Response to the review of J. Middelburg

The authors present a rather complex model allowing simulation of biogeochemical processes in coastal systems subject to seasonal anoxia. The paper has a few strengths and many weaknesses. Most numerical biogeochemical models focus ei- ther on the water column or on the sediments and very few couple these domains. The presented BROM model **does explicitly deal with the coupled system** and is therefore of value.

Strengths of this paper include the (a) coupling of pelagic and benthic modules, (b) the explicit resolution of the benthic boundary layer (BBL), (c) the focus on seasonal hypoxia and (d) its linkage to/integration with the Framework for Aquatic Biogeochemical Modeling. These characteristics make this an interesting paper and the presented model is potentially useful.

However, there are many issues to be resolved before publication of this paper and model. 1. The paper is poorly written in terms of organization, flow and **use of English**. A few examples of the latter (line 1: seawater and benthic sediments, benthic sys- tems or sediments are fine, but not benthic sediments; the use of the term protolithic processes: do you refer to stone age processes? or do you simply mean equilibrium processes, etc. etc.). There appear native speakers and/or UK/Canada based scientists among the authors: perhaps they should have another look at it. The text is also not prepared with utmost care: many typos, wrong equations etc. (see below in the list of detailed comments).

We apologize for the condition of the original submitted manuscript, and thank the Reviewer for nevertheless providing a detailed and constructive review which has contributed to a major improvement (in our opinion) in the model code and description. The new submission has been thoroughly revised to improve structure, language, and accuracy of the equations.

The model could be much better put in context and **existing literature** is poorly incorporated. I was missing references to other papers dealing with coupled benthic-pelagic models, the more simpler ones (Lancelot, Soetaert, Fennel, Reed and co-workers) and the highly complex ones from the ERSEM family. Soetaert and co-workers (Soetaert and Middelburg, 2009; Meire et al., 2013) have published on seasonal oxygen issues with coupled pelagic benthic models. There is also a large body of knowledge on the effect of oxygen in early diagenetic models; that literature is not covered. Extensive work on the role of sediments as moderating the timing of return fluxes (delay in return of N, P, Si after bloom) and the memory provided by stored reduced sulfur, iron and carbon in sediments is poorly covered (see work on Gulf of Mexico by Nancy Rabalais and co-workers).

We thank the reviewer for drawing our attention to this work, which is indeed highly relevant. The Background section has been extended to provide a more thorough summary of existing literature, including all of the models cited above. It remains, however, a summary and not an in-depth review; the latter is beyond our intended scope.

The model **description** is often incomplete and imprecise (see below for a far from complete list). The documentation is not sufficient. Boundary conditions of the model are not clearly described. Details about the coupling of the models are insufficient: e.g. the grid size is very likely changing, yet not provided. It is unclear whether particulate organic matter is modeled explicitly. Is it transported by bioturbation in the sediment. It is unclear how bio-irrigation and solid-phase mixing are treated. Sometimes parameters are introduced in the text, but appear as fixed value (hard-coded) in the tables.

We acknowledge and apologize for these shortcomings. The new submission offers a much more thorough description. Boundary conditions are now described in a dedicated section 2.2.5. The BROM-transport grid, which combines water column and sediment subgrids, is now described in a dedicated section 2.2.3. Dead particulate organic matter is explicitly modeled, as is now stated clearly in section 2.1.2. Particulate variables are diffused in the sediment by bioturbation – this is now clarified in section 2.2.1 which describes the BROM-transport model formulation. In BROM-transport, bio-irrigation is treated as a non-local exchange process following (Boudreau, 1997; Schluter et al., 2000; Meile et al., 2001) (see section 2.2.1). Mixing of solid phase constituents is only by bioturbation in the sediments. Mixing of the solid phase as a whole (interphase mixing) in BROM-transport may occur only by bioturbation at the sediment-water interface. These processes are now clearly described in the new section 2.2.1.

