**Some open points / things to double-check**

**Anonymous Referee #1**

**4. Comment:**

Methanogenesis: the 1/2 methane to DIC ratio seems to imply acetoclastic methanogenesis. What evidence is there to ignore hydrogenotrophic methanogenesis?

**Response:**

We thank the reviewer for this valid point. However, we are not aware of an approach that would allow split the two pathways in quantitative terms in a global context. Therefore, we assume that the acetoclastic pathway is the dominant methanogenic pathway on the global scale (REF?). However, OMEN-SED could be easily adapted to represent

hydrogenotrophic methanogenesis globally (i.e. by adapting stoichiometric factor ).

**5. Comment:**

For a globally applicable model, the lack of CaCO3 dissolution is an obvious issue. Thus, can you expand on what problems the modeling of CaCO3 dissolution would cause (page 18)? Is this linked to the calculation of pH? Why can pH (and then carbonate) not be estimated from DIC and alkalinity?

**Response:**

In general, the coupling between multiple reaction-transport equations (i.e. strongly coupled biogeochemical dynamics) make finding an analytical solution difficult or even impossible. Calcium carbonate dissolution is kinetically controlled by the amount of CaCO3 and thermodynamically controlled by the porewater concentrations of calcium ion, Ca2+, and carbonate ions, CO32-. The reaction terms of the CaCO3 , (the Ca2+), the DIC and balance equations would thus depend on the concentrations of CaCO3, Ca2+ and CO32- (DIC, pH/Alk). This set of strongly coupled equations does not have a simple analytical solution. Finding a solution to the problem requires some creativity and a number of assumptions that need to be independently tested and validated. This task thus requires some additional work and model development that go beyond the scope of this first model description paper centred on organic carbon and nutirents. However as pointed out in Section 5 “already planned future extensions of OMEN-SED include an explicit description of carbonate dissolution and iron.”

**DH: I changed it a little, okay like this? Sandra has an idea how to do it but does not necessarily want to give it away here.**

**6. Comment:**

Is there no P sorption on iron oxides below the oxic zone? If so, why?

**Response: DH: Okay like this?**

We here follow the approaches of Slomp et al. (1996) and Gypens et al. (2008) who both assume that HPO42- is released due to the reduction of Fe oxides throughout the reduced sediment (i.e. starting at zox).

**OLD:**

**Sandra: Because there are no iron oxides.**

DH: I suppose it refers to the denitrification zone!!?? Shouldn't there actually be still P sorption!? But it is anyway a tiny layer....

**SHALL WE CHANGE IT TO zno3 or leave zox and cite Gypens and Slomp papers?**

**8. Comment:**

A fraction of the sulfide produced is assumed to escape complete oxidation. Does this mimicking the effect of precipitation with iron, rather than escape from the sediment?

**Response:**

In the reviewed version of OMEN-SED, this fraction mimicked the escape from the sediment. However, in response to the first critical comment of reviewer 3 (K. Wallmann) we made the following changes to OMEN-SED:

When coupled to an ESM the γH2S value (fraction of H2S that is oxidised) becomes dependent on the bottom water oxygenation state. That is, γH2S = 1.0 for oxic bottom waters and a user defined value γH2S <1.0 for anoxic bottom waters. For simplicity and as oxygen will eventually serve as the final TEA this is still implemented as aerobic sulfide oxidation.

In addition, we introduce another parameter (γPyr) representing the fraction of sulfide that is precipitated as pyrite (i.e. 0.0 <= γPyr < 1 - γH2S) under anoxic bottom waters. The text, tables and equations (for SO4, H2S and alkalinity) are changed accordingly. The presented results have not been changed and we note that γPyr = 0.0 for all simulations.

Again, γPyr should really just be an auxiliary parameter we use as a quick fix (- I’d also call it gamma\_FeS as pyrite formation can be direct or- more often-via FeS formation). You apply this in the sulfate reduction zone. You just multiply the SRR term in the H2S equation with (1-gamma\_H2S) and also adapt the alkalinity term accordingly. We thus just assume that a user-defined fraction of the produced H2S precipitates as FeS(FeS2) in the sulfate reduction zone. If someone does not want to make any assumptions about FeS precipitation- fine they can set it to 0, if people feel they want to make assumptions, they can set it to whatever. You just make clear that we set it to 0 for all applications because we do not want to make any assumptions- and done!

