S. 1})$$

where T , R_{CO_2} , and t denote the global mean surface temperature (in $^{\circ}\text{C}$), the ratio of the atmospheric CO_2 partial pressure $p\text{CO}_2$ to $p\text{CO}_2^*$, and time (in Ma), respectively. ESS denotes Earth-system sensitivity set to 3°C , and W_s denotes the effect on ΔT of an increase in solar radiation over geological time set to 7.4°C . t is set to 0 Ma in this study. An asterisk denotes the present-day (pre-industrial) value, i.e., $T^* = 15^{\circ}\text{C}$ and $p\text{CO}_2^* = 280$ ppm.

Next, the continental weathering rate (in mol yr^{-1}) is formulated based on the GEOCARB model (e.g., Berner 2004). Carbonate weathering, $J_{\text{CaCO}_3}^w$, and silicate weathering,

74 $J_{\text{CaSiO}_3}^w$, are represented as follows:

$$75 \quad J_{\text{CaCO}_3}^w = f_{\text{Bc}}(t) f_{\text{Bb}}(t) J_{\text{CaCO}_3}^{w,*}, \quad (\text{S. 2})$$

$$76 \quad J_{\text{CaSiO}_3}^w = f_{\text{Bt}}(t) f_{\text{Bb}}(t) J_{\text{CaSiO}_3}^{w,*}. \quad (\text{S. 3})$$

77 Here, the temperature- and CO₂-dependent factors are described as follows:

$$78 \quad f_{\text{Bb}} = \left(\frac{2R_{\text{CO}_2}}{1 + R_{\text{CO}_2}} \right)^{0.4}, \quad (\text{S. 4})$$

$$79 \quad f_{\text{Bt}} = (1 + f_{\text{sil}}\Delta T)^{0.65} \exp\left(\frac{\Delta E}{R} \cdot \frac{\Delta T}{TT^*}\right), \quad (\text{S. 5})$$

$$80 \quad f_{\text{Bc}} = 1 + f_{\text{cal}}\Delta T. \quad (\text{S. 6})$$

81 For simplicity, we do not consider the weathering of organic matter and assume that $J_{\text{P}}^{\text{riv}}$ is

82 proportional to the sum of chemical weathering rates of carbonate and silicate; therefore, the

83 normalized riverine P input rate can be expressed as follows (Komar and Zeebe 2017):

$$84 \quad \frac{J_{\text{P}}^{\text{riv}}}{J_{\text{P}}^{\text{riv},*}} = \frac{J_{\text{CaCO}_3}^w + J_{\text{CaSiO}_3}^w}{J_{\text{CaCO}_3}^{w,*} + J_{\text{CaSiO}_3}^{w,*}}. \quad (\text{S. 7})$$