The model is very complex and detailed (perhaps too much) in some aspects and very rudimentary in other aspects. Regarding the latter, many detailed Mn, Fe, S transformations are included, chemoautotrophy is resolved for aerobic and anaerobic microbes (or only bacteria?), but important processes such as methane generation and anaerobic methane oxidation coupled to sulfate reduction are ignored. Another example particle settling velocities is corrected for the formation of Mn-oxides in the water column but other carrier phases such as calcium carbonate are not resolved. Clearly, the presented model is a version 1.0 and represents a first step, but the priorities of the authors do not match those of the majority of the audience. At the minimum some motivation for their particular choice should be communicated to the audience.

The motivation for the complexity of BROM is discussed in the new text (section 2.1.1):

"The model has 33 state variables (Ci), described in Table 1. This includes frequently measured components such as hydrogen sulfide (H2S) and phosphate (PO4), as well as rarely measured variables such as elemental sulfur (S0), thiosulfate (S2O3), trivalent manganese species Mn(III), and bacteria. Variables of the latter category were included because their contribution to biogeochemical transformations is believed to be substantial. For instance, bacteria play an important role in many modelled processes and can consume or release nutrients in organic and inorganic forms (Canfield et al., 2005; Kappler et al., 2005). We acknowledge that for many of these additional variables, site-specific estimates of associated model parameters and initial/boundary conditions may be difficult or impossible to obtain, and may in practice require some crude assumptions and approximations (e.g. universal default parameter values, no-flux boundary conditions, initial conditions from a steady annual cycle). Nevertheless, we believe that for many applications this will be a price worth paying for the additional process resolution/realism provided by BROM for important biogeochemical processes in the BBL and sediments."

The definition of the “bacteria” model compartment is made precise in the new text:

"We divide all the living OM (biota) into Phy (photosynthetic biota), Het (non-microbial heterotrophic biota), and 4 groups of "bacteria" which may be considered to include microbial fungi."

The processes of methanogenesis and methane oxidation with oxygen have been added to BROM-biogeochemistry.

The effect of accelerated particle settling velocities has in fact been removed in the new code, and the text has been adjusted accordingly.

Section 3.1 on model output **discussion** needs major revision. The link with the figures is unclear and the organization is suboptimal. You discuss the oxygenated winter period and then link to later periods or a few days later in the section on oxygenated winter period. There is no **story**. Try **to limit yourself to a few findings and discuss those**. The reader now has to digest all the computer output her or himself.

Section 3 was shortened and re-structured. Following the reviewers' recommendations we now just focus on describing the ability of BROM to simulate changes in the redox conditions and illustrating the rates of processes and transport fluxes.

Section 3.2 is not useful or convincing. The link with data is very poor. This is indeed a difficult job, but here serious work has been done. A comparison with just three to four papers is made and the extensive databases on oxygen uptake, oxygen penetration depth etc are not consulted. A statement like line 10 on page 20: “further observations under anoxic and suboxic conditions are rare as field and experimental studies generally focus on oxic conditions” is close to unacceptable. Consider all the work done on the Eastern Pacific ocean margins (Washington and Oregon shelves, California basins, Mexico/Peru/Chile margin), Indian ocean and shelves and multiple European systems (Black Sea, Baltic Seas). There are nice seasonal time series in coastal systems with low-oxygen events during summer (Kiel bight, etc.)

Section 3.2. was removed from the text.

Minor issues:

Page 3: - Line 2: benthic sediments? –

Modified to "benthic systems"

Line 3: directly affect and are impacted by.. –

Sentence modified to:

"Benthic fluxes of chemical elements (C, N, P, O, Si, Fe, Mn, S) alter redox state and acidification (i.e. pH and carbonate saturation), which in turn affect the functioning of benthic and pelagic ecosystems."

Line 7: fuzzy writing, rewrite

Sentence modified to:

"The redox state of the near bottom layer in many regions can change with time, responding to the supply of organic matter, physical regime and coastal discharge."

