

Supplementary Material to

“Model of Early Diagenesis in the Upper Sediment
with Adaptable complexity – MEDUSA (v. 2) :
a time-dependent biogeochemical
sediment module for Earth System Models,
process analysis and teaching”

Additional Results

Guy Munhoven

Dépt. d’Astrophysique, Géophysique et Océanographie,
Université de Liège,
B-4000 Liège, Belgium,
eMail: Guy.Munhoven@uliege.be

14th September 2020

Abstract

We provide here additional graphs and results to complete the experiments presented in the main paper. These include the O₂ profile adjustment results for the thirteen stations considered in the JEASIM application. We also report the calcite mass fractions in the deposition flux, produced by the fitting procedure and the resulting calcite mass fraction in the surface sediment.

1 JEASIM – Complex composition and reaction network model

1.1 Oxygen profiles

The O₂ microprofile data used in the JEASIM experiments are comparatively straightforward to fit as illustrated in Figs. S1 and S2, which show the oxygen profiles obtained by the fitting procedure described in the main text for all of the thirteen sites. The best-fit parameter results are given in the `jeasim.cl.ods` spreadsheet that can be found in `work/jeasim` in the directory tree of the code and data archive included in this Supplement. `jeasim.cl.ods` also includes sheets that were used to set the initial values for the iterative optimisations, for the first stage oxygen profile fit procedure and for each of the subsequent calcite dissolution rate order fits.

The fits obtained here are essentially indistinguishable from those of Jourabchi et al. (2008).

1.2 pH profile results

Tables S1 to S3 give the calcite mass fractions in the deposition flux that has been adjusted to fit the porewater pH profiles from Jourabchi et al. (2008) and the resulting surface sediment mass fraction of calcite, for each of the three rounds of fitting (see main text for details).

References

Jourabchi, P., Meile, C., Pasion, L. R., and Van Cappellen, P.: Quantitative interpretation of pore water O₂ and pH distributions in deep-sea sediments, *Geochim. Cosmochim. Ac.*, 72, 1350–1364, <https://doi.org/10.1016/j.gca.2007.12.012>, 2008.

