Reply to the second review of the manuscript "FESOM2.1-REcoM3-MEDUSA2: an ocean-sea ice-biogeochemistry model coupled to a sediment model"

We appreciate the reviewer's constructive suggestions as well as the critical points. Below we list the changes made in the revised manuscript and our answers to reviewer's questions, following the order of comments in the reviews.

In the following, reviewer comments start with a C: and are set in italics, while our responses start with a R:

Summary:

C: Ying Ye and colleagues resubmitted a revised version of their manuscript with significant changes to address the comments of both reviewers. Most notably, the authors changed the degradation rate constant for the low C:N OM class in MEDUSA2, they performed mass corrections to account for the asynchronous coupling of the models and the loss of nitrogen through denitrification in sediments, three new subsections were added to the Results (3.2.2–3.2.4, briefly describing MEDUSA2 results at the end of coupled simulation), and Figure 3 & Table 1 (summarizing their globally integrated results) has been revised and improved – even though problems still exist with the reported opal fluxes (see comment #1.3. I really appreciate the improved Fig. 5.

While the authors have made substantial improvements to the manuscript, there are still significant weaknesses that need to be addressed (some of which were raised in the previous reviews but have not been addressed in a satisfying manner). In my view, most importantly, it would be beneficial to include more and better "tuning" experiments (e.g., to enhance results for modern OM preservation + at least one idealized transient simulation). This will help to convince readers of the model framework's appropriateness to simulate not only appropriate steady-state modern and LGM conditions but also transient Earth system dynamics, as intended by the authors in future studies. Having a model configuration that simulates modern marine conditions well should be the minimum goal for such a GMD paper, especially considering that this configuration will be the reference for future studies!

Therefore, I still cannot support the publication of the manuscript in Geoscientific Model Development. I summarize my main concerns below and I hope that my general comments will help to improve the manuscript further.

R: We thank the reviewer for acknowledging the improvements of the manuscript.

One of the weaknesses of our model that the reviewer pointed out is the unsatisfying model-data fit of the sediment preservation, particularly the preservation of total particulate organic carbon (TOC) at high latitudes. During the revision we made much effort to improve the TOC preservation by:

- conducting sensitivity experiments with respect to the settling flux to the seafloor
- adding sulfate reduction as an additional organic matter (OM) degradation pathway;
- extending the sediment model to a greater depth (50 cm now, instead of 10 cm before) within

the sediment, resolved with more vertical layers (71 node-grid now, compared to 21-node grid before);

• and improving the global sedimentation rate distribution with an additional lithogenic ("clay") input, as it turned out that the dust input flux was insufficient to produce realistic mass accumulation rates at shallow seafloor depths.

These changes have clearly improved the model-data fit, especially through considering OM degradation by sulfate reduction and enhanced sedimentation rates in shallower waters. Details of model changes are given in the reply to the general comments. Based on these improvements, the coupled FESOM2.1-REcoM3-MEDUSA2 simulation ($R_{coupled}$) was rerun and all model results have been updated in the revised version.

The other major critical point that the reviewer raised was that we did not show any results of a LGM or transient simulation. In our previous response letter, we mentioned that LGM simulations have been started with the fully coupled setup–AWI-ESM2, and those results will be published in another paper focusing on mechanisms driving the glacial CO_2 draw-down. To demonstrate that the ocean-only setup with MEDUSA can be used to study transient climate changes, we now conducted two transient experiments which describe the reaction of the ocean–sediment system after adding 1000 and 2000 PgC into the atmosphere, respectively. With those experiments, the interactions between the atmosphere, ocean and sediment under perturbation in the atmospheric CO_2 can be examined. More details are provided below in the reply to the general comments. The results of those experiments are presented in the revised manuscript.

General comments:

C: Comment #1.1: Improve the simulation patterns of preservation in the sediments: The poor model-data fit in Fig. 6 can not only be explained by the lower resolution. As stated in the previous review: "Previous models with similar or even coarser resolution are able to simulate POC (and calcite) settling fluxes and preservation on the shelves much better (e.g., Palastanga et al., 2011; Hülse et al., 2018; Ridgwell & Hargreaves, 2007)."

Taking OM as an example, I think there a multiple reasons for why the wt% patterns are not very realistic (that could/should be addressed):

1. The settling fluxes at high latitudes are (potentially) too large (comparing your Fig. 4a with Fig. 5a of Dunne et al. – note, that their color scale is very different), whereas the global total seems to be way too small (see Tab. 1). So the pelagic POC degradation should be improved first as this will influence the OM available for benthic preservation.

