Geoscientific
Model Development
Discussions

Interactive comment on "Bottom RedOx Model (BROM, v.1.0): a coupled benthic-pelagic model for simulation of seasonal anoxia and its impact" *by* E. V. Yakushev et al.

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1 General comments

1.1 Appreciation of the manuscript

In this paper, E. V. Yakushev and co-authors present a highly complex model suitable to study the coupled biogeochemical processes at the bottom boundary layer, the sediment-water interface and the surface sediment. The model appears to provide an extremely complete description, considering all the processes and primary and

secondary chemical reactions that have been taken into account. It is integrated into the *Framework for Aquatic Biogeochemical Models*, FABM (Bruggeman and Bolding, 2014).

Although the model appears to have been skilfully designed and set up, the paper has, unfortunately, a number of weaknesses. It is not suitable for publication in *Geoscientific Model Development* in its current form – it should nevertheless be possible to **reconsider it after a major revision**.

This paper would definitely have benefited from another round or two of rereading and proofreading. Not even the name of the model is unambiguously given: in the title, the name is *Bottom RedOx Model*, in the model presentation (p. 2, ll. 2–3) it is *Bottom RedOx Layer Model*. The English of the paper needs some thorough revision. There are parts that are acceptable and others that are almost unsuitable for review. I am not going to point out all the English errors that I found – they are simply to numerous to key them all in here. There is one British co-author and two co-authors with affiliations to institutions in English-speaking countries or regions: could they please have a look at the manuscript and help to correct it and rewrite where necessary! There are errors (spelling, grammar, syntax, style) on nearly every single page, but sections 3.2.4 (Manganese) and 3.3 (Carbonate system) require particularly close attention.

The paper has been submitted as a "model description paper". Requirements for that type of paper are detailed in http://www.geoscientific-model-development.net/about/manuscript_types.html#item1. Quite some requirements are not met in this paper.

1. The model description is not well contextualized. The application presented is for a shallow-water environment, but one may ask where else it could be applicable, and which extensions or adaptations would be required or which simplifications would be possible. The authors mention, e. g., a possible coupling to NEMO,

which encompasses almost the complete range of marine environments that one can imagine.

2. The technical details of the implementation are incomplete, and therefore, the criterion of model reproducibility that the paper should aim for is not met. All to many details are not covered in the description.

3. The instructions about where to get the code are incomplete. Much guesswork is currently required to locate the relevant files inside the FABM distribution. This could easily be avoided by, say, three to five extra sentences.

4. There does not seem to exist a way to permanently access the precise model version described in this paper.

5. The limitations of the model and the fundamental software requirements are not given: if the model described here is really BROM-transport (this is not a name found in the paper, but it is the name of the only sensible source code collection that I could find), then the paper needs to state right away that:

   • the BROM source code can only be compiled with the Intel Fortran compiler for Windows

   • the current version can only use hydrodynamic conditions derived from GOTM (according to the Wiki at https://sourceforge.net/p/fabm/wiki/BROM_ FABM).

   Although it is reported on p. 16 (l. 5), that the model was run with the Intel compiler for Windows,[1] it is said nowhere that this is the only way to run it. This is obviously a extremely strongly limitation and I am wondering whether such a restriction is

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[1]It would be useful to provide the version number of the compiler used. FABM and BROM require some specific Fortran 2003 features and the Intel compiler only offers full support for Fortran 2003 since version 15. However, a subset offered by earlier versions might be sufficient here.

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fundamentally necessary. As far as I can see, FABM itself is written in standard-conforming Fortran 2003 in a portable manner (no hardcoded kind types, etc.) and does not seem to rely on a single compiler for a single platform.

I strongly encourage the authors to prepare a version of the source code that can be used on other platforms and with alternative compilers. It should be possible to do this quite rapidly by introducing a few pre-processor directives, which would switch off some extra functionality provided by the Intel Fortran compiler for Windows, but that is not fundamentally required for the model itself. This would increase the usefulness of BROM by orders of magnitude! Else, what is the point in emphasizing that the model code "[. . .] uses modern software standards: it is coded in object-oriented Fortran 2003, [. . .]" (p. 27, ll. 17–18) if in the end, it only compiles with one single compiler on one single platform.

