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”

Author’s Response

Guy Munhoven

20th April 2021

Dear Sandra,

please find below my point to point listing of the changes made to the manuscript in response to the referees’ comments and suggestions. For the sake of brevity, I do not repeat here the justifications that were given in the Author’s Comments in reply to the Referees Comments. A *latexdiff* version of the manuscript highlighting the insertions and deletions in the text has also been uploaded alongside the revised manuscript.

I hope the manuscript is now acceptable for publication.

Best regards,

Guy

Revisions in response to comments by Anonymous Referee #1

General Comments

2.2.2 Solution strategy
The different initial conditions for the iteration scheme are excellent and clear. However, I think it would be good if the convergence criteria is made more clear in the main manuscript. From your “Technical Reference” I understand that you test for a convergence of the (solid) concentration profiles. The second criterion, however, is difficult to comprehend. I think it would be good to include a clear description of both criteria in the main manuscript. Also, is the overall solution divided into different steps? E.g. is OM degradation and the resulting profile calculated first and from it MEDUSA deduces the O2 profile? Because the zonation of oxic and anoxic OM degradation has implications for the production of alkalinity and thus carbonate dissolution. Finally, does MEDUSA check for the convergence of burial velocity at the very end if the solid components are not declared as volumeless?

- Reorganised the contents of sections 2.1 and 2.2 and furthermore rewrote large parts of section 2.2 to improve the description of the solution strategy and the two-level convergence criterion.
- Also extended chapter 3 of the "MEDUSA *Technical Reference*" to include explicit details about the scaling of solutes' equations.

Specific/technical comments

ln. 21: I think it should read "the latter" here

OK, corrected.

ln. 46: Please give example reference for the meta-model approach.

Added references to Sigman et al. (1998) and Dunne et al. (2007) (as announced in the AC1) and furthermore to Ridgwell (2007) and Capet et al. (2016).

ln. 49 - 50: Please add references for examples for the "expert-chosen empirical parametric functions" and for the "system identification theory" approach

- "expert-chosen empirical parametric functions": added reference to Dunne et al. (2007);
- "system identification theory": added references to Crucifix (2012) and to Ermakov et al. (2013) and rephrased sentence.

Table 1+2 and in the corresponding text (e.g. ln 70 and first paragraph on pg. 5): For completeness please include OMEN-SED (Hülse et al., (2018) which is an analytical early diagenetic steady-state model for OM degradation dynamics with flexible resolution. OMEN-SED is available as standalone model and coupled to cGENIE and presents a noval approach to simulate benthic-pelagic coupling (i.e. different to the approaches presented in Table 1 and 2).

- Added OMEN-SED in Tables 1 and 2.
- Added information about the coupling of OMEN-SED to cGENIE at lines 119–126 in the *latexdiff* report.

Ln 127: "... during which some parts gets remineralised (i.e., oxidised or dissolved), and some parts gets buried." Please check the spelling here.

Text modified to read "... during which some parts get remineralised (i.e., oxidised or dissolved), and the rest gets buried."

Ln 130-133: Please add reference.

Added reference to Archer et al. (1998).

ln 134: "Previously buried carbonates will then return to the sedimentary mixed as a result of the bioturbation activity..." I guess the "sedimentary mixing" is a typo, please rephrase.

"the sedimentary mixed" modified to read "the sedimentary mixed layer".

Page 7: ln 142: I think the "instead of" can be deleted

OK, deleted.

Page 9: ln 197: So for solutes DBL is the same as REACLAY only that porosity equals 1? Could you please include a brief explanation why/when a DBL is important and when it should be used?

Added new section 2.5 "Code building and customisation options: taming the flexibility" which also discusses the role and importance of a DBL.

Page 10: ln 215: Pointing the reader here to you supplementary document "Early Diagenesis in Sediments "A one-dimensional model formulation" would be good as it provides more and very useful information for instance about the parameterisations for tortuosity and how the diffusion coefficients are calculated. Maybe also cite Ullman and Aller (1982) who did a lot of early work on diffusion coefficients and tortuosity parameterization.

