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Interactive comment on "OMEN-SED 0.9: A novel, numerically efficient organic matter sediment diagenesis module for coupling to Earth system models" *by* Dominik Hülse et al.

Anonymous Referee #1

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This manuscript presents an early diagenetic model that can be coupled to an Earth System Model to study biogeochemical cycling over 'climate relevant' timescales. It starts with a nice introduction and overview of the role of early diagenetic processes. Then the model is described, an extensive sensitivity analysis is presented, the model is applied to a number of sites, and then compared to numerical models. Finally, in section 4, an application in which the model is coupled to an Earth System Model is presented.

Overall, I consider the approach which relies on analytical solutions of simplified set of early diagenetic processes promising and useful, and the description of the model is

clear. Below I outline my criticism. The model builds on numerous assumptions which likely limits its applicability in the coastal ocean, where most of the mineralisation and benthic-pelagic coupling takes place.

Model formulation - The model assumes no overlap of mineralization reactions with different terminal electron acceptors, and assumes that secondary redox reactions can be collapsed onto the interfaces between different mineralization zones (p.9). This is probably ok in environments typically encountered at greater water depth, but there is ample evidence of 'overlapping' mineralization pathways in surficial sediments, in particular in permeable or bioturbated settings. - In the denitrification layer, all N goes to N2. However, in the suite of processes involved in the breakdown of organic matter, ammonium is produced as well, even if nitrate serves as TEA. Ammonium produced in the denitrification zone would need to be accounted for at the transition to the oxic zone as well, which may further reduced the O2 penetration depth. Also, processes such as DNRA or anammox are not included, even though literature surveys (e.g. Dalsgaard et al. 2005) indicate that anammox is relevant at shallower water depth. - Methane oxidation: All methane is assumed to be oxidized anaerobically. Is this done for simplicity? Is there no leakage term (gamma_CH4; comparable to incomplete sulfide and ammonium oxidation) because methane escaping from the anoxic zone is assumed to be removed by aerobic methane oxidation? - Methanogenesis: the 1/2 methane to DIC ratio seems to imply acetoclastic methanogenesis. What evidence is there to ignore hydrogenotrophic methanogenesis? - 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? - Is there no P sorption on iron oxides below the oxic zone? If so, why? - Why does some of the ammonium created below the oxic zone escape oxidation, but oxidation of ammonium to nitrate is complete in the oxic zone? - 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? - Iron cycling is not

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represented explicitly but some of the effect of iron cycling is parameterised. With its effect on sulphur cycling, P sorption and C mineralization (metal reduction can be the main mineralization pathway, see e.g. Canfield et al. 1993), I don't fully understand the reason for doing so (apart from the added complexity when dealing with another solid phase). - 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. - The 2G model is a sensible choice. Model parameterisation is a general concern (page 3, line 30), but I suggest to cite some promising new approaches to address this issues such as presented by https://www.biogeosciences-discuss.net/bg-2017-397

site comparison case studies: - Table 13: fix the depths for the SB and IM sites (SB is the 585m site ...). - Why are the stoichiometric factors set to default values when Epping et al. provide the C/N ratio of the surface sediment? - If a non-local exchange mechanism resulting from bioirrigation is invoked for the Canyon site, what is the source of the high ammonium (and DIC) leading to the observed increase in concentration at depth?

- global transect case study: I don't see the value of the 5% reoxidation case. This is simply unrealistic for the conditions considered here. A possible explanation why lower gammas are giving better match to the data in the shallow sites is that under those conditions, the conceptual model of a vertical separation of reaction zones is more and more violated, so the gamma become a 'fudge-factor' to account for this (see also above comments about the coastal ocean). - on page 43, it says that if fPOC is computed to be > 1 (more than 100% is preserved), then this is discarded and all POC is remineralized. Imposing constraints is fine, but what is the rationale for jumping from >100 to 0 % preservation?

- 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.

On p.54 it says "In theory, its scope of applicability thus ranges from the regional to the global and from the seasonal to the millennial time-scale. " - in the following paragraph they recognize that "This steady-state assumption is only valid if the variability in boundary conditions and fluxes is generally longer than the characteristic timescales of the reaction-transport processes. "

I recommend to be a little more cautious in the application of the model, since I am not convinced that violations of assumptions underlying the conceptual model and non-steady state effects can be ignored. The model clearly requires substantial tuning. It is clear that the authors are aware of the shortcomings, and they discuss that the model may not be adequate to assess seasonal patterns (and one can think of additional settings, where fluxes vary over timescales intrinsic to the POC profile in the top 50cm of sediment modeled here). My concern is that they largely ignore them in their application, before acknowledging them in the discussion. I also suggest to tone down the finding that "A comparison between simulated OM contents and observations indicates that depth dependent k-f relationships provide the best fit (Section 4.2.2), confirming more theoretical considerations regarding the different time and reactivity scales that need to be considered (see Section 4.2). " The age-reactivity relationship is pretty well established, without confirmation by this modeling effort.

The stated purpose of section 4 is "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." This section indeed illustrates the feasibility of the coupling, but I (and I assume most readers) would not have doubted that in the first place. The manuscript then presents two 2G approaches, in which the rate constants for the mineralization of POC are either fixed or varied based on an empirical relationship with the burial velocity. It is shown that the magnitude of the degradation rate constants

matter. This is clearly expected, because the POC degradation rate is key when the input fluxes are reasonable. Yet, to what extent benthic solute fluxes (other than O2, which is tightly linked to OM mineralisation) are captured in this model is less clear to me. In fact, the sensitivity analysis and figure 8 show that the gamma values matter substantially, and they are in my opinion largely lumping unresolved processes. Hence, they will likely require tuning from site to site. 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.

Figures 12 - 14: I gather the R2 values are for the bin averages. I don't see much value of that, as over- and underpredictions cancel each other out in the averaging. Why not compute statistics for the actual model results with the Seiter data directly?

Minor comments - page 8/ line 1: It is said that all parameters in Eq. 1 may vary with depth, but above it is stated that porosity and burial rates are constant with depth. - the fraction of POC buried is defined as the POC at z=0 relative to the POC at depth. Why is it not defined as the flux at z=0 vs. the flux at depth (it seems Eq. 5 ignores the diffusion flux)? Related to that, page 10, line 18 refers to a concentration/flux boundary conditions at the SWI. The following equations and Table 2 only show a known concentration, not a flux condition. However, the latter would be useful when connecting the sediment model to a model of the water column. On page 43, Eq. 51 this is addressed - make this clear earlier. - Can lines 21-23 on page 21 be deleted? - page 31, line 2: specify NH4, SO4 and H2S FLUXES - Figure 3 did not help me much. Does the green dashed vertical arrow indicate possible locations of zbio?

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