The model itself seems to be carefully designed and set up. There are a few assumptions regarding the physical environment that may be debatable and that would benefit from a few extra words of explanation (see specific comments below). The set of processes and coupled chemical reactions and equilibria that have been taken into account is extremely complex. It is not obvious if such a high degree of complexity is truly necessary. The model indeed seems to allow a rather accurate simulation of the environment chosen. However, to what extent does it contribute to improve our understanding of the way the environment evolves? It would be interesting to know which are the dominant actors of the system. Unfortunately, the paper does not address this kind of question at all.

2 Specific comments

2.1 Introduction

The scope of the model, i. e., the bottom boundary layer (BBL), (also known as the benthic boundary layer, or are there differences between those two BBLs?) deserves to be presented in more detail. What is its typical thickness? What influences that thickness? How does it change throughout the global ocean? What are the typical gradients across the BBL? Please do not forget that *Geoscientific Model Development* has a broad lectureship.

I am surprised to read that "the Bottom Boundary Layer (BBL) [...] is still understudied" (p. 5, l. 22). On my shelf I have the fine book *The Benthic Boundary Layer: Transport Processes and Biogeochemistry* (Boudreau and Jørgensen, 2001). It is nearly 15 years old and BBL research has certainly not come to a rest since that book got published. Please reconsider that statement and provide a fair representation of the existing literature.

2.2 General model presentation

2.2.1 Scope of the model

In the end, it is not entirely clear what the exact scope of BROM is. In the abstract, BROM is introduced as a model for the biogeochemical process in the bottom boundary layer; in the model description though, we read that "[t]he water column considered in our model spans the sea surface (upper boundary) down to user's defined sediment depth [...]". This is to some extent contradicting as this domain largely exceeds the bottom boundary layer. Please clarify.

2.2.2 Computational aspects

It is stated that numerical integration was carried out with the Eulerian scheme (the explicit or the implicit variant? – the extremely short time-steps chosen make me guess it is the former, but it would be good to state this). Is the same Eulerian scheme used for both space and time dimensions? Please specify all the schemes used.

Details about the pH solving algorithm can only be looked up in the code. The text only says that "[...] total pH was calculated using the Newton-Raphson method" (p. 11, ll. 20–21) and that "Carbonate system equilibration was parameterized using the standard approach (i.e. Lewis and Wallace, 1998)" (Table 2). This latter affirmation is meaningless: Lewis and Wallace (1998) neither provide information about the methods used in their program, nor do they define any standard approach. A few more details about how calculations are actually done in BROM would be of order here.

In general, the text really ought to be more complete and informative about numerical aspects of the model. This is what *Geoscientific Model Development* readers expect.

2.2.3 Rate law expressions

The tables that list all the processes considered in BROM and their rate laws, and that collect the different parameter values are among the most informative parts of the paper. They clearly represent one of its major strengths. Unfortunately no references are given for the parameter values presented in Table 3. There is a large variety of kinetic rate laws that are used in the model (Monod laws, squared Monod laws, laws in tanh, ...). I think it would be good to have a few words of explanation about the choices operated. Please also complete the references where missing (Table 2, on pp. 41–43 and Table 3, throughout).

As mentioned in the general appreciation already, I really wonder if all that complexity is really necessary, or, put the other way around: which minimalist set of process would be sufficient to obtain realistic results?

2.2.4 Miscellanea

Denitrification is considered, and nitrification, but I could not find anything about how nitrogen fixation is dealt with. I would expect that this process is required to avoid an unrealistic drift in the nitrogen inventory.

2.3 Total alkalinity

This part of the paper (p. 9) is one of the most disappointing ones. It is very approximate, completely overloaded with information that is ignored in the end. It furthermore contains several errors.

For clarity, it would be best to provide immediately the approximation actually used in the model, and not a hypothetical one, that could have been used. Alkalinity contributions that are not included or that are set to zero should be omitted. The text will be considerably simplified.

Whatever the expression chosen for total alkalinity, it will anyway always remain only an approximation. But even approximations need to be factually correct. Unlike written in the paper, . . .

- . . . H_3PO_4 is also part of alkalinity and $A_{TPO_4} = [HPO_4^{2-}] + 2[PO_4^{3-}] - [H_3PO_4]$ — interestingly this is correct in Table 6 (except for a typo) and also in the code;

- . . . NH_4^+ is not part of alkalinity (it is the zero-level species) and thus $A_{TNH3} = [NH_3]$;

- . . . it is the total borate concentration that is estimated from salinity and not $[B(OH)_4^-]$ — $[B(OH)_4^-]$ is calculated from the state variables just like to others (this is correctly done in the code, fortunately);

- . . . F^- is not part of alkalinity, only HF, so that $A_{THF} = [HF]$ — this is also wrong in Table 6 (at 68 μM, it would be barely negligible), but I suggest to discard the A_{THF} term from the alkalinity expression anyway, as it is not included in the model.

