

Supporting information for

RADIV1: a non-steady-state early diagenetic model for ocean sediments in Julia and MATLAB/GNU Octave

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Contents of this file

Tables S1 to S3

Figure S1

Supplementary references

Table S1. Environmental conditions, bottom-water and sediment properties for the North-western Atlantic Ocean station.

Variable	Value	Source
Station ID	Station #9	Hales et al. (1994)
Location	North Atlantic	Hales et al. (1994)
Coordinates	34.33N / 70.35W	Hales et al. (1994)
Depth	5210 m	Hales et al. (1994)
Temperature	2.2 °C	Hales et al. (1994)
Salinity	34.9	Hales et al. (1994)
DBL thickness	938 μm	Sulpis et al. (2018)
<i>Solid fluxes to the seafloor ($\text{mol m}^{-2} \text{a}^{-1}$)</i>		
POC flux (F_{POC})	0.18 (6.0 g POM $\text{m}^2 \text{a}^{-1}$)	Hales et al. (1994)
Fast-decay POC	0.70 x F_{POC}	Assumed
Slow-decay POC	0.27 x F_{POC}	Assumed
Refractory POC	0.03 x F_{POC}	Assumed
CaCO ₃ flux (F_{CaCO_3})	0.20 (20.02 g CaCO ₃ $\text{m}^2 \text{a}^{-1}$)	Hales et al. (1994)
Calcite	F_{CaCO_3}	Assumed
Aragonite	0	Assumed
MnO ₂ flux (F_{MnO_2})	0.0005	Assumed
Fe(OH) ₃ flux ($F_{\text{Fe(OH)}_3}$)	0.0005	Assumed
FeS flux (F_{FeS})	0	Boudreau (1996)
<i>Sediment surface properties</i>		
Surface [CaCO ₃]	27 dry wt %	Hales et al. (1994)
Surface [POC]	0.31 dry wt %	Hales et al. (1994)
Clay flux	26 g $\text{m}^{-2} \text{a}^{-1}$	Assumed
Surface porosity	0.91	Assumed
Porosity at depth	0.74	Assumed
<i>Bottom-water chemistry</i>		
TAlk	2342 $\mu\text{mol kg}^{-1}$	Hales et al. (1994)
ΣCO_2	2186 $\mu\text{mol kg}^{-1}$	Hales et al. (1994)
[O ₂]	266.6 $\mu\text{mol kg}^{-1}$	Hales et al. (1994)
[ΣNO_3]	20.0668 $\mu\text{mol kg}^{-1}$	GLODAPv2 (Lauvset et al., 2016)
[ΣSO_4]	29.180 mmol kg^{-1}	Computed from S (Millero, 2013)
[ΣPO_4]	1.3561 $\mu\text{mol kg}^{-1}$	GLODAPv2 (Lauvset et al., 2016)
[ΣNH_4]	0	Assumed
[$\Sigma\text{H}_2\text{S}$]	0	Assumed
[Mn ²⁺]	0.5 nmol kg^{-1}	Typical deep-sea value (Morton et al., 2019)
[Fe ²⁺]	0.5 nmol kg^{-1}	Typical deep-sea value (Abadie et al., 2017)
[Ca ²⁺]	10.255 mmol kg^{-1}	Computed from S (Riley and Tongudai, 1967)
[CO ₃ ²⁻] _{sw} ($\mu\text{mol kg}^{-1}$)	102.6 $\mu\text{mol kg}^{-1}$	Computed (RADI)
[CO ₃ ²⁻] _{eq Calcite} ($\mu\text{mol kg}^{-1}$)	117.6 $\mu\text{mol kg}^{-1}$	Computed (RADI)
[CO ₃ ²⁻] _{eq Arag.} ($\mu\text{mol kg}^{-1}$)	175.5 $\mu\text{mol kg}^{-1}$	Computed (RADI)
Ω_{ca}	0.88	Computed (RADI)
Ω_{ar}	0.59	Computed (RADI)

Table S2. Environmental conditions, bottom-water and sediment properties for the Southern Pacific station.