For a good quantitative overlook of why H2S trapping by FeS/FeS2 is important see Meyers, 2007.

<https://agupubs.onlinelibrary.wiley.com/doi/epdf/10.1029/2006PA001332>

Note: the conclusions about SO4 are bs, but the rest is extremely well done and informative!!!

**DH: Okay like this??? I just discussed it briefly with Andy and he does not like the new parameter. He'll have a look over the weekend. Maybe we can just state that the model currently can't capture pyrite formation and let the non-oxidised H2S escape to the water-column!!??**

**DH:**

SO we would never get an **H2S return flux???:**

OXIC: gamma=1.0: everything is oxidized

ANOXIC: gamma < 1.0:- non-oxidized H2S is going to pyrite??

e.g. WHAT IF NOT ENOUGH Fe TO FORM ALL THE PYRITE?

**10. Comment:**

transport processes: A 1D diffusion/bioturbation model clearly faces major challenges in the coastal ocean, where sediments one predominantly are permeable. And setting fir=1, implying no bioirrigation, is also a very strong assumption.

**Response:**

Most sediments on the globe are non-sandy, therefore we had decided to neglect sandy sediments. However, 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 16-18):

**TODO check pg + lines**

*“Soetaert et al. (1996) derived an empirical relationship between fir and seafloor depth (fir = Min{1; 15.9 · z −0.43 }) based on observations from Archer and Devol (1992) and Devol and Christensen (1993) which is used in OMEN-SED.“*

**DH: Shall we add something similar to Krumins e.g. in the limitations section or just in the response to the comment or in the paragraph on bioirrigation?**

**Both, but short!**

**17. Comment:**

- link to cGENIE. Page 44 discusses the challenges in applying the model in such a setting. In addition, deposition fluxes may change over time. At what point is the steady state assumption on the POC profile still valid under such settings? This is addressed summarily at of the bottom of page 54.

However, I think it is important to lead with this, before interpreting the data-model comparison.

**Response:**

As suggested by the reviewer the steady-state assumption is addressed earlier in the text.

We added the following sentence to Section “4.2 Parameterising the OM degradation rate constants in a global model” (pg 45, lines 10-11): **TODO check pg + lines**

*“Furthermore, by assuming steady-state in OMEN-SED we assume that deposition fluxes of OM are constant over the characteristic timescales of the reaction-transport processes.”*

**DH: Is this sufficient?**

**yes**

**OMEN-SED – cGENIE coupling**

**20. Comment:**

The stated purpose of section 4 is …

… The validation of the coupled model requires more work, and I wonder whether this was not better done in a separate paper, in which the coupling to cGENIE and the parameterization of POC mineralization was explored in more detail.

**Response:**

As stated in the manuscript (page 45):

“*Our objective is not to perform and discuss a detailed calibration of the coupled models as this is beyond the scope of this sediment model development paper. Rather we want to showcase the feasibility of the model coupling, illustrate the range of results and thus information that can be generated with OMEN-SED and verify that model results capture the main observed global benthic biogeochemical features*.”

We think that demonstrating how OMEN-SED can be coupled to an ESM and illustrating the type of output/information generated by OMEN-SED within such a coupling is a central aspect of the model description paper.

However, we agree with trimming down this section (as in the re-submitted version). We will discuss an improved model-data analysis (also using observations of SWI-fluxes) in a follow-up publication (as also suggested by reviewer #3 K. Wallmann).

Specifically, the sensitivity analysis for the spatially uniform degradation rate constants (Figure 12) and it's discussion has been removed (compare pages 47-50).

**DH: Should we remove more???- no**

**Anonymous Referee #2**

**1. Comment:**

The model neglects the effect of sediment compaction “due to mathematical con-

straints”. 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.