Rewrote text at lines 215*ff* (in the submitted manuscript, lines 268*ff* in the *latexdiff* report) and added footnote inviting to refer to the supplementary document for further details and references. Also included reference to Ullman and Aller (1982) to that document.

ln. 221: bioirrigation "constant". What are you using for alpha in the set-up used in your simulations for this manuscript? Is it a depth dependent approach (e.g. Soetaert et al. (1996))?

- Nothing changed around old l. 221, as the required information was already present.
- Added notice in the introductory paragraph of section 3 to precise that α is set to zero for the test case applications presented.

Page 11: Additional constraints: Maybe it makes sense to include the constraint that the porosity profile is prescribed (i.e. time independent, $d\varphi/dt = 0$) at this point?

Added short notice about the steady-state assumption on φ at the end of the paragraph that presents the equation for determining the advection rate profile (now eq. (3) in section 2.1.1, heading "Transport") and non-steady state φ would modify that equation.

Page 12: ln. 292: "...and the topmost interior node of REACLAY" Is this part of the sentence not redundant as this note is always below the top of REACLAY? The same applies for the bottom of DBL.

Nothing changed as I prefer the current text (see reply in AC1).

Ln 297: "but the spacing and extent of each of these may be different." Depending on what? E.g. if the user wants to have a higher resolution for shelf-sediments compared to the deep ocean?

No change required.

Page 16: ln 405: I think this should read: dissolved organic matter instead of "dissolved inorganic matter"

OK, corrected as suggested.

Page 17: ln 438: I think it should read: simulation experiments from Munhoven (2007)

Suggestion incorrect as explained in the AC1 – nothing changed.

ln 450-451: I guess the sentence could be changed to: "MBM is an eleven-box carbon cycle model of the carbon cycle in the ocean and the atmosphere"

Text changed to "MBM is an eleven-box model of the carbon cycle in the ocean and the atmosphere"

ln 453: close the parenthesis after Pacific

OK, corrected.

Section 3.2 COUPSIM — Coupling simulator page 21 ln. 519: why did you just simulate depths greater than 1000m below sea-level? And are the shallower observations in Seiter (where generally the highest TOC concentrations are observed) excluded from the data-set (or is there hardly any data for shallower settings because of the resolution of the observations)?

Added explanatory sentence regarding this choice (lines 700*ff* in the *latexdiff* document).

Fig. 3 : I think opal are the red triangles. In that case the caption needs to be corrected.

OK, corrected.

Ln 551: Your rate constants for OM degradation could be for instance compared to Palastanga et al. (2011) who used the HAMOCC model coupled to a diagenetic model using a 1G-approach for OM. They also compare their results to the Seiter et al. (2005) data and find the best fit using k_ox=0.005 yr-1 and k_anox=0.002 yr-1 for depths $>$ 2000m (k_ox=0.01 yr-1 and k_anox=0.008 yr-1 for depth $<$ 2000m).

Amended paragraph (see lines 735*ff* in the *latexdiff* report) to include that comparison.

page 27 ln 652: spelling: I think it should read: "... in order to allow..."

OK, corrected.

Revisions in response to comments by Anonymous Referee #2

General comments

(1) The model seems to apply different numerical schemes to different realms as inferred from Fig. 1. However, how the model does this is not 100% clear from the ms. Also, there seems to be some options that could affect the overall solution scheme/sequence, e.g., whether the model includes diffusion boundary layer or not; whether the advection is solved or not; whether the model tracks time or not, etc. Although the details are referred to the Supplement when relevant, a flow chart of the calculation scheme/sequence including branches for some important model options would be very helpful for the reader to grasp what is going on in the model.

> Reorganised the contents of sections 2.1 and 2.2 and rewrote large parts of section 2.2 to provide more details about the solution strategy. No flow chart added, as I am not convinced about the usefulness of such a scheme for a complex model such as MEDUSA.

