Replies to Anonymous Referee #2 on “OMEN-SED 0.9: A novel, numerically efficient organic matter sediment diagenesis module for coupling to Earth system models”

1. Comment:
The model neglects the effect of sediment compaction “due to mathematical constraints”. I understand the rational for this and accept a consistency of this assumption to near-seafloor (bioturbated) sediments; however, this might be a problem for deeper sediments discussed in the paper (down to 50 or 100cm). The authors should either define different porosity values for different depth-zones or to demonstrate that the results are not particularly sensitive to the value of this parameter.

Response:
Assuming constant porosity is required to solve the diagenetic equation analytically. It is a mathematical limitation and it will induce a certain error. However, the error is not very large and we have already shown this by comparing the performance of OMEN-SED against observed data (Section 3.2) and against model results from a fully formulated RTM with depth-varying porosity (Section 3.3). The comparison of OMEN-SED with the results of the numerically solved RTM (Section 3.3) allows evaluating to which extend simplifying assumptions (e.g. constant porosity, non-overlapping redox zones etc) affect simulation results and, thus, quantitatively test the performance of the computationally efficient OMEN-SED approach against the computationally expensive numerical approach.

We also want to reiterate that OMEN-SED is designed for the coupling to ESMs and thus for global scale applications (see responses to reviewer #1). The novel model represents a big advance compared to the description of benthic-pelagic exchange processes currently incorporated into ESMs (Hülse et al., 2017; also see comment by the K. Wallmann). Conservative and reflective boundaries, as well as simple box models are characterized by much stronger, simplifying assumptions and far bigger limitations than constant porosity.

We included a little paragraph on this in the limitation section (pg 54 lines 3-8):
“Furthermore, by their very nature, analytical models do not allow for overlapping biogeochemical zones or depth dependent porosity, which introduces a certain error to simulation results. However, the energy yield dependent sequence of oxidants is generally valid (e.g. Hensen et al., 2006) and the good agreement between OMEN-SED and the results obtained with a fully formulated numerical RTM (allowing for overlapping TEA use and depth dependent porosity, Section 3.3) shows that these are not critical limitations of OMEN-SED - even for shallow sediments.”

2. Comment:
Dividing the sediment column into functional zones in such a strict manner does not always represent reality well. Thus, “nitrogenous” zone may overlap with “oxic” zone. This assumption, as far as I understand, made it impossible to simulate nitrate SWI flux directed into the sediments in oxygenated environment, which is definitely not true. Validation of the model against measured benthic fluxes would probably demonstrate to some extent accordance of suggested method with real benthic system.

Response:
First, it is possible to simulate nitrate influx into the sediments in oxygenated environments with
OMEN-SED (see e.g. Fig. 6C).

In the following we repeat the response given to the 1\textsuperscript{st} comment of Reviewer #1:

We agree with the reviewer that different biogeochemical zones can overlap. However, as stated in the text, OMEN-SED is designed for the coupling to ESMs and its formulation is thus first and foremost guided by achieving numerical efficiency while retaining biogeochemical reality. As summarized in the manuscript, there are essentially two approaches that can be used to describe biogeochemical processes in models. The first approach solves the general diagenetic equation numerically on a regular or irregular grid and biogeochemical zonation emerges in response to inhibition terms allowing a certain degree of overlap between biogeochemical zones. This approach is highly flexible and thus preferable. Yet, its excessive computational demand unfortunately renders its application within a three-dimensional Earth System Model framework impossible. On the other hand, analytical models that subdivide the sediment into distinct biogeochemical zones are computationally efficient and thus ideally suited to describe diagenetic dynamics in ESM.

By their very nature, analytical models do not allow for overlapping biogeochemical zones. As stated in the manuscript, this is a simplification. However, we disagree with the reviewer that this simplification would \textit{per-se} prevent the application of such analytical approaches in shallower aquatic environments. In fact, OMEN-SED builds on a number of analytical models that were developed to investigate local, coupled nutrient and oxygen cycles in coastal sediments (e.g. Billen, 1982; Goloway and Bender, 1982; Jahnke et al., 1982; Slomp et al. 1996). Similar approaches were later successfully applied from oxic to anoxic sediments and at the regional coastal ocean scale (e.g. Ruardij and Van Raaphorst, 1995; Tromp et al., 1995; Gypens et al., 2008). In particular, Gypens et al., (2008) points out that accounting for secondary redox process in the boundary condition induces little error as: “Using a numerical model, Soetaert et al. (1996) showed that this re-oxidation mainly occurs at the oxic-anoxic transition interface.”

