

## Response to anonymous reviewer comments RC3

Please see our responses in blue below.

In this paper, a new tool is presented that couples a low-resolution pelagic biogeochemical model with a low resolution benthic biological model for the Baltic sea. The (vertically integrated) benthic state variables are then used to calculate impacts on biogeochemistry using presumed effects of bioturbation and water-column conditions on denitrification and phosphorus dynamics. My main doubts with this paper are connected to the biological focus of the model.

Essentially there exist two schools of modelers: some modelers take a *biological* approach and ignore or strongly parameterize biogeochemistry. Their models disregard the small-scale vertical gradients of solutes in the sediment and often consider only surface-averaged concentrations of particulate substances (e.g. organic matter). Moreover, their models operate on seasonal time scales, as organisms usually react on these time scales. Opposed to this are the modelers that tackle sediment dynamics from a *biogeochemical* perspective and strongly parameterize biology. These modelers take into account the fine-scaled vertical gradients of solids and solutes that are observed in the sediment, and their dynamics includes reactions operating at very different timescales, from very short (< seconds) up to very long time scales (multi-years). In these models, the metabolism of the (higher) organisms is included as “oxic mineralization” of organic matter, while their bioturbation activity is included as a “coefficient”. Thus, these models strongly parameterize the biology, and only explicitly account for the biogeochemistry. As long as the main conclusions of these models are stated in the area of the model focus, there is nothing wrong with any of these approaches. For instance, it is reasonable to assume that a biogeochemical model can rather faithfully reproduce the impacts of certain external conditions on sedimentary nitrogen or phosphorus removal rates, but it is questionable whether such models can also well represent the distribution of the benthic organisms that drive the biogeochemical cycles. Similarly, why would we put a lot of faith in biogeochemical conclusions that come from a model that focusses on biology and parameterizes the biogeochemistry? This is in a nutshell the doubts I have on this paper. While the conclusions seem logical, I am still to be convinced that the tool used to arrive at them is appropriate.

Because of the biological focus, there are quite some assumptions with respect to biogeochemistry that are not dealt with in the manuscript. For instance: the paper talks about the sediment pools of C, N and P, and Si. Biogeochemically one distinguishes between particulate and dissolved pools – here I had to guess that the pools refer only to particles (the ‘food’ of the organisms). Thus, the transient (within season) storage of dissolved components is ignored. Is this a reasonable assumption? (I could not find any evidence for this). In addition, historical eutrophication in the Baltic may have caused significant storage of dissolved nutrients deep in the sediment (i.e. ammonia, phosphate, sulphide), which are not accounted for in the model. Can these be ignored – what is the effect of ignoring these on long-term simulations?

In addition, the dependencies of the biogeochemical processes on the model variables are so complex that it is very difficult to see how these processes are affected. For instance the formula (5), which essentially describes the dependency of denitrification on water-column oxygen and biota, has 4 “fitting” parameters – to what data have these been fitted? The P-sequestration formula (formula 7) has even 8 “fitting” parameters. On

line 187, it is said that it is difficult to constrain the new parameters. Does this mean that these parameters have not been fitted at all – and if they have, on which data? And why would instead running sensitivity analyses by changing the E<sub>bio</sub> parameter be a valid alternative? A little more effort in showing that these dependencies are realistic is required. (and where is formula 6?).

I also find the lack of any comparison of model output with biogeochemical sediment data worrisome. On L 313, the authors claim that they cannot “properly validate the simulated sediment stocks or fluxes due to a lack of large-scale data and insufficient understanding of the multitude of mechanisms underlying the biogeochemical transformations and fluxes”. The first part (lack of data) does not do justice to the multiple biogeochemical studies in the Baltic that have recorded sediment-water exchange fluxes, and measured sediment concentration profiles in great detail. Also, I do not agree with the statement that there is “insufficient understanding” of biogeochemistry. As a quantitative science, biogeochemistry is at least as (and probably much more) advanced as biology! And even if it were true that we do not understand the biogeochemistry, why would we then trust the simple parameterisations that are used in this manuscript?

In summary, as much as I like the conclusions from this paper, the authors need to try a bit harder to convince that biogeochemistry in the Baltic can be predicted based on presumed effects of biological activity on N and P removal.