Variable	Value	Source
Station ID	Station #7.3	Sayles et al. (2001)
Location	Southern Pacific	Sayles et al. (2001)
Coordinates	60.15S / 170.11W	Sayles et al. (2001)
Depth	3860 m	Sayles et al. (2001)
Temperature	0.84 °C	Sayles et al. (2001)
Salinity	34.696	Sayles et al. (2001)
DBL thickness	715 μm	Sulpis et al. (2018)
<i>Solid fluxes to the seafloor ($\text{mol m}^{-2} \text{a}^{-1}$)</i>		
POC flux (F_{POC})	0.138 (4.6 g POM $\text{m}^2 \text{a}^{-1}$)	Assumed
Fast-decay POC	0.70 x F_{POC}	Assumed
Slow-decay POC	0.27 x F_{POC}	Assumed
Refractory POC	0.03 x F_{POC}	Assumed
CaCO ₃ flux (F_{CaCO_3})	0.25 (25.02 g CaCO ₃ $\text{m}^2 \text{a}^{-1}$)	Assumed
Calcite	F_{CaCO_3}	Assumed
Aragonite	0	Assumed
MnO ₂ flux (F_{MnO_2})	0.0005	Assumed
Fe(OH) ₃ flux ($F_{\text{Fe(OH)}_3}$)	0.0005	Assumed
FeS flux (F_{FeS})	0	Boudreau (1996)
<i>Sediment surface properties</i>		
Surface [CaCO ₃]	37.7 dry wt %	Sayles et al. (2001)
Surface [POC]	0.37 dry wt %	Sayles et al. (2001)
Clay flux	32 g $\text{m}^{-2} \text{a}^{-1}$	Sayles et al. (2001), November – February average
Surface porosity	0.91	Sayles et al. (2001)
Porosity at depth	0.87	Assumed
<i>Bottom-water chemistry</i>		
TAlk	2365 $\mu\text{mol kg}^{-1}$	GLODAPv2 (Lauvset et al., 2016)
ΣCO_2	2260 $\mu\text{mol kg}^{-1}$	GLODAPv2 (Lauvset et al., 2016)
[O ₂]	215.7 $\mu\text{mol kg}^{-1}$	GLODAPv2 (Lauvset et al., 2016)
[ΣNO_3]	32.2416 $\mu\text{mol kg}^{-1}$	GLODAPv2 (Lauvset et al., 2016)
[ΣSO_4]	29.010 mmol kg^{-1}	Computed from S (Millero, 2013)
[ΣPO_4]	2.2428 $\mu\text{mol kg}^{-1}$	GLODAPv2 (Lauvset et al., 2016)
[ΣNH_4]	0	Assumed
[$\Sigma\text{H}_2\text{S}$]	0	Assumed
[Mn ²⁺]	0.5 nmol kg^{-1}	Typical deep-sea value (Morton et al., 2019)
[Fe ²⁺]	0.5 nmol kg^{-1}	Typical deep-sea value (Abadie et al., 2017)
[Ca ²⁺]	10.196 mmol kg^{-1}	Computed from S (Riley and Tongudai, 1967)
[CO ₃ ²⁻] _{sw} ($\mu\text{mol kg}^{-1}$)	77.5 $\mu\text{mol kg}^{-1}$	Computed (RADI)
[CO ₃ ²⁻] _{eq Calcite} ($\mu\text{mol kg}^{-1}$)	91.7 $\mu\text{mol kg}^{-1}$	Computed (RADI)
[CO ₃ ²⁻] _{eq Arag.} ($\mu\text{mol kg}^{-1}$)	138.9 $\mu\text{mol kg}^{-1}$	Computed (RADI)
Ω_{ca}	0.85	Computed (RADI)
Ω_{ar}	0.56	Computed (RADI)

Table S3. Environmental conditions, bottom-water and sediment properties for the Central Equatorial Pacific station.

