



# ***Interactive comment on “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” by Guy Munhoven***

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I thank the referee for their careful and in-depth reading of my manuscript and their constructive comments. For the sake of conciseness, I reply here only to questions and comments where extra information was requested. I gladly accept all the other suggestions and corrections and will take them into account for the revision of the

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## 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 O<sub>2</sub> 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?*

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The adopted **convergence criteria** are standard practice in the numerical solution of non-linear equations and equation systems (e.g., Antia, 2002). When iteratively solving an equation or equation system, there are essentially two main types of iteration stopping criteria that can be adopted: one based upon the differences between subsequent iterates and one based upon the magnitude of the function residual. None of these is universally adequate and it is generally advisable to use a combination of the two. For safety reasons, they should furthermore be complemented by a limitation of the total number of iterations (Kincaid and Cheney, 1991). With MEDUSA, I found that monitoring the difference between subsequent iterates and stopping iterations once this difference fell below a given (small) threshold value

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would not always provide an acceptable solution to the equation system. In some instances, where iterations were only slowly progressing at a high function residual value, iterations would often be stopped prematurely on the basis of that criterion alone and convergence falsely diagnosed. We therefore first of all require that the function residual value is sufficiently small. “Sufficiently small” clearly makes sense only if the scales of the equations can be properly estimated. Once the scaled function residual is sufficiently small (first criterion), it is interesting to perform some root refinement (**second criterion**). Here, this is only done if the total number of iterations has not yet been exceeded. In general, the second criterion requires a few extra iterations only and may further reduce the function residual by several orders of magnitude. As suggested by the referee, this will be made more explicit in the revised manuscript.

Regarding the actual implementation of the convergence test, the *Technical Reference* is possibly misleading in its current form as the scaling of the equations is only detailed for solids therein. Similar scaling is nevertheless applied for solutes and it is straightforward to derive the scaled expressions of the solutes’ equations from those of the solids. It is sufficient to notice that solute diffusion is an intraphase type diffusion, and  $w$  may be substituted for by  $u$ . The convergence test considers all the scaled equations for all the solids and all the solutes (criterion 1) and all the scaled increments of all the solids’ and solutes’ concentrations (criterion 2). This will be made more explicit in the *Technical Reference*, by also providing detailed expressions for solutes.

The **solution strategy** is an all-at-once one – no separate process-based steps. As the framework system must be able to cope with any composition and reaction network, all processes are treated on par, and except for positivity of the concentrations, no further a priori assumptions are made.

If organic matter is included as a component and other oxidation pathways than the oxic one are considered, the redox zonation emerges automatically in the solution of the equation system, once that solution becomes sufficiently precise.

The **convergence of the solids' advection rate profile** is currently not explicitly checked for. It is expected that constituent concentrations keep changing as long as the advection rate profile changes from one iteration to another. It is therefore unlikely that iterations get stopped unless the advection rate profile stabilises. For extra security, it might nevertheless be interesting to include a test for the convergence of the advection rate profile as well. So far, this has, however, not been necessary.

### Specific/technical comments

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

References to Sigman et al. (1998) and Dunne et al. (2007) will be added.

*In. 49 - 50: Please add references for examples for the “expert-chosen empirical parametric functions” and for the “system identification theory” approach*

For the “expert-chosen empirical parametric functions,” reference will be made to Dunne et al. (2007). The “system identification theory” approach was actually meant as a future perspective. It has to my best knowledge so far only been used at a more global scale for ESMs, but not yet to sediment models. A reference to Crucifix (2012) will be added for the fundamentals

of this approach in that more general context and to Ermakov et al. (2013) for an pilot application of this technique to MBM-MEDUSA.

*Ln 130-133: Please add reference.*

Added reference to Archer et al. (1998).

*In 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” should actually have read “the sedimentary mixed layer” — corrected.

*Page 9: In 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?*

Yes, exactly: solutes are treated the same way in the DBL and in REACLAY, with porosity set to 1 in the DBL. To keep the structure of the equation system simple, equations for solids are nevertheless included in the DBL, but their concentrations are forced to zero there. The DBL acts as a transport barrier for the exchange of solutes between the sediment and the overlying seawater across the sediment-water interface: the thicker it is, the stronger the resistance it exerts. The existence of a DBL is merely due to the presence of a sediment-water interface that delimits a turbulent medium. As such, it should actually be included in any model configuration a priori.

However, including a DBL slows down a model. An important question is then to what extent the model results are influenced by the presence or absence of a DBL. I am currently writing up a manuscript on that subject and it seems that there is no unequivocal response to that question. The presence of a DBL turns out to play an important role with reduced complexity model compositions (such as the classical calcite–clay–CO<sub>3</sub> composition of Keir (1982), recently used by Sulpis et al. (2018)). With sediment compositions commonly used in sediment modules included in ocean biogeochemical models (with calcite, clay and organic matter as solids and CO<sub>2</sub>, HCO<sub>3</sub><sup>-</sup>, CO<sub>3</sub><sup>2-</sup>, O<sub>2</sub> and possibly NO<sub>3</sub><sup>-</sup> as solutes, the role of a DBL, even of 1 mm thickness, on the preservation patterns of sedimentary material is very limited. In other configurations, it may nevertheless be important again. Sulpis et al. (2018) have calculated the global distribution of the DBL thickness over the seafloor. They find a wide range of values, from 100 to 10,000 μm, with a most probable value close to 1000 μm though.