Page 4: - Line 3: enrichment with OM or do you mean deposition of labile organic matter –

Sentence modified to:

"The sediment generally consumes oxygen due to deposition of labile OM and presence of reduced forms of chemical elements"

Line 26-27: animals can die, migrate or change their behavior: revise text accordingly

Modified to:

"This may lead to death, migration, or changed behavior of the benthic macro- and meiofaunal organisms responsible for bioturbation and bioirrigation…"

Page 5: - Line 4-15: **additional literature** incorporation required. How does your model differ from those. Where are the improvements etc.

Additional literature has been incorporated in the new Background section. The ways in which BROM differs from existing models are now explicitly listed in the final paragraph of this section.

- Line 22: the benthic boundary layer is a major strength. Introduce it better. Delineate the features, etc. –

The BBL is now better introduced in the second last paragraph of the Background:

"The BROM model described herein is a fully coupled benthic-pelagic model with a special focus on deoxygenation and redox biogeochemistry in the sediments and Benthic Boundary Layer (BBL). The BBL is "the part of the marine environment that is directly influenced by the presence of the interface between the bed and its overlying water" (Dade et al., 2001). Physical scientists tend to prefer the term "bottom boundary layer", but this is largely synonymous with the BBL (Thorpe, 2005). Within BROM, the term BBL is used to refer to the lower parts of the fluid bottom boundary layer where bottom friction strongly inhibits current speed and vertical mixing, hence including the viscous and logarithmic sublayers up to at most a few metres above the sediment. This calm-water layer plays a critical role in mediating the interaction of the water column and sediment biogeochemistry and in determining e.g. near-bottom oxygen levels, yet it remains poorly resolved in most physical circulation models. For BROM we have developed an accompanying offline transport module "BROM-transport" that uses output from hydrodynamic water column models but solves the advection-diffusion-reaction equations for a "full" grid including both water column and sediments. BROM-transport uses greatly increased spatial resolution near to the SWI, and thereby provides explicit spatial resolution of the BBL and sediments."

Line 24: at the BBL: do you exclude the sediments here?

Our BBL definition does exclude the sediments (see above), but the scope of BROM does not. This scope or goal is now better defined:

"The goal of this work was to develop a model that captures key biogeochemical processes in the water and sediment and to analyze the changes occurring in the BBL and SWI."

Page 6: - line 9-10: it is unclear whether organic C is also modeled or is it just inorganic

C. - Line 12: No nitrogen transformations?

Only inorganic C is explicitly modeled (state variable name DIC). Organic matter (dissolved and particulate) is modeled only in nitrogen currency (variable names DON and PON) so to derive organic C estimates from model output would require use of a stoichiometric ratio C:N. Nitrogen transformations are modelled. The new manuscript reads:

"BROM considers interconnected transformations of species of (N, P, Si, C, O, S, Mn, Fe) and resolves OM in nitrogen currency. OM dynamics include parameterizations of OM production (via photosynthesis and chemosynthesis) and OM decay via oxic mineralization, denitrification, metal reduction, sulfate reduction and methanogenesis."

Page 7: - Line 2: delete consists

Done

- Line 26 and all through: replace protolithic processes with **equilibrium processes/reactions or acid-base reactions**

Done

Page 8: - Line 11: provide the number of state variables to the reader

Done (33).

Page 9: - Line 1: chemoautotrophy is resolved, but overall **secondary production** is ignored. There may be good reasons for this, but communicate this then to the reader

Secondary production is resolved. The state variable 'Het' represents all non-microbial heterotrophs. These graze the phytoplankton as well as bacteria and detritus, and they reach significant concentrations in both pelagic and benthic parts of the model domain. The new section 2.1.2 reads:

"…We divide all the living OM (biota) into Phy (photosynthetic biota), Het (non-microbial heterotrophic biota), and 4 groups of "bacteria" which may be considered to include microbial fungi. These latter are: Baae (aerobic chemoautotrophic bacteria), Baan (anaerobic chemoautotrophic bacteria), Bhae (aerobic heterotrophic bacteria), and Bhan (anaerobic heterotrophic bacteria). OM is produced photosynthetically by Phy and chemosynthetically by bacteria, specifically by Baae in oxic conditions and by Baan in anoxic conditions. Growth of heterotrophic bacteria is tied to mineralization of OM, favouring Bhae in oxic conditions and Bhan in anoxic conditions. Secondary production is represented by Het which consumes phytoplankton as well as all types of bacteria and detritus…"

- Line 8-10: why is methanogenesis excluded? This is probably related to the way you model organic matter. Conceptually most simple is to turn all labile organic matter remaining after depletion of all oxidants into methane and carbon dioxide.

Methanogenesis is included in the new, modified version

- Line 15- 25: the alkalinity equations as given are wrong: the phosphate alkalinity term should include a H3PO4 term, the ammonium alkalinity term should not include NH4+, etc. Please check whether you have implemented it correctly into your model.

Checked and corrected.

Page 10:-Line 2: I guess you mean Atom was set to zero and not TOM.

Correct. In the new text, the TOM alkalinity is removed.

Page 11: -Line 1-10: quite a number of the reactions are not balanced and inconsistent with Table 2: e.g. denitrification with hydrogen sulfide and the line above represent two reactions of which the latter misses a two before OH-. Check carefully. -Line 11: Table 2 not 3.

Apologies for our sloppy editing. All equations have now been carefully checked and corrected.

Page 12: middle of page: a distinction is made between settling velocity of particulate matter and of particles with Fe and Mn oxides. Why not write particle settling velocities (w) as a sum of various contributing terms. Why the focus on Fe and Mn? Just a Black Sea model heritage?

In the new version, all the inorganic particles sink at the same constant velocity, and this velocity is larger than all organic matter sinking velocities.

Page 13: - Line 8: the eddy diffusion coefficient was assumed constant in the BBL. As a first coupled model that resolves the BBL **it may be done like this**, but given the **lognormal velocity profiles,** would one not expect a depth profile in Kz as well. This can be incorporated quite easily.

A good suggestion, thanks. In the new version, Kz (now D, to be more conventional) can have a linear depth variation either if it is treated dynamically or assuming a static log layer. This is now described in section 2.2.7:

"The vertical diffusivity needs a more careful treatment as it is the main defining characteristic of the pelagic vs. BBL vs. sediment environments. Within the water column, the total vertical diffusivity D = Dm + De for solutes and D = De for particulates, where Dm is a constant molecular diffusivity at infinite dilution, and De is the eddy diffusivity read from the input file for the pelagic water column. For the BBL, De can be defined as "dynamic", in which case it is linearly interpolated for each day between the deepest input forcing value above the SWI and zero at a depth h¬DBL above the SWI, where h¬DBL is the diffusive boundary layer (DBL) thickness (default value 0.5 mm). This option is likely appropriate for shallow water applications where De may be strongly time-dependent within the user-defined BBL (default thickness 0.5 m). Alternatively, a static, fixed profile D¬eBBL(z) may be more appropriate for deep water BBLs, where time dependence may be weak and deepest values from hydrodynamic models may be relatively far above the SWI. In this case, BROM-transport offers two options for D¬eBBL(z): 1) a constant value, dropping to zero in the DBL, or 2) a linear variation between a fixed value at the top of the BBL and zero at the top of the DBL. Option 1) defines a simplest-possible assumption, while option 2) corresponds to the assumption of a log layer for the current speed (e.g. Boudreau and Jorgensen, 2001). Eddy diffusivity is strictly zero in the DBL, on the SWI, and within the sediments. Diffusivity in the sediments is due to molecular diffusion and bioturbation and is parameterized as described in section 2.2.1."

- Line 15-20: the description of bioturbation/bioirrigation is difficult to follow. As written above are solid phase and solutes transported separately or together? This is unclear. Bioturbation depth are very shallow for fully oxic conditions.