Finally, the good agreement between OMEN-SED and the results obtained with a fully formulated numerical RTM (compare Section 3.3, allowing for overlapping TEA use) shows that this is not a critical limitation of OMEN-SED - even for shallow sediments.

We again want to refer to the paragraph we added to the limitations section (see last comment, pg 54 lines 3-8).

\textbf{3. Comment:}

Nitrogen dynamics include “the metabolic production of ammonium, nitrification, denitrification as well as ammonium adsorption”. Denitrification is considered as a single-step process ignoring NO2- production/consumption and anaerobic ammonium oxidation (Anammox) which is undoubtedly a significant component of the biogeochemical nitrogen cycle (Devol, 2015). In other words, nitrogen dynamics is somewhat simplified. This simplification should be quantified/discussed in more details.

\textbf{Response:}

In the following we repeat the response given to the 2nd comment of Reviewer #1:

Anammox is implicitly included in the model. The organic nitrogen released during the denitrification process is assumed to be directly oxidized with nitrite to N\textsubscript{2} through a coupling between denitrification and anaerobic ammonium oxidation.

However, we would like to stress again that OMEN-SED is a benthic model designed for the coupling
Most ESMs do not even explicitly resolve N-dynamics. In addition, OMEN-SED is a system/global scale model that aims to resolve the most pertinent biogeochemical dynamics on a global scale (including a paleoenvironmental context) and estimate the main SWI-fluxes and not a model that aims at resolving specific local scale dynamics. Even most local scale RTM applications do not resolve DNRA and anammox explicitly. However, OMEN-SED could be easily adapted to explicitly resolve these processes if the specific application requires their representation (e.g. coastal ocean).

We included a sentence on this in the Section 2.2.3 “Nitrate and Ammonium” (pg. 12, lines 22-24):

“Anaerobic ammonium oxidation (anammox) is implicitly included in the model. The organic nitrogen released during denitrification is assumed to be directly oxidized with nitrite to N2 through a coupling between denitrification and anammox.”

4. Comment:
The efficiency of binning procedure discussed in section 4.2.1 is doubtful. First of all, such binning assumes presence of STD bars on the plots. Also, I think that it would be more logical to group POC content into POC rain rate (RRPOC) classes rather than WD classes as RRPOC may significantly vary at different regions of the ocean of the same WD. Finally this binning gives a false impression of a good POC content fit. I realize that parameterization of multi-G model is beyond the scope of this sediment model development paper, therefore I suggest to use existing way to parameterize multi-G models and validate your model against the databases suggested in those studies (for example Stolpovsky et al., (submitted) https://www.biogeosciences-discuss.net/bg-2017-397/).

Response:
We thank the reviewer for the suggestion. We decided to follow suggestions from reviewer #1 and #3 (K. Wallmann) and shortened the cGENIE coupling section. Figure 12 (and its discussion) has been deleted from the manuscript. The R2 values in Figures 13 and 14 (as well as their discussion in the text) has been removed as well. Compare changes on pages 47-50.

The ranges of simulated SWI-fluxes from the stand-alone OMEN-SED model are already compared to the Stolpovsky et al., (2015) database in Figure 6.

If binned by RRPOC for uniform k-values, all grid-cells with same RRPOC have the same preservation in OMEN-SED. Therefore, this would not be very useful.

5. Comment:
POC is not a very good constraint, since measured POC is in large part the less reactive stuff that is left over after mineralization of the more reactive fractions. This was shown in Stolpovsky et al., 2015 paper (see the discussion in section 4.3). Fluxes at the SWI are believed to be a better constraint.