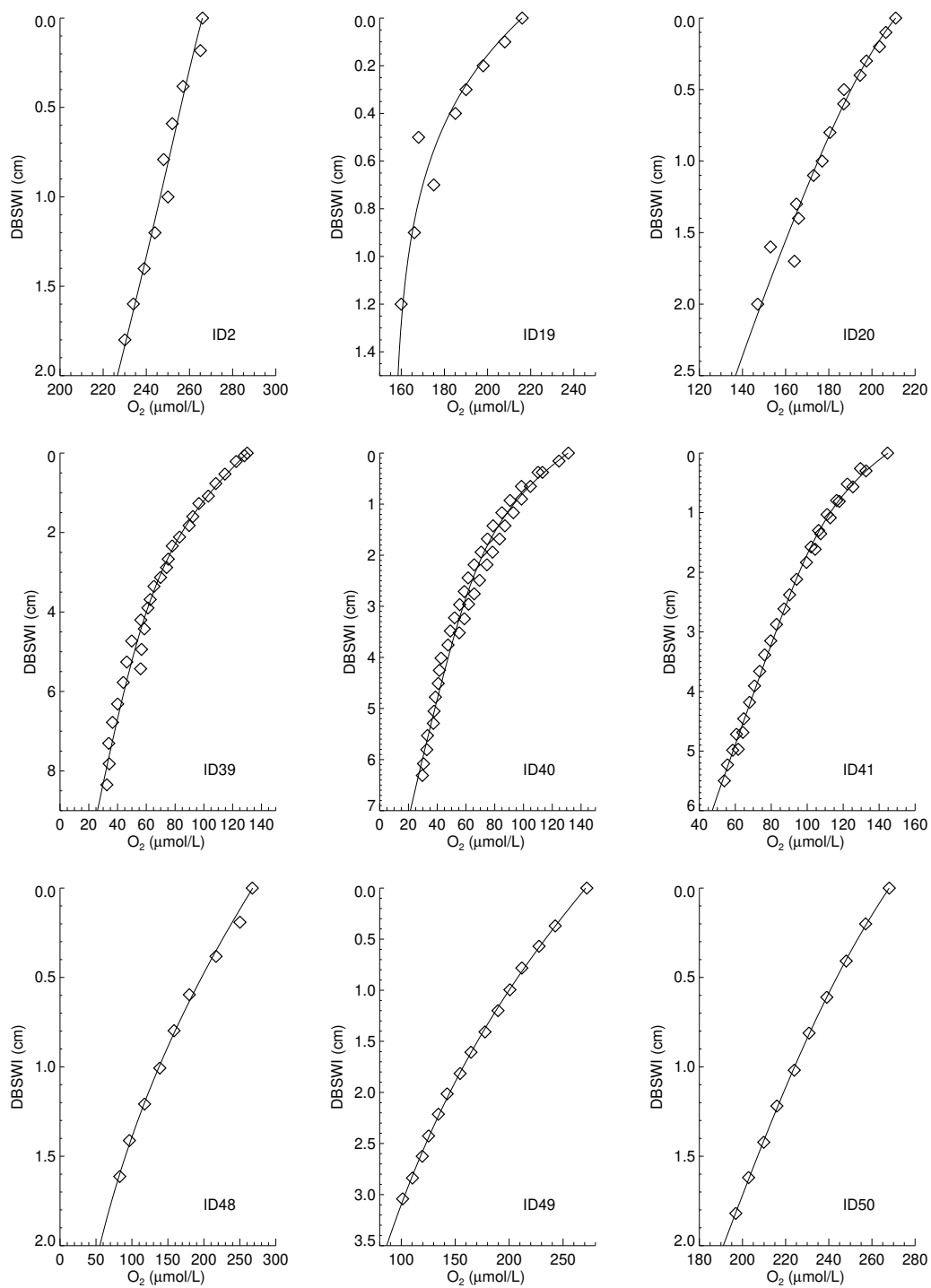


Figure S1: O_2 profiles for sites 2–50.

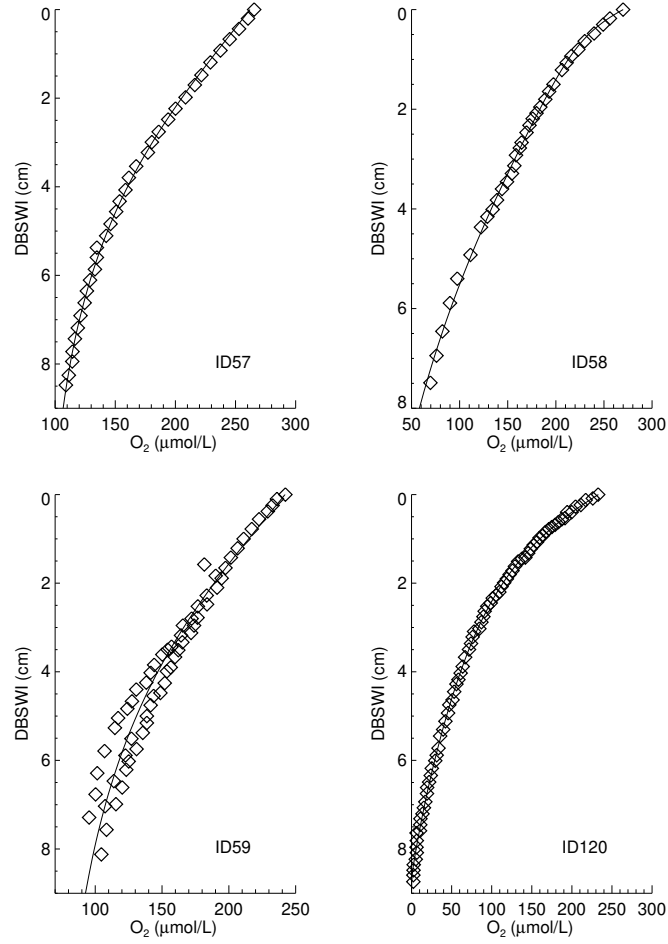


Figure S2: O₂ profiles for sites 57–120.