Variable	Value	Source
Station ID	Station #W-2	Berelson et al. (1994) / Hammond et al. (1996)
Location	Equatorial Pacific	Berelson et al. (1994) / Hammond et al. (1996)
Coordinates	0.0N / 139.9W	Berelson et al. (1994) / Hammond et al. (1996)
Depth	4370 m	Berelson et al. (1994) / Hammond et al. (1996)
Temperature	1.4 °C	GLODAPv2 (Lauvset et al., 2016)
Salinity	34.69	GLODAPv2 (Lauvset et al., 2016)
DBL thickness	1 mm	Assumed
<i>Solid fluxes to the seafloor (mol m⁻² a⁻¹)</i>		
POC flux (F_{POC})	0.20 (6.6 g POM m ² a ⁻¹)	Assumed
Fast-decay POC	0.70 x F_{POC}	Assumed
Slow-decay POC	0.27 x F_{POC}	Assumed
Refractory POC	0.03 x F_{POC}	Assumed
CaCO ₃ flux (F_{CaCO_3})	0.22 (22.02 g CaCO ₃ m ² a ⁻¹)	Assumed
Calcite	F_{CaCO_3}	Assumed
Aragonite	0	Assumed
MnO ₂ flux (F_{MnO_2})	0.0005	Assumed
Fe(OH) ₃ flux ($F_{\text{Fe(OH)}_3}$)	0.0005	Assumed
FeS flux (F_{FeS})	0	Boudreau (1996)
<i>Sediment surface properties</i>		
Surface [CaCO ₃]	76.1 dry wt %	Hammond et al (1996) Table 1
Surface [POC]	0.24 dry wt %	Hammond et al (1996) Table 1
Clay flux	2 g m ⁻² a ⁻¹	Hammond et al (1996)
Surface porosity	0.85	Hammond et al (1996)
Porosity at depth	0.74 (4cm)	Berelson et al. (1994)
<i>Bottom-water chemistry</i>		
TAlk	2426.0 μmol kg ⁻¹	GLODAPv2 (Lauvset et al., 2016)
ΣCO ₂	2324.3 μmol kg ⁻¹	GLODAPv2 (Lauvset et al., 2016)
[O ₂]	159.7 μmol kg ⁻¹	GLODAPv2 (Lauvset et al., 2016)
[ΣNO ₃]	36.93 μmol kg ⁻¹	GLODAPv2 (Lauvset et al., 2016)
[ΣSO ₄]	29.005 mmol kg ⁻¹	Computed from S (Millero, 2013)
[ΣPO ₄]	2.39 μmol kg ⁻¹	GLODAPv2 (Lauvset et al., 2016)
[ΣNH ₄]	0	Assumed
[ΣH ₂ S]	0	Assumed
[Mn ²⁺]	0.5 nmol kg ⁻¹	Typical deep-sea value (Morton et al., 2019)
[Fe ²⁺]	0.5 nmol kg ⁻¹	Typical deep-sea value (Abadie et al., 2017)
[Ca ²⁺]	10.193 mmol kg ⁻¹	Computed from S (Riley and Tongudai, 1967)
[CO ₃ ²⁻] _{sw} (μmol kg ⁻¹)	77.9 μmol kg ⁻¹	Computed (RADI)
[CO ₃ ²⁻] _{eq Calcite} (μmol kg ⁻¹)	100.0 μmol kg ⁻¹	Computed (RADI)
[CO ₃ ²⁻] _{eq Arag.} (μmol kg ⁻¹)	150.7 μmol kg ⁻¹	Computed (RADI)
Ω _{ca}	0.78	Computed (RADI)
Ω _{ar}	0.52	Computed (RADI)