85

Figures

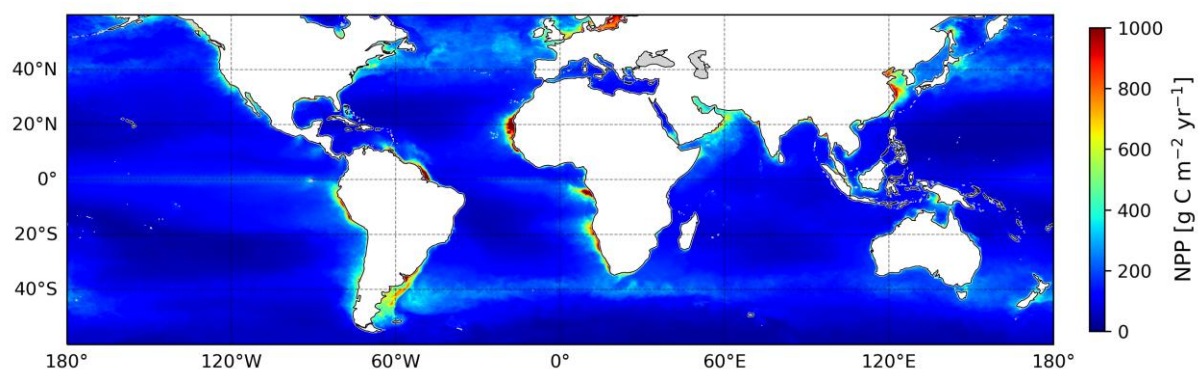
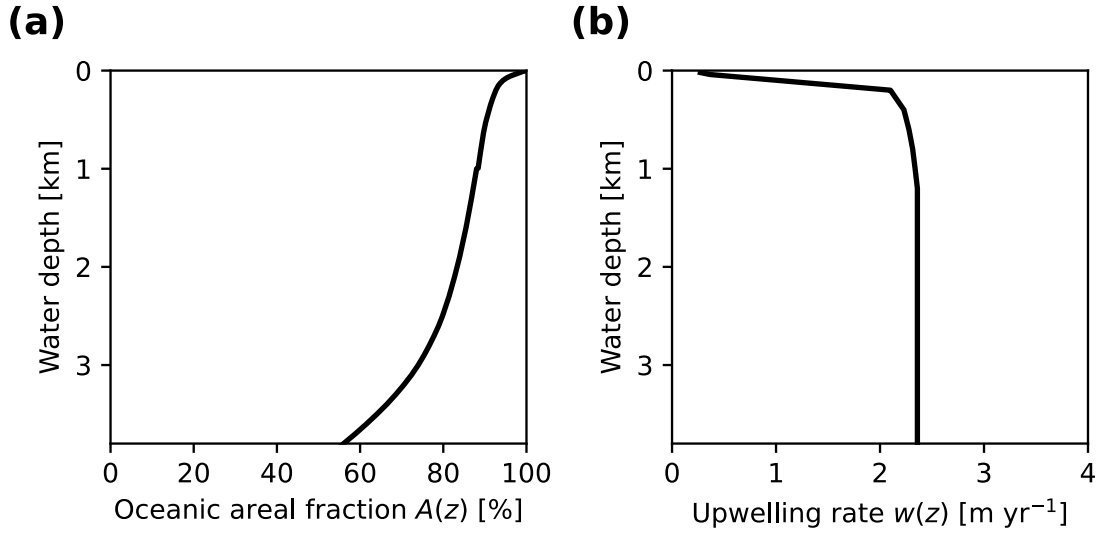


Figure S1. Global distribution of annual net primary production in 2021. Data were obtained from Ocean Productivity (<https://orca.science.oregonstate.edu/index.php>) and estimated using the vertically generalized productivity model (VGPM; Behrenfeld and Falkowski 1997) based on MODIS dataset.



93

94 Figure S2. Oceanic bathymetry and upwelling rate in the open ocean. (a) Oceanic areal fraction

95 $A(z)$ (normalized by sea surface area) (GEBCO Bathymetric Compilation Group 2025). (b)