**TODO pg and line:**

We included a little paragraph on this in the limitation section (pg 55 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.”*

**DH: I changed the sentence. Is it better/okay like this?**

**DH: OLD version:**

*“The depth invariant porosity introduces a certain error to simulation results as in reality porosity decreases with sediment depth. However, 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. From this we deduce that the results are not particularly sensitive to porosity changes****.”***

**TODO:** E.g. The depth invariant porosity introduces a certain error as in reality porosity decreases with sediment depth. However, the error is not very large as has been shown 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).

**Referee #3: K. Wallmann:**

**1. Comment:**

The model ignores sulfide precipitation and pyrite formation. Consequently, dis-

solved sulfide produced by sulfate reduction and AOM at depth diffuses upward to be

either oxidized by oxygen or released into ambient bottom waters. This is a very un-

realistic set-up. In most sediments dissolved sulfide is removed from the pore water

by pyrite precipitation while the remaining sulfide is oxidized with ferric iron, nitrate and

nitrite before it can reach the oxic surface layer or the ocean. Aerobic sulfide oxidation

is only important in highly reactive surface sediments where the diagenetic sequence

is not maintained but several electron acceptors are used simultaneously. The model

is based on the assumption that electron acceptors are used sequentially rather than

simultaneously. Hence, it cannot simulate situations where aerobic sulfide oxidation

is important but creates high rates of aerobic sulfide oxidation in geological settings

where this process does in fact not occur. The authors should try to fix this problem.

They could for example abandon the model parameter that defines the fraction of dis-

solved sulfide that escapes into bottom waters. In the modern ocean, sulfide leakage

from sediments occurs only in very rare situations and it does not make sense to sim-

ulate these anoxic sediments with a model that ignores iron cycling, pyrite formation

and sulfide precipitation. The authors could instead introduce a parameter that de-

fines the fraction of sulfide that is precipitated as pyrite and update the alkalinity model

accordingly.

**Response:**

We thank Prof. Wallmann for this very valid suggestion. At this rather advanced stage of the model development and evaluation processes we decided to implement the following changes to OMEN-SED: When coupled to an ESM we have made γH2S (fraction of H2S that is oxidised) dependent on the bottom water oxygenation state. That is, γH2S = 1.0 for oxic bottom waters and a user defined value γH2S <1.0 for anoxic bottom waters. For simplicity and as oxygen will eventually serve as the final TEA this is still implemented as aerobic sulfide oxidation.

In addition, we introduce another parameter (γPyr) representing the fraction of sulfide that is precipitated as pyrite (i.e. 0.0 <= γPyr < 1 - γH2S) when bottom waters are anoxic. The text, tables and equations (for SO4, H2S and alkalinity) are changed accordingly. The presented results have not been changed and we note that γPyr = 0.0 for all simulations.

**DH: Okay like this??? I just discussed it briefly with Andy and he does not like the new parameter. He'll have a look over the weekend. Maybe we can just state that the model currently can't capture pyrite formation and let the non-oxidised H2S escape to the water-column!!??**

See above

**OLD:**

**???** So should I assume that under oxic conditions all H2S gets oxidized? But still with O2 and not with nitrate? But we could leave γH2S in for anoxic environments and introduce a new parameter that defines the fraction of sulfide that is precipitated as pyrite (you wanted that anyway ;) ).

**How to update the alkalinity model?**

**Comment 3.3:** I would encourage the authors to delete the entire section 4 of the paper because it

does not add useful information but presents rather misleading results. They shouldaim to present other more useful applications of their highly innovative analytical model in follow-up publications.

**Response:**

Here, we repeat parts of the response to comment 20 of reviewer #1:

We think that demonstrating how OMEN-SED can be coupled to an ESM and illustrating the type of output/information generated by OMEN-SED within such a coupling is a central aspect of the model description paper.

However, we are fine with trimming down this section (as in the re-submitted version). We will discuss an improved model-data analysis (also using observations of SWI-fluxes) in a follow-up publication.

Specifically, the sensitivity analysis for the spatially uniform degradation rate constants (Figure 12) and it's discussion has been removed (compare pages 47-50).

**DH: Should we remove more???**