We agree with the reviewer that organic matter processing in sediments has traditionally been studied in different fields of science with differing foci and assumptions. An excellent treatise of this subject can be found in the recent review by Middelburg (2018). As stated by Middelburg, we also believe that while there is merit in the traditional approaches, there is added benefit in interdisciplinary approaches bridging this gap. For example, most biogeochemical models of sediment diagenesis include the bioturbation of animals, but only represent their consumption of organic matter and secondary production implicitly in a bulk formulation. On the other hand, few biological models resolve the dynamic coupling between benthic animals and their sedimentary resources. In addition to Middelburg (2018), several other recent reviews and perspectives have called for interdisciplinary approaches merging the biological and biogeochemical as well as benthic and pelagic research traditions (Ehrnsten, 2020; Lessin et al., 2018; Snelgrove et al., 2014, 2018). We believe that our approach should be well suited for the current journal, as its aim is to “cover interactions between the biological, chemical, and physical processes”. Or to cite the concluding remark of Middelburg (2018): “I hope that colleagues studying marine sediments are aware that “bio-” in sediment biogeochemistry is more than just microbiology”.

We have added several justifications of our choice of approach and methodology to the introduction, as also requested by Reviewer 1. The new introduction is reproduced below:

#### “1. Introduction

Coastal ecosystems are highly productive, consist of diverse biological communities and carry out important functions including those supporting a growing world population (Costanza et al., 1997, 2014). However, they are facing multiple anthropogenic pressures such as nutrient loading and climate change (Cloern et al., 2016; Halpern et al., 2008). Elucidating the mechanisms of the coupled biogeochemical cycling of carbon

(C), nitrogen (N) and phosphorous (P) in these systems is important to understand how they respond to current and future pressures, but also because they contribute to the regulation of global climate and nutrient cycles by processing anthropogenic emissions from land before they reach the ocean (Ramesh et al., 2015; Regnier et al., 2013a, 2013b; Seitzinger, 1988).

In contrast to the deep open ocean, benthic-pelagic coupling plays a large role in biogeochemical cycling in coastal and estuarine ecosystems (Soetaert and Middelburg, 2009). Coastal sediments act as hotspots for organic matter degradation and permanent removal of elements from biological cycling through burial and denitrification (Asmala et al., 2017; Regnier et al., 2013a; Seitzinger, 1988). The bioturbating activities of benthic fauna alter the physical and chemical properties of surface sediments, which in turn strongly influence organic matter degradation processes and benthic–pelagic biogeochemical fluxes (Aller, 1982; Rhoads, 1974; Stief, 2013). Here, we define bioturbation as all biological processes that affect the sediment matrix, including burrow ventilation (bio-irrigation) and reworking of particles (Kristensen et al., 2012). Additionally, benthic fauna retain carbon and nutrients in its biomass and transform them between organic and inorganic forms through metabolic processes (Ehrnsten et al., 2020b and references therein; Herman et al., 1999; Josefson and Rasmussen, 2000). Together, these direct and indirect effects of benthic fauna have far-reaching consequences for ecosystem functioning in the benthic and pelagic realms (Griffiths et al., 2017; Lohrer et al., 2004).

Even though the importance of benthic fauna for sediment biogeochemistry and benthic–pelagic fluxes has long been recognized (Rhoads, 1974), the combined effects of animal bioturbation and metabolism have seldom been studied together (Ehrnsten et al., 2020b; Middelburg, 2018; Snelgrove et al., 2018). A long-standing assumption in biogeochemical sediment research is that animals contribute considerably to transport of solids and solutes through bioturbation, but their consumption of organic matter is of minor importance (Middelburg, 2018). However, several studies show that this assumption does not hold in many shallow coastal systems, as recently reviewed by Middelburg (2018) and Ehrnsten et al. (2020b).

Further, empirical studies of faunal effects often focus on temporally and spatially limited parts of the system, omitting important interactions and variability occurring in natural ecosystems (Snelgrove et al., 2014). It is logistically challenging to study multiple drivers and interactions in the benthic and pelagic realms, such as the interactions between benthic and pelagic production, empirically. Mechanistic or process-based models are powerful tools to conduct such studies (Seidl, 2017). Here, we extend a physical–biogeochemical model of the Baltic Sea ecosystem (BALTSEM; Gustafsson et al., 2014; Savchuk et al., 2012) with benthic fauna components based on the Benthic Macrofauna Model (BMM; Ehrnsten et al., 2020a). We include both the direct feedbacks from animal growth and metabolism and the indirect effects of their bioturbating activities on biogeochemical cycling to evaluate their relative contributions.