This part of the model was significantly improved and is clearly described in the new section 2.2.1. Solid and liquid phases are diffused separately (intraphase mixing) except possibly at the sediment-water interface if the option to allow bioturbation across the SWI is enabled. Solute diffusivity in the sediments is a sum of molecular diffusivity, corrected for tortuosity and relative viscosity following Boudreau (1997), and bioturbation diffusivity, depending on a fixed vertical profile and a time-dependent oxygen status of the bottom layer of the water column (fluff layer). Particulate diffusivity in the sediments is just the bioturbation diffusivity. Solute burial velocity also now differs from particulate burial velocity due to the effects of compaction (Boudreau, 1997). Burial velocities now also depend on depth under an assumption of steady state compaction (Berner, 1970, 1981; Boudreau 1997; Meysman et al., 2005) and additional velocity components can optionally be added to account for modelled particulate fluxes to the SWI and particulate reactions in the sediments (see section 2.2.1 and Appendix B).

The current default "mixed layer" depth for bioturbation is 2 cm (cf. values 5 cm and 1 cm used by Soetaert and Middelburg (2009) for well-mixed and anoxic conditions respectively). The default decay scale for bioturbation diffusivity below the mixed layer is 1 cm, following Soetaert and Middelburg (2009). This information is now included in the run-time input file brom.yaml (see Appendix D). We agree that a 2 cm mixed layer may be too shallow for fully oxic conditions; in such cases the user should increase the mixed layer depth parameter in the brom.yaml file.

Section 2.3. The description of boundary conditions needs more attention. It appears that you use flux boundary conditions for the gases and constant or fixed (at least im- posed) boundary for the others. This may lead to mass balance issues. The boundary conditions at the bottom (depth 12 cm in sediments) are not described: no flux or **no gradient** or fixed concentration? The assumed sulfate concentration is either close to zero or do you mean 25 10-3M? Basically all external sources such as atmosphere and rivers are added to surface layer.

In the new BROM-transport code we allow four different options to define boundary conditions (upper and lower) for each variable. For the upper boundary (air-sea interface) the default option is no flux, unless the flux is specifically parameterized by the (FABM) biogeochemical model. For BROM-biogeochemistry this means that, by default, all variables have no flux surface boundary conditions except oxygen and DIC, which have fluxes parameterized using atmospheric oxygen and CO_2 levels prescribed in the brom.yaml file (see Appendix D). Optional fixed (Dirichlet) boundary conditions do indeed imply mass fluxes into or out of the modelled water column, but this need not be unrealistic. We have found in fjord and lake applications that fixed (possibly time-dependent) surface boundary condition can provide a way of modelling missing net influxes of nutrients from rivers. Boundary conditions at depth are no-gradient by default (advective outfluxes can still occur due to burial velocity). External sources (e.g. from rivers) can also be allowed to contribute directly to the model interior by setting the "horizontal mixing" forcings, rather than by setting boundary conditions. This all described in the new section 2.2.5:

"BROM-transport presently allows the user to chose between four different types of boundary condition for each variable and for upper and lower boundaries: 1) no-gradient at the bottom boundary (no diffusive flux) or no-flux at the surface boundary, except where parameterized by the FABM biogeochemical model (i.e. for O2 and DIC in the case of BROM-biogeochemistry); 2) a fixed constant value; 3) a fixed sinusoidal variation in time defined by amplitude, mean value, and phase parameters; or 4) an arbitrary fixed variation in time read from the input netCDF file. All boundary condition options and parameters are set in the brom.yaml file (see Appendix D). Note that options 2-4 are Dirichlet boundary conditions which define implicit fluxes of matter into and out of the model domain, and that all boundary concentrations should be in units [mmol/m3 total volume (water+solids)]. The default option 1 is generally the preferred choice, but the Dirichlet options can also be useful to allow a simple representation of e.g. fluxes of nutrients into and out of the surface layer due to lateral riverine input. A possible alternative is to use the forcings parameters for horizontal mixing (see equation (1)) to specify horizontal exchanges or restoring terms to observed climatology (see section 2.2.7)."