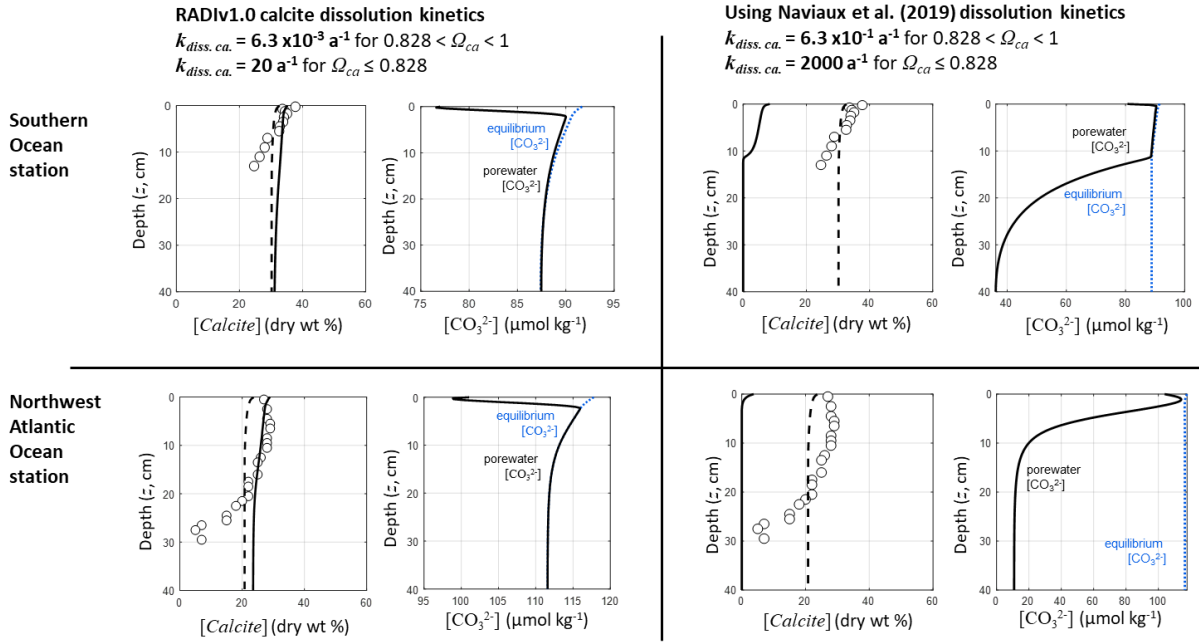


Figure S1. Comparison of predicted calcite and CO_3^{2-} concentration profiles using the calcite dissolution kinetics implemented in RADiv1 (left) and using the rate constants from the original publication (Naviaux et al., 2019a) coupled with the surface area of foraminifera ($400 \text{ m}^2 \text{ mol}^{-1}$, from Subhas et al., 2018). The dashed line represents results from the MUDS model.

Supplementary references

- Abadie, C., Lacan, F., Radic, A., Pradoux, C. and Poitrasson, F. (2017) Iron isotopes reveal distinct dissolved iron sources and pathways in the intermediate versus deep Southern Ocean. *Proceedings of the National Academy of Sciences* 114, 858-863.
- Berelson, W.M., Hammond, D.E., McManus, J. and Kilgore, T.E. (1994) Dissolution kinetics of calcium carbonate in equatorial Pacific sediments. *Global Biogeochemical Cycles* 8, 219-235.
- Boudreau, B.P. (1996) A method-of-lines code for carbon and nutrient diagenesis in aquatic sediments. *Computers & Geosciences* 22, 479-496.
- Hales, B., Emerson, S. and Archer, D. (1994) Respiration and dissolution in the sediments of the western North Atlantic: estimates from models of in situ microelectrode measurements of porewater oxygen and pH. *Deep Sea Research Part I: Oceanographic Research Papers* 41, 695-719.
- Hammond, D.E., McManus, J., Berelson, W.M., Kilgore, T.E. and Pope, R.H. (1996) Early diagenesis of organic material in equatorial Pacific sediments: stoichiometry and kinetics. *Deep Sea Research Part II: Topical Studies in Oceanography* 43, 1365-1412.
- Lauvset, S.K., Key, R.M., Olsen, A., van Heuven, S., Velo, A., Lin, X., Schirnick, C., Kozyr, A., Tanhua, T., Hoppema, M., Jutterström, S., Steinfeldt, R., Jeansson, E., Ishii, M., Perez, F.F., Suzuki, T. and Watelet, S. (2016) A new global interior ocean mapped climatology: the $1^\circ \times 1^\circ$ GLODAP version 2. *Earth System Science Data* 8, 325-340.
- Millero, F.J. (2013) *Chemical Oceanography*, Fourth Edition. CRC Press - Taylor & Francis Group, Boca Raton.
- Morton, P.L., Landing, W.M., Shiller, A.M., Moody, A., Kelly, T.D., Bizimis, M., Donat, J.R., De Carlo, E.H. and Shacat, J. (2019) Shelf Inputs and Lateral Transport of Mn, Co, and Ce in the Western North Pacific Ocean. *Frontiers in Marine Science* 6.
- Naviaux, J.D., Subhas, A.V., Dong, S., Rollins, N.E., Liu, X., Byrne, R.H., Berelson, W.M. and Adkins, J.F. (2019a) Calcite dissolution rates in seawater: Lab vs. in-situ measurements and inhibition by organic matter. *Marine Chemistry* 215.
- Riley, J.P. and Tongudai, M. (1967) The major cation/chlorinity ratios in sea water. *Chemical Geology* 2, 263-269.
- Sayles, F.L., Martin, W.R., Chase, Z. and Anderson, R.F. (2001) Benthic remineralization and burial of biogenic SiO_2 , CaCO_3 , organic carbon, and detrital material in the Southern Ocean along a transect at 170 West. *Deep Sea Research II* 48, 4323-4383.
- Subhas, A.V., Rollins, N.E., Berelson, W.M., Erez, J., Ziveri, P., Langer, G. and Adkins, J.F. (2018) The dissolution behavior of biogenic calcites in seawater and a possible role for magnesium and organic carbon. *Marine Chemistry* 205, 100-112.
- Sulpis, O., Boudreau, B.P., Mucci, A., Jenkins, C.J., Trossman, D.S., Arbic, B.K. and Key, R.M. (2018) Current CaCO_3 dissolution at the seafloor caused by anthropogenic CO_2 . *Proceedings of the National Academy of Sciences* 115, 11700-11705.