96 Upwelling rate in the open ocean (m yr⁻¹) of the standard run.

97

98

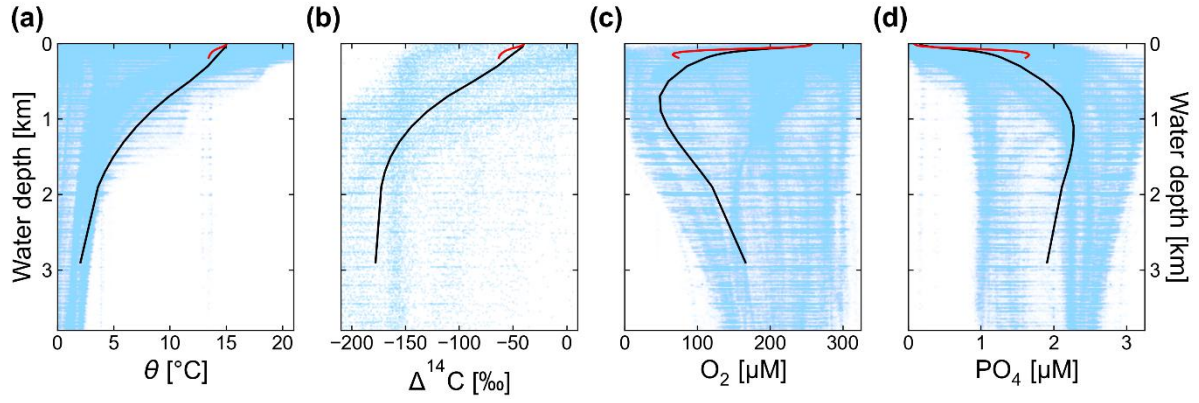
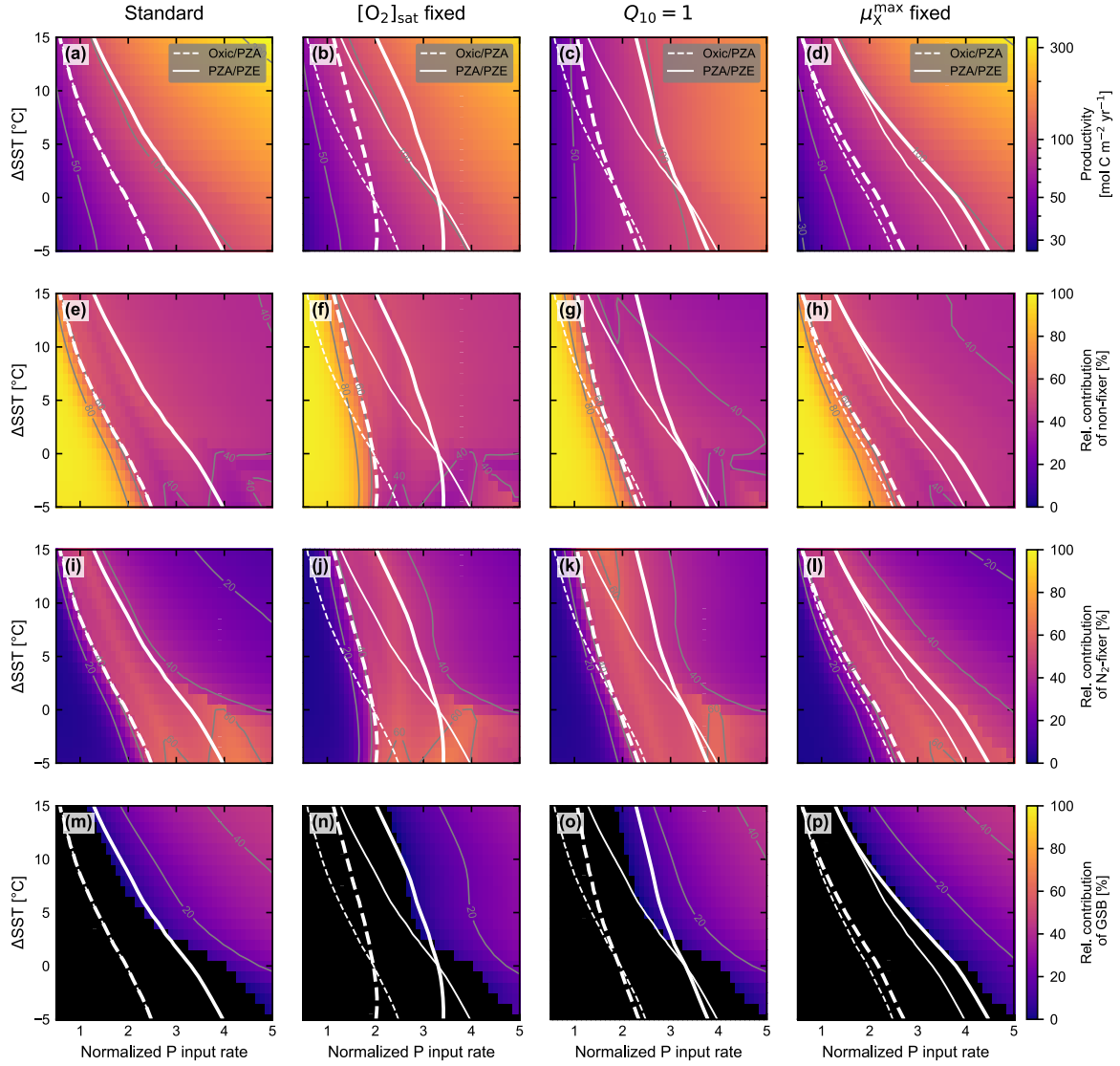


Figure S3. Vertical profiles of physical and biogeochemical tracers in the standard case. Panels show (a) potential temperature θ ($^{\circ}\text{C}$), (b) radiocarbon $\Delta^{14}\text{C}$ (‰), (c) dissolved O_2 (μM), and (d) PO_4 (μM). Solid black and red lines denote the simulated profiles in the open ocean and upwelling region, respectively. Observational data from the Global Ocean Data Analysis Project (GLODAP) database are also shown as scatter plots (Key et al. 2015; Olsen et al. 2016).