We use the Baltic Sea as a model area for three reasons: (i) the shallow depth (mean depth 57 m) and enclosed geography with a long water residence time (about 33 years) contribute to strong benthic-pelagic coupling (Snoeijs-Leijonmalm et al., 2017; Stigebrandt and Gustafsson, 2003), (ii) the relatively simple, species-poor benthic communities facilitate model development, and (iii) the major features of biogeochemical cycling of C, N and P in the Baltic Sea are well known due to a wealth of oceanographic measurements and studies performed over the past century, making it an ideal system

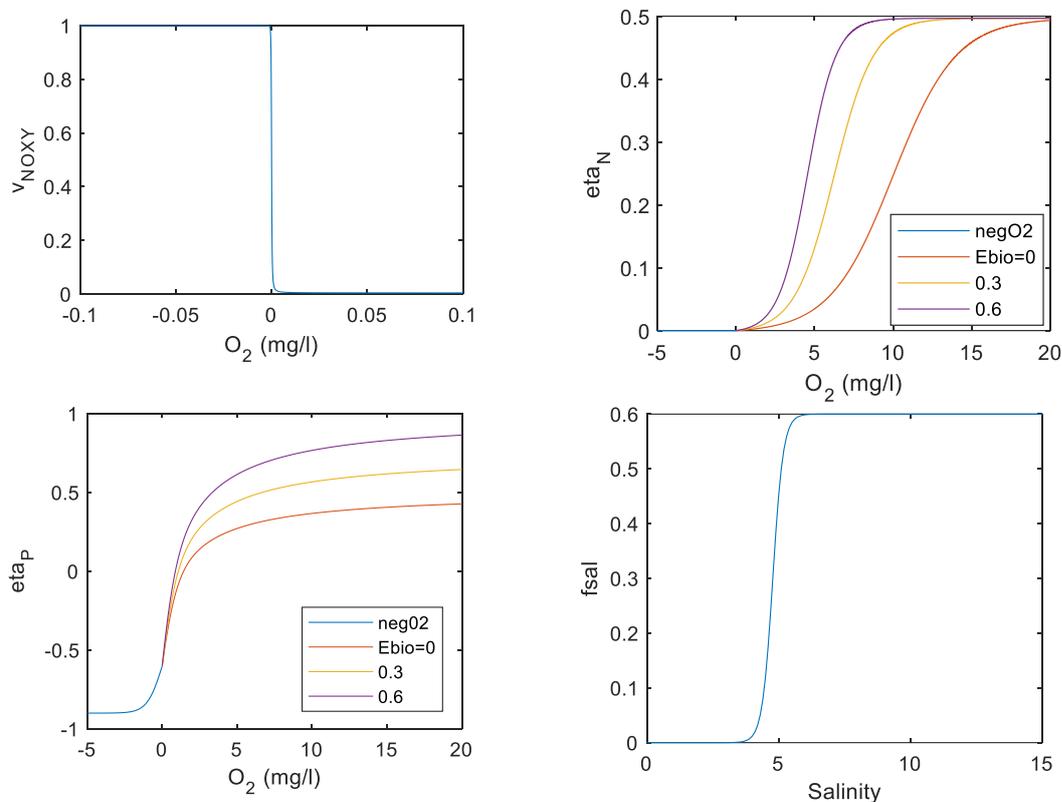
for process-based modelling (Eilola et al., 2011; Gustafsson et al., 2017; Savchuk and Wulff, 2009, 2001). However, the sediment pools and the role of sediment processes in benthic–pelagic exchange are not as well quantified as pelagic pools and fluxes. The higher uncertainty in benthic compared to pelagic processes as well as the traditional focus on pelagic eutrophication are probable reasons why physical-biogeochemical models of the Baltic Sea have omitted benthic fauna as state variables (e.g. Eilola et al., 2011; Lessin et al., 2018). Here, we aim to fill this knowledge gap and explore the role of benthic fauna in biogeochemical cycling of C, N and P on a long-term ecosystem-level scale.”