Site	$n = 4.5$		$n = 2$		$n = 1$	
	$J_{\%Calc}$	%Calc	$J_{\%Calc}$	%Calc	$J_{\%Calc}$	%Calc
2	<u>5391</u>	<u>4081</u>	<u>188</u>	<u>117</u>	<u>949</u>	<u>916</u>
19	<u>832</u>	1.0	<u>746</u>	0.16	<u>709</u>	0.14
20	<u>299</u>	6.7	<u>283</u>	1.5	<u>277</u>	1.2
39	<u>337</u>	<u>334</u>	<u>288</u>	<u>286</u>	9.2	7.0
40	3.4	0.08	3.7	0.01	3.6	0.01
41	81	77	5.6	0.04	5.5	0.04
48	7.9	2.2	5.9	0.01	5.9	0.01
49	<u>2329</u>	<u>2293</u>	<u>2329</u>	<u>2291</u>	<u>403</u>	<u>363</u>
50	53	25	31	0.07	31	0.08
57	<u>497</u>	<u>495</u>	<u>497</u>	<u>495</u>	<u>497</u>	<u>495</u>
58	40	19	22	0.22	21	0.21
59	44	0.3	36	0.32	34	0.32
120	1.0	0.01	1.0	0.01	1.1	0.01

Table S1: Fitting step 1 – no constraints. $J_{\%Calc}$ is the calcite mass fraction in the deposition flux and %Calc that fraction in the surface sediment (top 10 cm), both in percent. Underlined figures are physically unrealistic results.

Site	$n = 4.5$		$n = 2$		$n = 1$	
	$J_{\%Calc}$	%Calc	$J_{\%Calc}$	%Calc	$J_{\%Calc}$	%Calc
2	90	7.8	90	41	90	56
19	90	1.9	90	1.8	90	1.5
20	90	4.9	90	4.8	90	11
39	90	87	90	88	9.2	7.0
40	3.4	0.08	3.7	0.01	3.6	0.01
41	81	77	5.6	0.04	5.5	0.04
48	7.9	2.2	5.9	0.01	5.9	0.01
49	90	53	90	50	90	50
50	53	25	31	0.07	31	0.08
57	90	88	90	88	90	88
58	40	19	22	0.22	21	0.21
59	44	0.3	36	0.32	34	0.32
120	1.0	0.01	1.0	0.01	1.1	0.01

Table S2: Fitting step 2 – calcite mass fraction in the deposition capped at 90%. $J_{\%Calc}$ is the calcite mass fraction in the deposition flux and %Calc that in the surface sediment (top 10 cm), both in percent. Figures set in boldface are prescribed.

Site	$n = 4.5$		$n = 2$		$n = 1$	
	$J_{\%Calc}$	%Calc	$J_{\%Calc}$	%Calc	$J_{\%Calc}$	%Calc
2	<u>143</u>	22	72	22	56	22
19	<u>728</u>	10	<u>584</u>	10	<u>525</u>	10
20	<u>298</u>	10	<u>262</u>	10	<u>247</u>	10
39	93	90	92	90	92	90
40	93	90	93	90	93	90
41	92	87	92	87	91	87
48	27	21	27	21	27	21
49	63	26	66	26	63	26
50	59	31	59	31	58	31
57	68	66	68	66	68	66
58	85	64	85	64	86	64
59	75	43	71	43	68	43
120	3.9	3.2	4.0	3.2	4.0	3.2

Table S3: Fitting step 3 – calcite mass fraction in the top 10 cm of the sediment constrained by the observations. $J_{\%Calc}$ is the calcite mass fraction in the deposition flux and %Calc that in the surface sediment (top 10 cm), both in percent. Figures set in boldface are prescribed; underlined figures are physically unrealistic results.