106

107

108

109

110

111

112

Figure S4. Sensitivity analysis of the structures of marine microbial ecosystem, decomposed by individual temperature-dependent factors. The results for the coastal upwelling region are shown. The contour plots show (a–d) NPP ($\text{mol C m}^{-2} \text{ yr}^{-1}$), and the relative contribution to NPP for (e–h) oxygenic photoautotrophs, (i–l) N_2 -fixing cyanobacteria, and (m–p) GSB. The columns correspond to different experimental settings. “Standard” represents the full model run including all temperature-dependent factors (identical to Fig. 7). The other columns represent

113 sensitivity experiments where specific temperature-dependent factors were disabled: “[O₂]_{sat}
114 fixed” (O₂ solubility fixed at ΔSST = 0 °C), “ $Q_{10} = 1$ ” (constant organic matter decomposition
115 rates), and “ $\mu_X^{\max}$ fixed” (maximum growth rate fixed at 15 °C). The thick dashed and solid
116 white contours indicate the boundaries of oxic/PZA and PZA/PZE for each experiment,
117 respectively. For comparison, in the right three columns, the boundaries of oxic/PZA and
118 PZA/PZE for the "Standard" case are overlaid as thin dashed and solid white contours,
119 respectively. Black shaded areas denote conditions where no GSB activity occurs.

120

References

- Behrenfeld MJ, Boss E, Siegel DA, Shea DM (2005) Carbon-based ocean productivity and phytoplankton physiology from space. *Global Biogeochem Cycles* 19:GB1006. doi:10.1029/2004gb002299.
- Behrenfeld MJ, Falkowski PG (1997) Photosynthetic rates derived from satellite - based chlorophyll concentration. *Limnol Oceanogr* 42:1-20. doi:10.4319/lo.1997.42.1.0001.
- Berelson WM, Balch WM, Najjar R, Feely RA, Sabine C, Lee K (2007) Relating estimates of CaCO₃ production, export, and dissolution in the water column to measurements of CaCO₃ rain into sediment traps and dissolution on the sea floor: A revised global carbonate budget. *Global Biogeochem Cycles* 21:GB1024. doi:10.1029/2006GB002803.
- Berner RA (1982) Burial of organic carbon and pyrite sulfur in the modern ocean; its geochemical and environmental significance. *Am J Sci* 282:451-473. doi:10.2475/ajs.282.4.451.
- Berner RA (2004) *The Phanerozoic carbon cycle: CO₂ and O₂*. Oxford University Press, New York, NY. doi:10.1093/oso/9780195173338.001.0001.
- Berner RA, Kothavala Z (2001) GEOCARB III: A revised model of atmospheric CO₂ over Phanerozoic time. *Am J Sci* 301:182-204. doi:10.2475/ajs.301.2.182.
- Carr M-E, Friedrichs MAM, Schmeltz M, Noguchi Aita M, Antoine D, Arrigo KR, Asanuma I, Aumont O, Barber R, Behrenfeld M, Bidigare R, Buitenhuis ET, Campbell J, Ciotti A, Dierssen H, Dowell M, Dunne J, Esaias W, Gentili B, Gregg W, Groom S, Hoepffner N, Ishizaka J, Kameda T, Le Quéré C, Lohrenz S, Marra J, Mélin F, Moore K, Morel A, et al. (2006) A comparison of global estimates of marine primary production from ocean color. *Deep Sea Res Part 2 Top Stud Oceanogr* 53:741-770. doi:10.1016/j.dsr2.2006.01.028.
- Dunne JP, Sarmiento JL, Gnanadesikan A (2007) A synthesis of global particle export from the surface ocean and cycling through the ocean interior and on the seafloor. *Global Biogeochem Cycles* 21:GB4006. doi:10.1029/2006GB002907.
- GEBCO Bathymetric Compilation Group 2025 (2025) *The GEBCO_2025 Grid - a continuous terrain model for oceans and land at 15 arc-second intervals*.