It is true that all models are simplified representations of reality, and the level of complexity and detail frames the questions that a model can answer reliably. Therefore, great care should be taken in choosing the appropriate model formulations based on the question(s) being asked. Here, our main focus is on the biogeochemistry of the Baltic Sea as a coupled benthic-pelagic system. This means that we are primarily focussing on basin-wide spatial and long temporal (days to decades) scales. Many physical-biogeochemical ecosystem models working on similar scales choose to treat the sediments as a reactive boundary layer, where sinking organic matter is immediately transformed to inorganic compounds and returned to the pelagic. Soetaert, Middleburg, Herman & Buis (2000) reviewed and tested different approaches to couple benthic and pelagic biogeochemical models in coastal shelf systems (from no to vertically resolved sediment models), and concluded that the best choice is a vertically integrated dynamic sediment model of the type used in BALTSEM, because of an optimal balance between computational demand and accuracy attained in terms of e.g. mass budgeting and seasonality of benthic-pelagic solute fluxes. Two decades later, computational resources have increased, but we still argue that including a vertically resolved Reactive-Transport-Model (RTM) or similar for the sediments remains suboptimal. In the case of BALTSEM, each sediment variable is resolved at each depth meter in thirteen basins, amounting to 1349 individual RTMs that would need to be run in parallel. In addition to the increased running time, parameterisation would be difficult and time-consuming and the added complexity would reduce interpretability and traceability of results (Levins, 1966; Robinson, 2008). Some development in the integration of vertically resolved sediment and pelagic biogeochemistry is ongoing, but these models generally need to trade off complexity in other parts. For example, Radtke et al. (2019) implement such a model in one dimension at a few individual sites and omit dynamical modelling of the physics.

In the early days of BALTSEM development, Savchuk & Wulff (1996) developed and tested the use of a detailed process-oriented sediment model in BALTSEM with solids and solutes as separate state variables. However, they found that data to parameterize and verify the various processes on a system level were largely lacking. They also found that a simplified version with only one state variable for each sediment nutrient pool gave comparable results. In the approach used in BALTSEM since then, the solutes in the sediments are not prognostic state variables, hence, solutes produced or consumed in the sediments are directly causing exchange with the water column. We would argue that on a long-term ecosystem scale, the omission of short-term storage of solutes in pore waters does not significantly hamper model functionality. For further discussion and reasoning behind the formulations, we refer the reader to previous BALTSEM publications (Savchuk et al., 2012; Savchuk and Wulff, 1996, 2001) as well as other model descriptions using similar formulations (Capet et al., 2016; Isaev et al., 2020; Samuelson et al., 2015).

Regarding the ability of BALTSEM to reproduce the long-term storage of nutrients in sediments in response to eutrophication, we would like to point to two previous studies, showing the simulated build-up of nutrient stores in sediments (Gustafsson et al., 2012) and the consequent increase in benthic fauna (Ehrnsten et al., 2020). While quantitative data to validate the sediment pools themselves is scarce, BALTSEM has been shown to accurately reproduce the long-term development of pelagic nutrient pools (Gustafsson et al., 2012; Savchuk et al., 2012). We consider this important indirect validation of sediment pools and dynamics, as it would not be possible to reproduce the time-lag in pelagic nutrient pools compared to inputs without a proper representation of sediment pools and processes.

The reviewer shows some concern regarding the complexity of sediment biogeochemical model formulation, in particular the equations for apportionment of mineralized N into NH, NO and N<sub>2</sub> ( $v_{NOXY}$  and  $\eta_N$ ) and mineralized P into release versus sequestration ( $\eta_P$ ). These mathematical formulations are indeed not the most accessible, and we would therefore like to open them up with a graphical presentation of the shape of the curves in relation to bottom water oxygen concentration below.  $v_{NOXY}$  gives the fraction of mineralized N released as NH in relation to oxygen concentration.  $\eta_N$  (“eta<sub>N</sub>”) defines the fraction of oxidized N released as NO. The other fraction is denitrified.  $\eta_P$  gives the fraction of mineralized P that is sequestered in the sediments. Here, the curve is shown for salinity > 5. The second term in  $\eta_P$ ,  $fsal$  is a step-like function which leads to higher P sequestration in the Bothnian Bay compared to all other basins. This is used as a proxy for the higher availability of phosphate-binding agents in this basin.