R: We agree that the modelled TOC wt% in Fig. 6 in the submitted version does not really match the observations. The reviewer is also right that the settling flux onto the sediment surface and the OM degradation in sediments are the two factors affecting the TOC content in sediments. We first compared the export production in our simulation with observation-driven model results (Clements et al., 2023, and studies compared there) and our result is within the range of those studies and relatively close to (Dunne et al., 2007). Estimated settling fluxes on seafloor vary over at least one order of magnitude at high latitudes (Dunne et al., 2007; Hayes et al., 2021). It is thus difficult to judge if the fluxes in our model are too high.

In REcoM3, settling fluxes onto the sediment surface are determined by sinking velocity and rem-

ineralisation of POC and the latter is a function of temperature and POC concentration. Sinking velocity of POC was already tuned to match the observed basin averaged vertical profiles of DIC, Alk, O₂, DIN and DSi (Fig. 3 in the submitted version) which show a good agreement with observations. And further changes in the sinking velocity will not affect the contrast between high and low latitudes. Thus, our tuning work focused on the temperature dependence of remineralisation. Several sensitivity experiments were conducted where Q10 for microbial degradation of POC in the water column was lowered step-wise from 2.3 to 1.5 so that OM degradation becomes faster at low temperatures (high latitudes) and slower at high temperatures. The settling fluxes of POC show correspondingly a stronger decline in large areas at high latitudes, while they are also reduced almost in the entire global ocean (Fig. 1). The contrast of sediment carbon preservation between the high-latitude shallower waters and the large area of the global open ocean does not change as much as the settling flux and much smaller areas at high latitudes are affected. A Q10 value much lower than 1.5 would be not reasonable for known microbial activities (Laufkötter et al., 2017).

Furthermore, the good agreement of basin-wise averaged profiles of DIC, Alk, O_2 , DIN and DSi with GLODAPv2 and WOA data also provides an evidence for a realistic water-column degradation of OM in our model. Therefore, we did not further tune the model regarding the settling fluxes but focused on the degradation processes in sediments.



Figure 1: Differences in the settling flux of POC onto the sediment surface $(\text{mmolC m}^{-2} \text{day}^{-1})$ and TOC wt% in sediments between the sensitivity experiment with Q10=1.5 and R_{init} in the submitted version.

C: 2. OM is not further oxidized when nitrate is exhausted – this is not correct and will cause too much OM preservation in these grid-cells: Judging by Fig. 7 (right, or Fig. 4 in replies to reviewers), NO3 is zero in a large fraction of higher latitude cells \rightarrow in these grid-cells too much OM is preserved (see Fig. 6)

R: Too much TOC is indeed preserved at high latitudes where NO_3 is exhausted. Unlike the the models cited above, MEDUSA includes a consistent NO_3 balance. If a simple first order approach is used for anoxic degradation (as, e.g., Palastanga do), the implicit assumption is that there are always enough oxidants besides O_2 . However, the oxidant balance is not closed, and since NO_3 is an oxidant and a nutrient, the nutrient cycle is unbalanced as well. Therefore, we closed the nutrient balance which results in a side-effect of excessive OM preservation in the submitted manuscript.

To better simulate OM degradation when NO_3 is exhausted, we now added SO_4 reduction into the reaction network after aerobic degradation and nitrate reduction. The same reaction rate constants

are applied for all degradation pathways, while they differ between the two OM classes over two orders of magnitude. A series of sensitivity runs were conducted to by varying the reaction rate constants to fit the observed TOC content in the surface sediment. SO_4 reduction substantially reduced the OM preservation at high latitudes and with the enhanced sedimentation rate in shallower waters together, the too strong contrast between the high-latitude shallower waters and the open ocean has been clearly improved as well (Fig. 2a and b).

Model details of SO_4 reduction and the new simulations are provided in the revised manuscript. Additionally, a detailed documentation is provided as supplementary material to describe the MEDUSA2 configuration used in the study.



Figure 2: TOC wt% averaged over the upper 10 cm of the surface sediment in R_{init} in the submitted version (a), in the new simulations considering SO₄ reduction (b) and additionally with improved clay input (c), and TOC wt% in Hayes et al. (2021) (d).

C: 3. Better tuning of the OM fractions and degradation rate constants in MEDUSA2 will also help. (For the revision the authors simply increased one degradation rate constant by a factor of 5 and 10.) Instead, rate constants could depend on seafloor depth, sedimentation rate or OM settling flux (see e.g., Boudreau, Springer Berlin, 1997). This would potentially not only improve the model-data fit but also responds to changing environmental conditions when simulating paleo-conditions.