For the sulfate upper and lower boundary conditions we have used Dirichlet conditions of 25000 uM (or mmol/m3) for both.

Section 3: I stop making detailed feedback because there are too many issues and the referee already spent double the amount of time normally needed for an evaluation.

Again we sincerely apologize for the condition of the original submitted manuscript. We are confident that the new version will not require so much correction.

p. 26, line 5-9: chemoautotrophy indeed involves CO2 consumption and thus has the potential to increase pH. However, the energy required for CO2 fixation is obtained from oxidation of reduced products: usually an acid producing process. With typical growth efficiencies one would produce more acid linked for the energy than consumption of acid by organic matter production. Cable-bacteria spatially disconnect half reactions and can therefore cause a real pH increase. Without detailed model investigations, I suggest removing these sentences. The authors might be right because of the com- plexity of reactions and the many buffering reactions, but it is not convincing as pre- sented here.

This part of discussions was removed from the modified version.

Table 1: it is stated that oxygen is presented in microM O, but sometimes it might be, at other places it is definitely in microM O2.

Corrected. O2 is now always present in microM O2.

Table 2: - Aerobic respiration and denitrification are treated different than Fe, Mn and sulfate reduction regarding DON and PON separation. - For Mn reduction where does the 0.5 come from (half saturation constant hard-coded?) - There are multiple typos which complicate checking. - Where is the (1+ftD(t)) term coming from. ftD is not defined. - Page 41: I guess that NO3 dependence should depend on nitrate and not on ammonia?

Apologies again. Table 2 has now been checked and corrected.

The factor 0.5 in the Mn reduction formulations is not a hard-coded half saturation constant (all half saturation constants are input parameters in fabm.yaml). It is rather there to ensure that the specific Mn reduction rates at high Mn concentration (tanh function tending to unity) and high H_2S concentration (Michaelis-Menten function tending to unity) are indeed set by the limiting rate parameters K_mn_rd1 and K_mn_rd2.

The variable ftD(t) and its corresponding dependence have been removed in the new version.

Apologies for the typo in NO3 dependence. This should have been a combined function of nitrate and ammonium (nitrate uptake suppressed at high ammonium concentrations). It is correct in the new Table 2.4.

Table 3: - I guess that K_Mn_rds should be K_Mnrd_HS? - There are many values assumed, some literature citations would be helpful. I guess that the model is rather insensitive to most of these parameters and their value should therefore be based on literature values.

Sorry, K_Mn_rds was a typo.

Literature citations have been added to the new tables. Table 3 has been checked, corrected, and divided into several tables.

- Why did you choose 2.7 for the Fe/P ratio and not the conventional 10?

Table 4: check carefully: e.g. for phosphate you have hard-coded 2.7 for Fe/P and 0.67 for Mn/P rather than a parameter. Taking stoichiometry as a constant is fine, but do not present

An explanation has been added to the text. We refer to assumptions and numerical experiments described in (Yakushev et al., 2007), where we aimed to analyze the reasons for formation of a typical "phosphate dipole" in the water column, with a minimum just above, and a maximum just beneath the hydrogen sulfide onset. We used extreme values of Fe/P and Mn/P to demonstrate that this phenomenon cannot be explained by Fe (even if Fe/P = 2.7, and not 10), but can be explained by Mn(III).

Table 5: this table is unuseful and I doubt whether the fluxes are all in the right units. Table 6: could be deleted.

Both tables have been deleted.

Figures. All captions need more documentation. For instance it is not even mentioned why some concentrations are presented on two different scales. As written above, reconsider to focus on a few results and elaborate the model results in another paper. The figures as presented now appear more like raw model output.

The figures has been redrawn and carefully selected. As recommended we focus on demonstrating of the model possibilities and not on analyzing the model results.

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