The sigmoid form of the curves requires several parameters. We realize that calling these parameters “fitting constants” was misleading, as they are not independent parameters resulting from curve fitting to a specific dataset. Instead they are based on a general understanding of these processes put into mathematical terms (Savchuk and Wulff, 1996). We will therefore refer to them as just parameters in the future.

The addition of bioturbation enhancement to these formulations is also based on a qualitative understanding rather than fitting to data. As explained in the manuscript in more detail, we assume that bioturbation increases oxygen penetration into the sediments, thus shifting the curves in relation to bottom water oxygen concentration. As we do not know exactly how much the curves should be shifted, we performed a sensitivity analysis with a range of values for the parameter  $E_{max}$  in the bioturbation enhancement formulation.

We realize that the statement on line 313 about lack of data was badly formulated and we have now removed it from the manuscript. There is indeed a wealth of research on sediment biogeochemistry in the Baltic Sea. What we meant to say is that a comprehensive compilation of data on sediment stocks and fluxes on the scale needed for model validation is missing. It would be beyond the scope of this study to compile such a validation dataset. When writing the original manuscript, we considered citing a range of benthic-pelagic fluxes measured in the Baltic as validation for our model estimates, but concluded that citing fluxes out of context does not do justice to the research performed and does not add much scientific value to the current study. For example, a recent compilation of sediment-water dissolved inorganic P fluxes measured in the Baltic Sea (Berezina et al., 2019) gives a range of ca -29 to +87 mg P m<sup>-2</sup> d<sup>-1</sup>. Without a proper upscaling exercise accounting for the context of each study (which would be the subject of a comprehensive review), we do not believe that these numbers are of much value as validation.

Thus, beyond the validation of benthic fauna stocks and comparison to sediment C:N:P compiled by Cederwall and Elmgren (2001), we refrain from formal validation of sediment stocks and fluxes. However, a qualitative, and partly quantitative, comparison of model results to the current understanding of sediment processes and the impact of benthic fauna on them is included in the discussion section 4.2. As stated above, we also believe that the validation of pelagic biogeochemistry (Appendix B) is an indirect validation for sediment stocks and fluxes, as the benthic and pelagic are strongly coupled in this system. We have also added a discussion on ways forward to improve model validation and reliability to the last chapter “5. Conclusion and outlook”:

“Even though these large-scale simulations contain a large degree of uncertainty, they are an important complement to empirical studies, which for practical reasons can only consider temporally and spatially limited parts of the system (Boyd et al., 2018; Snelgrove et al., 2014). To improve the confidence in simulation results, we see two major ways forward. First, as all models contain different formulations, assumptions and uncertainties, implementing benthic fauna components in other physical-biogeochemical models and comparing the results would greatly increase the strength of evidence for those results where different models agree. This kind of ensemble modelling is increasingly used in climate change research, and has also been applied in the context of Baltic Sea biogeochemistry (Meier et al., 2012, 2018; Murphy et al., 2004). We hope that the publication of the benthic model formulations stimulates the development of benthic fauna modules in other models of the Baltic Sea ecosystem and beyond. Even though the current model implementation is only applicable to the brackish parts of the Baltic Sea due to a lack of functional groups present in the marine parts, the inclusion of additional functional groups using the existing groups as a template would be straightforward technically. The main challenges are the parameterisation of group-specific rates as well as managing the increased complexity.

Second, a comprehensive compilation of observational data on sediment stocks and fluxes would be needed for improved model validation. Such data is collected for monitoring and research purposes by a great number of institutions around the Baltic Sea, but a comprehensive, open-access, quality-controlled collection of this data is lacking. The Baltic Environment Database (BED) has been invaluable for both model development and validation of pelagic physics and chemistry. While this data can be used as indirect validation of benthic model processes in the strongly coupled system, we call for the development of a “Benthic BED” to facilitate future model development. A comprehensive collection of observational data would also facilitate the identification of knowledge gaps and future research priorities.”

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