Response:
We shortened the coupling section of the manuscript (we removed the sensitivity analysis with the spatially uniform degradation rate constants, compare pages 47-50) and we will discuss an improved model-data analysis of the coupled model, using existing parameterizations and maps of SWI-fluxes, in a follow-up publication. Also compare response to comment 20 of reviewer #1:

As stated in the manuscript (page 45, lines 23-26):

“Our objective is not to perform and discuss a detailed calibration of the coupled models as this is
Minor comments.

6. Comment:
Eq. 1: As a time and depth independent parameter, porosity should be moved out of differential in order to emphasize that it is constant: Porosity*dC/dt instead of d(Porosity*C)/dt.
Response: This has been changed as indicated.

7. Comment:
P. 8, L. 1: It is not immediately clear that the authors are talking about water (not sediment) depth.
Response: We agree that this is a bit misleading. We are actually talking about sediment depth. This has been changed in the revised manuscript to (pg. 8 lines 1-2):
“All parameters in Eq. (1), apart from porosity and burial rate, may vary with sediment depth and many reaction rate expressions depend on the concentration of other species.”

8. Comment:
Eq. 5: This representation sounds a bit odd. I think z∞ should be replaced with zmax, as POC content at infinite depth believed to be zero.
Response: The POC content of marine sediments does not tend to zero. A significant amount of POC is buried in marine sediments and enters the longterm C cycle (rock cycle). Without this imbalance between production and respiration, no O2 would have accumulated in the atmosphere. But we agree that the use of z∞ is not ideal, as the sediment column in OMEN-SED is not modeled until infinite depth. We have replaced z∞ with zmax in the entire manuscript.

9. Comment:
P. 9, L. 25: SWI is given without initial explanation.
Response: The explanation has been added at this part in the manuscript: “… sediment-water interface (SWI) …”

10. Comment:
P. 25, L. 6 – 13: I agree that bioirrigation may enhance SWI fluxes of dissolved species, therefore I do not understand why this way of transport is technically ignored for all water depths (fir=1)?
Response: In the following we repeat the answer given to Comment 10 of Reviewer #1:
The bioirrigation coefficient has been changed and is now represented by the empirical relationship with seafloor depth derived by Soetaert et al. (1996): fir = Min{1; 15.9 · z−0.43 }.
The text has been changed to (pg. 25 lines 21-23):
“Soetaert et al. (1996) derived an empirical relationship between fir and seafloor depth (fir = Min{1;
11. Comment:
P. 27, L. 28: PAWN is given without explanation.
Response:
As the name PAWN is derived from the authors names and not an acronym we do not think this information is of any value here.

12. Comment:
Fig. 7: Please add ticks and numbers to X-axis on H2S at 2213 and 4298m and NH4 at 108m. Some plates have very inconvenient ranges on horizontal axis, for example H2S at 4298m.
Response:
This has been changed as indicated.

13. Comment:
Sec. 3.3.2: I do not understand the rational for comparing OMEN-SED results with another model (Thullner et al. 2009). I would suggest comparing it to existing SWI flux database mentioned before (Stolpovsky et al., 2015). Also, reporting global denitrification rate modeled with OMEN-SED and its comparison with previous studies would support the model.
Response:
We evaluate the performance of OMEN-SED by comparing model results with data (section 3.2), as well as the results of a fully-formulated, numerical RTM (section 3.3). The comparison of OMEN-SED with the results of the numerically solved RTM allows evaluating to which extend simplifying assumptions (e.g. constant porosity, non-overlapping redox zones etc) affect simulation results and, thus, quantitatively test the performance of the computationally efficient OMEN-SED approach against the computationally expensive numerical approach. The ranges of simulated SWI-fluxes from the stand-alone OMEN-SED model are already compared to the Stolpovsky et al., (2015) database in Figure 6.

14. Comment:
P. 55, L. 24 – 25: Bold assumption, I suggest to avoid such formulations. The major advantage of OMEN-SED is its tremendously low computation time which is so important for ESMs. As always, only two options of the following three can be true the same time: “quickly”, “cheaply (super-computer is not needed)” or “qualitatively”.
Response:
This is not an assumption, but the conclusion from the model-data and model-model comparison at the system scale. To clarify this, the sentence as been changed to (pg. 55 lines 5-6):
“We have shown that the performance of OMEN-SED at the system scale is similar to that of a fully formulated, multi-component numerical model.”