(2) Pros and cons of options are discussed but it is not 100% obvious to the reader when to adopt which option. For example, in the ALL experiment, the author discussed the difference between the tracked time and actual time and the cause of it, but not sure when/why we should use the tracked time. Also, the author described that the implementation of mineral volume options (related to advection scheme) does not affect the overall results, which will make the reader to wonder when/why to adopt which option regarding mineral volumes. Furthermore, under what conditions should we adopt the option of DBL? As a model description paper, providing a conclusion on the options may not be obligation, but guiding the reader a little bit more could be desired.

> Added a new section 2.5 ("Code building and customisation options: taming the flexibility") to offer some guidance to potential users about the most common options, including a discussion on the importance of a DBL

Specific comments

Table 1: In my understanding $CaCO_3$ and clay are not vertically resolved in Archer's original model (1991); only porewater chemistry and OM are vertically resolved. How do you define the layer number when layer numbers are different between different species as is the case for Archer (1991)?

> - Added notice to the caption of Table 1 regarding the meaning of the number of layers/nodes.
> - Amended information about the model composition in Archer (1991) in Table 2. Similarly corrected information about Archer (1996).

Line 248: Are you saying that one of solid species is treated as a dilatant material and does not necessarily complies with advection law (e.g., Eq. (1) + equation in line 205)? I thought iterative implementation of Eqs. (1) and (6) and equation in line 205 could satisfy Eq. (4) (e.g., Archer et al., 2002).

> Added explanatory paragraph in section 2.2.1 (at the end of "Discrete equations", ll. 377–392 in the *latexdff* report below) about the over-determination of the equation system, making one of the equations redundant.

Lines 258-270: Not sure whether the equations for different realms are solved at once or in a sequence with/without iterations. Is it appropriate to define a boundary condition for TRANSLAY as done for the above layers?

Section 2.2 largely rewritten to make it clearer how the equation systems for the different realms are solved, and how their solutions influence each other.

Line 327: Do you mean w is calculated time-explicitly but solids-solutes are calculated time-implicitly? Also, I suppose Newton iteration is conducted only in REACLAY and DBL? Do you separate calculations between REACLAY and DBL or at once?

Solution strategy described in more detail in the reorganised and extensively rewritten section 2.2

Line 499: Is MEDUSA fully coupled to BEC (allowing exchange fluxes passed between the two models/modules) or are you just using the BEC output as boundary conditions and not returning any fluxes to BEC? The steady-state results of sedimentary profiles between the above two cases could different.

No changes made, as this information was already included in the text.

Table 3, cap. L1: Isn't 1 L = 1 dm^3 universally correct? If so this does not have to be assumed?

Deleted sentence regarding this "assumption" in the caption to Table 3.

Technical comments

Line 134: 'the sedimentary mixed' should be replaced with 'the sedimentary mixed layer'?

OK, corrected.

Line 453: Right parenthesis is missing.

OK, corrected.

Tables 1 and 2: 'BRNS-global' or 'BRNS-GLOBAL'?

Spelling changed to 'BRNS-global' throughout.

Fig. 3 caption L2: %Opal should be red triangles?

Yes, they should – corrected.

Author's own changes

Line 16 (also line 16 in the *latexdiff* report):

> "Ocean-atmosphere exchange schemes" corrected to read "Ocean-sediment exchange schemes"

Table 2:

> Added missing CO_2 and HCO_3^- to the list of solutes in MUDS.

Table 2:

> Added notice to the caption stating that "Clay" stands for inert, detrital or dilutant material.