R: Our configuration for the submitted version considered different degradation rates for the two OM classes: OM with a higher C:N ratio is 100-fold more slowly degraded through reaction with oxygen than OM with a lower C:N ratios. Degradation of different OM classes by nitrate reduction, however, had the same rate constant. In the revised version, the same rate constants are used for

oxic degradation, nitrate and sulfate reduction, but they differ between OM classes. With the additional degradation through sulfate reduction combined with the deepening of the sediment to 50 cm, we managed to well reproduce the observed pattern of TOC preservation.

C: Also, as the pelagic model only represents one OM fraction: How do you specify the two OM fractions in MEDUSA2 from this? I don't think this is discussed in the manuscript.

R: The ocean model REcoM3 simulates only one POM but with a flexible C:N ratio. To represent the entire range of the variable stoichiometry in the ocean model and keep the mass conserved between the ocean and sediment, we defined two POM classes in MEDUSA with the minimum and maximum C:N ratio found in settling fluxes produced by REcoM3 and partitioned the settling fluxes of PON (particulate organic nitrogen) into these two classes and then calculated the corresponding POC fluxes based on the fixed C:N ratios of the two POM classes. This was described in detail in the submitted manuscript from L170 to L182.

C: The results, of course, don't need to be perfect but should be better than presented in Fig. 6. And considering a run time of "2-3 weeks for 1000 model years" a few more experiments to improve the configuration are reasonable.

R: We agreed to carry out more experiments to improve the configuration, but this assessment of time that is needed was not realistic. It is true that calculating 1000 model years requires about 2 weeks. However, a lot of simulations have to be done for tuning a model and they can not always be run at the same time (due to the limit of available computing resources and logical sequence). After the model tuning, the production simulations for the manuscript were redone and the analysis and discussion of the results needed to be revised in the manuscript. We had therefore asked for an extension of three months for a thorough revision.

C: Comment #1.2: The global burial fluxes of POC (110 PgC kyr-1) and calcite (115 PgC kyr-1) look good (see Table 1). Please check the highest POC data estimate in Tab. 1 (i.e., 2600 PgC kyr-1) is this not a settling flux?

R: It is indeed the burial flux reported by Burdige (2007) and the high numbers refer to the continental margin sediments.

C: Comment #1.3: There seems to be something wrong with the opal fluxes: How can the opal settling flux in areas $\gtrsim 1 \text{km}$ (79-84 Pmol Si kyr-1) be larger than the global flux (22-40 Pmol Si kyr-1) in Table1? Also the units are different in the text (Tmol Si yr-1) and the Tab. 1 (Pmol Si kyr-1). And why is the global opal burial flux even larger (82 Pmol Si kyr-1). And compared to this the observed global burial is tiny (7.1 Pmol Si kyr-1).

R: We thank the reviewer for pointing out the different units used in the table and text. In the revised version we only use $Pmol \, kyr^{-1}$ in Tab. 1 and the related text.

The opal burial in $R_{coupled}$ is 12 Pmol kyr⁻¹, not 82. We apologize for the typo. The same number (12.1) can be found again in Tab. 2.

The deep-water settling fluxes of opal in Tab. 1 are higher than the global ones, because the numbers stem from different studies and none of them reported both for the deep-water and global sediments, except for Treguer et al. (1995) who reported an opal burial in deep-water sediments of 5.9 and in the global sediments of $7.1 \text{ Pmol kyr}^{-1}$. This was discussed in L335–L340 in the submitted version



Figure 3: Temporal evolution of the atmospheric pCO_2 in the experiments with an addition of 1000 (R_{pert1k}) and 2000 PgC (R_{pert2k}) in the atmosphere (a); and the change of calcite content in sediments relative to the state before the CO₂ perturbation in R_{pert1k} (b) and R_{pert2k} (c).

and we rephrased it to make it clearer.

C: Comment #2: Figure 6: The new color-bars for the model results (right) are finer than the colorbar for the observations (left). Therefore, model and observations cannot properly be compared as more features appear in the model results than in the observations (this was introduced to address one of the comments of reviewer #1).

R: Thanks! This inconsistency was overlooked in the submitted manuscript. The plots are redone now with the same color bar.

