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

Guy Munhoven

guy.munhoven@uliege.be

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I thank the referee for their careful consideration of my manuscript and for pointing out several shortcomings in the text. Please find below my replies to those comments that asked for information or clarification. All the other suggestions and corrections not mentioned here will be integrated in the revised text as recommended.

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.

After rereading the text I agree that the description of how the different realms are connected to each other is incomplete in the text has to be improved. The different options do actually not always imply special branching, but generally lead to different codes to be generated, or to differ by small details only. The *volumeless* option, e.g., only uses a pre-compiler switch that adapts code at several places: it deactivates the evaluation and integration of the reaction rate term at the right-hand side of eq. (6) in one subroutine and switches between calculating the specific partial volumes of solids from their respective intrinsic densities, and setting them to zero in another. A flow chart would thus have to be very detailed, which would limit its usefulness, in my opinion. I think that these aspects can be more conveniently described in the text.

(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.

Tracked time is rather expensive, as it adds a tracer to one solid and it requires all the processes that relate to that solid to be duplicated. If MEDUSA is only used as a ocean-sediment boundary scheme in a global biogeochemical cycle model, there is not stringent need to implement time tracking with CART in the sediment. However, if the produced sediment cores are meant to be compared to actual sediment data, tracked time would be recommended as it provides a reliable "age model" for the synthetic cores generated by the model. So, including or not including tracked time depends on the needs of the user.

The *volumeless* mineral option was only introduced to allow for a meaningful intercomparison with results derived from other models that do not take the effect of chemical reactions on the advection rate profile into account, but directly link the advection rate profile to the porosity profile via $w(z)(1 - \varphi(z)) = w_{\mathsf{SWI}}(1 - \varphi_{\mathsf{SWI}})$. Accordingly $w(z)$ is typically reduced by a factor of 2 to 2.5 only at depth, compared to w_{SWI}. When the effect of chemical reactions is into account, that reduction can easily exceed a factor of 10. Volumeless solids are therefore not used by default. In the applications reported in the paper, the volumeless solids option is only used for the JEASIM, since the original model by Jourabchi et al. (2008) used such prescribed solids' advection rate profiles.

It is not entirely clear to me what is meant here by "does not affect the overall results". Selecting the volumeless option leads to significantly different advection rate profiles (easily different by a factor of five and more), and thus different concentration profiles (see lines 252*ff* and discussion in the

previous paragraph of this reply). If this comment refers to the statement at line 638 ("Both approaches are mathematically equivalent"), then this must be a misunderstanding. What is meant there is that prescribing a flux of inert material that matches the prescribed burial rate when the volumeless solids option leads to exactly the same advection rate profile that would be derived from the $w(z)(1 - \varphi(z)) = w_{\mathsf{SWI}}(1 - \varphi_{\mathsf{SWI}})$ identity.

The revised manuscript will include a new section discussing the role of a DBL (see also reply to comments by Anonymous Referee #1). That section will also provide guidance regarding other options offered by MEDUSA, and the volumeless option in particular.

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)?

This is indeed correct–thank you for pointing out this imprecision. The number of grid points/layers is always taken as reported in the respective papers. In this particular case, that number relates thus only to solutes and organic carbon. Organic carbon distribution is furthermore calculated from the model of Emerson (1985), and used as a forcing function. Similar simplifications were made in the follow-up version (Archer, 1996): here again, calcite and detrital material were assumed to be homogeneous in the sedimentary mixed-layer, but this time the organic carbon profile was determined interactively. The relevant information will be amended in the Tables.

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).

At first sight, one might indeed think that the solid species whose evolution equation is replaced by that for static volume conservation would possibly not comply to its original evolution equation. This is, however, fortunately not the case. The complete equation system at each grid point, which includes the evolution equations for the concentrations of all the solids and solutes under consideration (one instance of eq. (1) for each constituent), the equation for the advection rate at that grid point (eq. (6)) and the static volume equation (eq. (4)) is actually overdetermined. There is one more equation than there are unknowns (the constituents' concentrations and the advection rate). The equations are, however, not independent of each other: eq. (6) is obtained from the weighted average of the solids' evolution equations, weighted by the partial specific volumes of the respective solids, and taking the static volume equation into account, followed by vertical integration. Details about the relationships between these different equations are provided in the technical report '*Early Diagenesis in Sediments. A one-dimensional model formulation*' in the Supplement. One of the equations is thus redundant. We have chosen to strictly enforce the static volume conservation throughout the iterations and thus to keep its equation and drop one of the solids' evolution equations – the equation for the main inert material.