Line 259 (line 306 in the *latexdiff* report):

> "ovelying" corrected to read "overlying"

Line 263 (line 310 in the *latexdiff* report):

> "accross" corrected to read "across"

Line 270 (line 318 in the *latexdiff* report):

> "wz_B^+" corrected to read "w_B^+"

Line 596 (line 781 in the *latexdiff* report):

> "oxygen concentration rates" corrected to read "oxygen concentrations"

Throughout:

> Changed "seafloor" to read "sea-floor"

Code availability section:

> Archived the codes in three archives on Zenodo and amended the section text accordingly, giving the DOIs of the three archives, that had to be uploaded separately because of the different licenses.

Supplement:

- Added reference manual for the μXML library in `muxml/doc`.
- Updated `buildandrun.pdf` to include information on getting and assembling the codes from three Zenodo code archives in order to run the test case applications.
- Cosmetic changes in `medusa-cocogen.pdf` to fix overfull lines.
- Code archive `medusa_v2.tar.gz`: corrected a glitch in `apps/jeasim/Makefile` that prevented the JEASIM application from compiling.
- Updated `smcontents.pdf` to reflect the above changes; also added versions and/or dates of the different documents.

References

Archer, D.: A data-driven model of the global calcite lysocline, Global Biogeochem. Cy., 10, 511–526, https://doi.org/10.1029/96GB01521, 1996.

Archer, D., Kheshgi, H., and Maier-Reimer, E.: Dynamics of Fossil Fuel CO_2 Neutralization by Marine $CaCO_3$, Global Biogeochem. Cy., 12, 259–276, https://doi.org/10.1029/98GB00744, 1998.

Archer, D., Morford, J. L., and Emerson, S. R.: A model of suboxic sedimentary diagenesis suitable for automatic tuning and gridded domains, Global Biogeochem. Cy., 16, 1017, https://doi.org/10.1029/2000GB001288, 2002.

Archer, D. E.: Modeling the Calcite Lysocline, J. Geophys. Res., 96, 17 037–17 050, https://doi.org/10.1029/91JC01812, 1991.

Capet, A., Meysman, F. J. R., Akoumianaki, I., Soetaert, K., and Grégoire, M.: Integrating sediment biogeochemistry into 3D oceanic models : A study of benthic-pelagic coupling in the Black Sea, Ocean Model., 101, 83–100, https://doi.org/10.1016/j.ocemod.2016.03.006, 2016.

Crucifix, M.: Traditional and novel approaches to palaeoclimate modelling, Quaternary Sci. Rev., 57, 1–16, https://doi.org/10.1016/j.quascirev.2012.09.010, 2012.

Dunne, J. P., Sarmiento, and Gnanadesikan, A.: A synthesis of global particle export from the surface ocean and cycling through the ocean interior and on the seafloor, Global Biogeochem. Cy., 21, GB4006, https://doi.org/10.1029/2006GB002907, 2007.

Ermakov, I., Crucifix, M., and Munhoven, G.: Emulation of the MBM-MEDUSA model: exploring the sea level and the basin-to-shelf transfer influence on the system dynamics, Geophysical Research Abstracts, EGU2013-9011-2, URL `https://meetingorganizer.copernicus.org/EGU2013/EGU2013-9011-2.pdf`, 2013.

Palastanga, V., Slomp, C. P., and Heinze, C.: Long-term controls on ocean phosphorus and oxygen in a global biogeochemical model, Global Biogeochem. Cy., 25, GB3024, https://doi.org/10.1029/2010GB003827, 2011.

Ridgwell, A.: Interpreting transient carbonate compensation depth changes by marine sediment core modeling, Paleoceanography, 22, PA4102, https://doi.org/10.1029/2006PA001372, 2007.

Sigman, D. M., McCorkle, D. C., and Martin, W. R.: The calcite lysocline as a constraint on glacial/interglacial low-latitude production changes, Global Biogeochem. Cy., 12, 409–427, https://doi.org/10.1029/98GB01184, 1998.

Ullman, W. J. and Aller, R. C.: Diffusion coefficients in nearshore marine sediments1, Limnol. Oceanogr., 27, 552–556, https://doi.org/10.4319/lo.1982.27.3.0552, 1982.