C: Comment #3: A transient experiment or paleo-application. This would be highly informative and was suggested by both reviewers (e.g., 1st comment of Reviewer #1) but has not been addressed. At least the model could be used to simulate an idealised perturbation experiment to showcase that it can be used for transient applications and that the sediment properties respond. In particular, because this is mentioned as one of the main motivations for configuring this model.

R: Please also see the reply to the general comment above. To demonstrate how the model responds to perturbation in the carbon system, we added 1000 (R_{pert1k}) and 2000 PgC (R_{pert2k}) into the atmosphere at the end of the coupled simulation $R_{coupled}$ and let them run for another 2000 years. The interactions between the atmosphere, ocean and sediment carbon pools, particularly in the form of calcite, were examined. Calcite in sediments are strongly dissolved (Fig. 3b and c) and the atmospheric CO₂ declines from 1235 ppm to 490 ppm in R_{pert2k} and from 765 ppm to 380 ppm in R_{pert1k} after 2000 years (Fig. 3a), showing the effect of carbonate compensation feedback. New sections have been added in the method and result chapter in the revised manuscript to describe these new experiments.

C: Comment #4: I was also not very convinced by the authors reasoning for why they did not include some output of C-isotopes. This was also suggested by both reviewers and is highly relevant for a model that will be applied to paleo-applications.

R: We agree – with both reviewers – that having isotopes in a coupled ocean–carbon cycle–sediment is highly relevant for a model that is intended to be used for paleo-applications, the more since the sediment model allows for the construction of synthetic cores that could be directly used for model-data comparisons. However, contrary to what the comment suggests, there are not such results, there is no "output of C-isotopes" that we could possibly present. The coupling has been technically realised (the code exists), but has neither been tested, nor calibrated. First of all, the calibration

and validation of the carbon isotopic part of the model is obviously dependent on that of the underlying carbon cycle and it goes without saying that there is no point in starting to calibrate the isotopic part as long as the fundamental C cycle does not yield satisfactory results (we are convinced that the present revision is now bringing us closer to this milestone). It is furthermore well-known that an ocean-only model (without sediments) already takes an order of magnitude longer to equilibrate its C isotope distributions than it requires to equilibrate its DIC and ALK distributions (see, e.g., Lynch-Stieglitz et al. (1995)); adding ocean-sediment exchange processes further extends this time. Besides these timescale constraints, which are inherent to the system under study, it should not be forgotten that additional tracers will also lead to longer computation times: for the sediment part alone, adding ¹³C and ¹⁴C will increase the computation time by $\sim 180\%$ (computation time roughly scales with the square of the number of tracers considered). Adding robust C-isotope results in this paper would simply require such a large amount of time, alone for the computations. Practically speaking, requiring us to include isotope results at this stage raises an unrealistic, if not impossible expectation.

Please rest assured though that tackling the isotopic related parts in the coupled model is one of our first priorities once the fundamental carbon cycle is deemed to operate in a satisfactory way, the more since isotopes also offer further means to improve the calibration of the sedimentary process representations.

C: Comment #5: Why a mass correction to account for the asynchronous coupling is necessary is unclear to me. Please explain and justify this better in the text. My understanding is, that while this might affect the inventories & fluxes during the spin-up phase the system should eventually come to a (new) steady- state.

R: We thank the reviewer for insisting on this mass-conservation issue, which was actually addressed in response to a comment to the initial version of the manuscript, but unfortunately incompletely assessed in the previous revision. The reviewer's understanding about the asymptotic behaviour of the asymptotic error due to the asynchronous coupling is justified: this error should fade away when steady-state is approached (at least on average over a few coupling intervals)

For the current revision, we further examined the mass conservation in the different compartments of the coupled model. Mass conservation in MEDUSA2 is very strong (the relative error between the actually calculated global inventory change and that calculated from the globally integrated transport and reaction terms is typically $10^{-9}-10^{-12}$). Decreasing the coupling interval by a factor of 5 (from 50 to 10 years) only improves the inventory imbalance from 0.53% kyr⁻¹ to 0.4% kyr⁻¹ Although the shorter time step clearly contributes to reduce the diagnosed imbalance, the improvement is comparatively small. We therefore conclude that the asynchronous coupling cannot be the main reason for the imbalance. It is most likely due to the (known) tracer conservation issues related to the use of an unstructured grid in FESOM. This will be further investigated and improved in future development work of FESOM-REcoM. In the meantime the mass correction helps us to ensure that the total tracer inventories in the ocean is strictly conserved, considering the globally integrated in- and output fluxes of the different tracers.