<http://dx.doi.org/10.5285/37c52e96-24ea-67ce-e063-7086abc05f29>.

Heinze C, Kriest I, Maier-Reimer E (2009) Age offsets among different biogenic and lithogenic components of sediment cores revealed by numerical modeling. *Paleoceanography* 24:PA4214. doi:10.1029/2008pa001662.

Johnson KS, Bif MB (2021) Constraint on net primary productivity of the global ocean by Argo oxygen measurements. *Nat Geosci* 14:769–774. doi:10.1038/s41561-021-00807-z.

Key RM, Olsen A, van Heuven S, Lauvset SK, Velo A, Lin X, Schirnick C, Kozyr A, Tanhua T, Hoppema M, Jutterström S, Steinfeldt R, Jeansson E, Ishii M, Perez FF, Suzuki T (2015) Global Ocean Data Analysis Project, Version 2 (GLODAPv2). Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, US Dept. of Energy, Oak Ridge, Tennessee. ORNL/CDIAC-162, NDP-093. doi:10.3334/CDIAC/OTG.NDP093_GLODAPv2.

Komar N, Zeebe RE (2017) Redox-controlled carbon and phosphorus burial: A mechanism for enhanced organic carbon sequestration during the PETM. *Earth Planet Sci Lett* 479:71–82. doi:10.1016/j.epsl.2017.09.011.

Laws EA, Falkowski PG, Smith WO Jr, Ducklow H, McCarthy JJ (2000) Temperature effects on export production in the open ocean. *Global Biogeochem Cycles* 14:1231–1246. doi:10.1029/1999GB001229.

Olsen A, Key RM, van Heuven S, Lauvset SK, Velo A, Lin X, Schirnick C, Kozyr A, Tanhua T, Hoppema M, Jutterström S, Steinfeldt R, Jeansson E, Ishii M, Pérez FF, Suzuki T (2016) The Global Ocean Data Analysis Project version 2 (GLODAPv2) – an internally consistent data product for the world ocean. *Earth Syst Sci Data* 8:297–323. doi:10.5194/essd-8-297-2016.

Ryan-Keogh TJ, Thomalla SJ, Chang N, Moalusi T (2023) A new global oceanic multi-model net primary productivity data product. *Earth Syst Sci Data* 15:4829–4848. doi:10.5194/essd-15-4829-2023.

Sarmiento JL, Gruber N (2006) *Ocean Biogeochemical Dynamics*. Princeton University Press, Princeton, NJ. doi:10.2307/j.ctt3fgxqx.

Shao Z, Xu Y, Wang H, Luo W, Wang L, Huang Y, Agawin NSR, Ahmed A, Benavides M, Bentzon-Tilia M, Berman-Frank I, Berthelot H, Biegala IC, Bif MB, Bode A, Bonnet S, Bronk DA, Brown MV, Campbell L, Capone DG, Carpenter EJ, Cassar N, Chang BX,

- 182 Chappell D, Chen Y-LL, Church MJ, Cornejo-Castillo FM, Detoni AMS, Doney SC,
183 Dupouy C, et al. (2023) Global oceanic diazotroph database version 2 and elevated
184 estimate of global oceanic N₂ fixation. *Earth Syst Sci Data* 15:3673–3709.
185 doi:10.5194/essd-15-3673-2023.
- 186 Steinfeldt R, Sültenfuß J, Dengler M, Fischer T, Rhein M (2015) Coastal upwelling off Peru
187 and Mauritania inferred from helium isotope disequilibrium. *Biogeosciences* 12:7519–
188 7533. doi:10.5194/bg-12-7519-2015.
- 189 Testa G, Masotti I, Farías L (2018) Temporal variability in net primary production in an
190 upwelling area off central Chile (36°S). *Front Mar Sci* 5:361275.
191 doi:10.3389/fmars.2018.00179.