The procedure from Archer et al. (2002) is not guaranteed to always work out in a general purpose model. As reported by Archer et al. (2002) the actual total solid phase concentrations in MUDS could deviate by as much as $\pm 50\%$ from the actually required 1 g/g during the iterations. In a general

purpose approach as the one adopted in MEDUSA, where the complete process network is solved at once, such large deviations may lead to failure of the iterative process without any guardrails (here the static volume conservation equation). Furthermore, conserving mass to within 2% only may be sufficient for steady-state calculations, but could cause considerable model drift in transient simulation experiments. In MEDUSA, mass is typically conserved to within 10^{-12} and better for each constituent in each column and to within 10^{-10} or better globally for set-ups with several thousands of columns typical for 3D biogeochemical cycle models.

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?

All equations in the REACLAY realm (or in the combined REACLAY-DBL realms if a DBL is included) are solved at once. TRANLAY is indeed only a buffer reservoir that collects material leaving REACLAY through its bottom, or that feeds REACLAY. The equations that describe the evolution of its contents are thus ordinary differential equations (mass balance equations) that do indeed not require a boundary condition, but only source-minus-sink terms. This will be corrected in the text.

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?

No, just like all the concentrations profiles, the w **profile** is calculated time-implicitly.

Yes, **Newton iterations** are only used in the REACLAY and the DBL realms. The w_k (k denoting the grid vertices) could be calculated together with all the concentration profiles. During the early development stages of MEDUSA, the advection rates w_k were treated on par with the concentrations of the model sediment components. The Newton-Raphson scheme was then based upon a Jacobian that also included derivatives of the equations with respect to the w_k's. Please notice though that it was not eq. (6) that was used at that time to calculate the solids' advection rate profile, but its derivative (eq. (2.49) in the technical report *Early Diagenesis in Sediments – A one-dimensional model formulation* in the Supplement) which depends only on the local concentrations and not all of those above. The resulting discrete equation system too often became singular in the course of the iterations, preventing convergence. This is why we switched to eq. (6), which directly provides $w(z)$, but has the disadvantage of being dependent not only on local concentrations, but on all the concentrations above the level where $w(z)$ is calculated. The Jacobian of the equation system would thus be lower triangular with in addition some super-diagonal blocks, leading to Newton-Raphson steps that are computationally speaking orders of magnitude more expensive than the solution of a block tri-diagonal system. The iterative solution procedure for the system of equations was therefore split up: each iteration starts by updating the advection rate profile given the currently best available concentration profiles (a fixed-point approach for the w_k) and then a Newton-Raphson step is taken for the concentration values with that advection rate profile taken as given. For the next iteration, the advection rates are then again first updated using the new concentration profiles, followed by a Newton-Raphson step for the concentrations, etc.

In the revised manuscript, the contents of sections 2.1.1, 2.1.2 and 2.2 will be reorganised and section 2.2 partially rewritten to improve the description (also in reply to the comments by Anonymous Referee #1).

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.

Here, we are just using `BEC` output as boundary conditions for `MEDUSA`, as explained on lines 503–509: the coupling simulator only reads in the data from a file that would otherwise (i.e., in an actually coupled setup) provided by the host biogeochemical model. So there are no return fluxes to `BEC` (please notice that the `BEC` output used for the forcing dates from 2005).

Results from a fully coupled `BEC-MEDUSA` setup, albeit with a more recent version of `BEC` and further including ^{13}C and ^{14}C isotopes, with bi-directional exchange fluxes between the two models have been presented elsewhere (Kurahashi-Nakamura et al., 2020). As discussed at lines 567–570 in the manuscript, the results between the two cases are indeed strongly different and the two-way coupling reduces if not solves some of the shortcomings diagnosed here.

For the `COUPSIM` application, I actually consider that the model code is the central contribution to the paper as it illustrates how to couple `MEDUSA` to a biogeochemical model.

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

It actually *is* ... and has been so since 1964 already[1] ... So, there is indeed absolutely no need to assume this. That notice will be deleted in the revised manuscript.

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[1]See https://www.bipm.org/en/CGPM/db/12/6/.

Technical comments

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

> 'BRNS-global' appears to be the correct spelling (Jourabchi, 2007). Corrected throughout.

I gladly accept all the other suggestions and corrections and will include them in the revised text.

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