The paragraph on the mass conservation issue and how it was addressed has been rewritten and moved to the section on FESOM2.1-REcoM3p in the model description chapter.

C: Comment #6: The higher spatial resolution result (Rhigh): I understand, that this was included

to address parts of the 2nd comment of Reviewer #2. However, these results are rather out of place here. Also the authors argument that this experiment shows that the coarse model resolution of Recoupled is mainly responsible for the low settling fluxes (lines 316-320) is at least insufficient: It is unclear if model resolution is the only boundary condition/parameter that changes between both configurations. Anyhow, there are multiple ways to increase the POC settling fluxes in the lower resolution Recoupled configuration (e.g., by increasing the low export production as acknowledged by the authors, or decreasing pelagic POC remineralization rates).

R: The resolution in this run was indeed not the only difference between those simulations. The ecosystem is a bit different in the high-resolution run, including a second zooplankton class which affects the cycling of nutrients. During the revision we conducted one simulation with the same code version but a much higher resolution (with ca. 127,000 surface grids) and updated the numbers for R_{high} in Tab. 1. The fraction of shallower-water POC settling is about 70% of the global flux, supporting the argument that the low resolution of simulations in this study is mainly responsible for the underestimation of the fraction of the shallower-water POC flux. The reviewer is right that results of the high-resolution run in the table seems to be out of place, since it is not the focus of this study and not discussed anywhere else in the manuscript. However, it is an important evidence for the considerable role of model resolution which can be better illustrated when comparing with the low-resolution run in numbers. Thus, we kept it in the table but added a short explanation in the table caption.

C: Comment #7: Fig. 3: I suggest including the profiles at the end of Rcoupled here as well because these are the new results presented and tested in the manuscript.

R: Agreed. The profiles of $R_{coupled}$ are moved from the appendix to Sect. 3.2.5 'Impact of the complex sediment on productivity and nutrient supply' and those of R_{sedbox} to the appendix.

A few minor comments:

C: Fig. 6: What is the simulated wt% here? Is it mean over the bioturbated layer, at 10cm, or something else? And what are the corresponding values of Hayes et al. (2021) representing?

R: Our model result was shown as the averaged sediment wt% over the surface 10 cm, while Hayes et al. (2021) shows the averaged wt% over the Holocene age if the age constraints are available and otherwise the measured compositions reported for the surface sediment. In the revised manuscript, for the comparability to data, we still calculated the averaged sediment wt% over the surface 10 cm, even when the reactive layer in our MEDUSA application is extended to 50 cm.

C: Fig. 7: I find it not very intuitive why you show RNO3 here. Can you please motivate this. If sulfate reduction would be included in the model (more important than Mn, or Fe-reduction on a global scale) then one could nicely show the different fractions.

R: Following the referee's implicit suggestion, we included sulfate reduction (skipping Mn(IV) and Fe(IV) reduction) as a further redox process in the revised version of the model. In the wake of this extension, Fig. 7 has been replaced with the carbon degradation rate by aerobic respiration, nitrate and sulfate reduction and the corresponding discussion in the manuscript has been updated.

C: Fig. C1: Why is there such a large drop in the calcite burial flux even though the calcite settling flux increases over the experiment?

R: In the submitted version there was no drop in calcite burial but in opal burial. Since the coupled simulation was rerun, all the related figures have been updated. In the new Fig. C1 the change in burial flux of opal is around 0% during the entire coupled simulation. Only POC burial shows a drop at the beginning of the simulation which can be explained by the drop of POM settling flux on top sediment.

We show this figure in the appendix to provide evidence that the ocean-sediment system starts to move towards a new steady state after a relative rapid adjustment during the first one or two coupling cycles. The small trend at the end of 2000 years indicates that a system including the complex representation of the seafloor sediments needs much longer to reach the steady state. The main focus here is the long-term trend, not the larger change during the adjustment. Thus, the figure does not resolve the first 200 years with more details. The large changes in the beginning of the simulation are caused by the large gradients at the water-sediment interface, since the starting conditions used here were obtained with REcoM3p run with the sedimentary input from the original one-box sediment layer and with no riverine input. Once the coupled simulation with the (precharged) sediment start, the in- and output flux patterns in the ocean completely change. Since the sediment now buries POC, less DIN is returned to ocean bottom, and less oxygen is consumed there. Also already during the first coupling cycle, biological productivity adjusts due to changes in nutrient supply. Accordingly the deposition, and thus degradation and diffusive return flux patterns adapt, and the whole system evolves towards a new steady-state, as shown on these graphs.

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