Interestingly, early instances of simple carbonate diagenesis models generally included a DBL (e.g., Schink and Guinasso Jr., 1977). Later, DBLs “vanished” from such models (e.g., Keir, 1982) without any explicit reason. This evolution might, however, possibly be linked to the progressive adoption of non-linear calcite dissolution kinetics in such models around that time: with the linear kinetics, they can be solved analytically with or without a DBL; with non-linear kinetics, a DBL prevents such an analytical solution and even without a DBL, they only allow an approximative analytical solution. In the later developed more complex early diagenesis models for which numerical solution procedures are adopted that can just as well handle configurations with and without DBLs, DBLs are still not widespread: on one hand, CANDI (Boudreau, 1996) and OMEXDIA (Soetaert et al., 1996) include one; on the other hand Archer (1991, 1996), Dhakar and Burdige (1996), STEADYSED1 (Van Cappellen and Wang, 1996) MUDS (Archer et al.,

2002) or Jourabchi et al. (2005) do not include one.

The equation system becomes to some extent “cleaner” at the sediment water interface, SWI, once a DBL is included. Without a DBL the SWI lies on a grid node, which is ideal for a prescribed concentration boundary condition (used for solutes) but less so for a flux boundary condition (used for solids), although the discretized equations remain mathematically consistent, which is not the case when concentrations have to be prescribed at a grid vertex (Hundsdoerfer and Verwer, 2003). With a DBL, the SWI lies on a grid vertex, which is then perfect for both solids and solutes, as they have to fulfil flux continuity equations in this case.

Bottom line: I recommend to include a DBL. For site-related applications, this nevertheless requires the knowledge of the thickness; for global applications, an average value of 1 mm should be adequate in most situations. For backwards compatibility with the interfaces to several biogeochemical cycle models that MEDUSA has been coupled to and that link to the MEDUSA’s SUBVERSION repository for this purpose, the default in the code will nevertheless remain “no DBL” for the time being.

The revised manuscript will include a new section about the importance of a DBL and some other options that MEDUSA offers (see also comments by Anonymous Referee #2)

*Page 10: In 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.*

Thank you for this suggestion. I will refer to that document and include a

reference to Ullman and Aller (1982) therein.

*In. 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))?*

The simulation experiments presented in the manuscript use  $\alpha \equiv 0$ . The original MBM-MEDUSA did not include bioirrigation and neither did Jourabchi et al. (2008) upon which JEASIM was based; COUPSIM is mostly focusing on great depths, where bioirrigation is negligible (Glud, 2008). As mentioned on the line 222, the bioirrigation “constant”  $\alpha$  may be depth-dependent. It may even be time-dependent and it may also depend on other parameters, such as the supply rate of organic matter or other constituent concentrations. Its value is updated at each iteration at the same time as the solids’ advection rate profile.

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

The porosity profile is not a constraint in the same sense as the volume conservation equation. While the basic set of equations used in the model could be adapted to deal with time-dependent porosity (either prescribed or composition dependent, such as in Zeebe and Zachos (2007)), the volume conservation equation will always remain valid. I thus keep this part unchanged.

*Page 12: In. 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.*



This observation is indeed correct. I nevertheless prefer to keep the current text as it is to remind that the grid node distribution on REACLAY is different in the model configurations with and without a DBL.

*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?*

Yes exactly: spacing and extent can be changed depending on the users' needs, and one typical usage of this facility would be different grid-point distributions at shallow and at great depths.

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

No, the text is correct. Munhoven (2007) included three different experiments: CRR, BST and ALL. Here, only the ALL experiment is revisited.

*In 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”*

This will be changed to “MBM is an eleven-box model of the carbon cycle in the ocean and the atmosphere”

*Section 3.2 COUPSIM — Coupling simulator page 21 In. 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)?*

Here we limit ourselves to depths of 1000 m and greater for the simulation experiment because the input data read in from the BEC results lead to even more unrealistic results at shallower depths. The model works without any problems for depths shallower than 1000 m as can be easily verified by setting `dlimzw_top` in the `&nml_regridding` namelist in the configuration file `medusa_coupsim_setup.nml` in `medmbm/work/coupsim_bec` to a value lower than `1000.0D+00`. However, with shallower threshold depths one ends up with TOC contents of 40% and more (equivalent to about 90% of organic matter) in the Kara Sea, the Sea of Okhotsk and in the South China Sea, far above the highest observed value (15% in one single grid point). The 1-G approach may not be adequate here and the adopted redox process network not sufficiently complete. The model complexity for COUPSIM was chosen to match the available boundary conditions as far as possible.

The complete TOC dataset of Seiter et al. (2004) actually includes 36,236 data points on a  $1^\circ \times 1^\circ$  longitude-latitude grid (64,800 grid points). Only 4 of these had TOC contents greater than 10%; about 30 of them present TOC contents between 5 and 10%. For the model-data comparison, only data for seafloor depths greater than 1000 m have been included on the maps in Figure 4, to be consistent with the seafloor extent considered.

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