Although it is specified later on that the stoichiometric constants of Roy et al. (1993) are used for the carbonate system, references for the other constants (e. g., dissociation constants for boric, phosphoric and silicic acids) required to solve the total alkalinity-pH equation are missing. Please provide references for those as well.

Finally, the pH scale used in the paper turns out to be the total scale. This should be stated more clearly than it is currently done (at my third reading, I discovered on p. 11 (l. 20) that "total pH was calculated". Please state this more obviously.

2.4 Physical environment

2.4.1 Porosity

Variable porosity is not included in the current version of BROM. The affirmation that "[. . .] its effect on [the] vertical transport is incorporated in[to] the values of K_z and $K_{z_{bio}}$, [. . .]" (p. 13, l. 17) is rather obscure. $K_{z_{mol}}$ is actually constant so it is not clear how it could take porosity variations into account. I am furthermore not certain that this simplification is really necessary, given the complexity and detailed representation of the rest of the model. Variable porosity should not significantly increase the model's compleity.

Furthermore, it appears that a tortuosity corresponding to the porosity value of 90%

was used, with reference to a "value from Boudreau, 1997" (p. 13, l. 22). This is not very meaningful. Boudreau (1997) lists eight theoretically based tortuosity-porosity relationships and three empirical ones. Please specify which one was used here and then cite the original reference.

2.4.2 Molecular diffusion

BROM uses a species-independent molecular diffusion coefficient. This considerably simplifies the advection-diffusion-reaction equations, as the total concentrations a, such as DIC and alkalinity can be transported directly. The reported value $K_{z_{mol}} = 1 \times 10^{-11}\,\mathrm{m^2s^{-1}}$ is, however, almost two orders of magnitude lower than those for typical ions: e. g., from Boudreau (1997, Table 4.8), we may calculate diffusion coefficient values of $0.781 \times 10^{-9}\,\mathrm{m^2s^{-1}}$ for HCO_3^-, $0.632 \times 10^{-9}\,\mathrm{m^2s^{-1}}$ for CO_3^{2-} and even $1.313 \times 10^{-9}\,\mathrm{m^2s^{-1}}$ for HS^- (each one for $t = 10\,°C$). These are infinite dilution diffusion coefficients, but correcting them for tortuosity and for the dynamic viscosity of seawater does not reduce these values by more than 15–20%. How would results change if these much higher values would be used?

2.4.3 Bioturbation

Biotubation is parametrized as a diffusive process, as is common usage. For the biodiffusion coefficient, it is only stated that it takes a constant value over the top 2 cm and that it decreases exponentially afterwards. However, I have not been able to find the length scale of this decrease anywhere in the text. Now, one may ask whether it is realistic to consider any bioturbation at all in anoxic parts of the sediment, the more since the text already indicates that the maximal bioturbation depth was only 0.5–2.2 cm (p. 13, ll. 15–16). How would this change your conclusions?

2.4.4 Bioirrigation

BROM takes the important process of bioirrigation into account. It is, however, represented as a purely diffusive process. Boudreau (1997) and Aller (2001) make a strong case that it would be more appropriate to represent bioirrigation as a non-local exchange process instead.

2.5 Code

On p. 7 (ll. 24–25), it is said that BROM consists of three modules. I did not want to download and install the complete FABM, but nevertheless wanted to inspect the BROM code, to find out more about the technical details that were missing from the paper. This was, however, not entirely straightforward.

2.5.1 Accessibility

After having opened http://fabm.org (which redirects to the FABM project page on SourceForge), I started to search for references to BROM. After some searching around, I detected the first trace of BROM under the "Wiki" tab: section 7 of chapter 2 of the User's Guide has the title "BROM-transport + FABM". BROM-transport is most probably the transport model mentioned in the paper (p. 7, l. 2), but that is not clear, since the paper always mentions BROM only. That section provides at least the first useful hint about where to find the BROM biogeochemical modules: under `src/models/niva/brom` in FABM. Proceeding to the "Code" tab then allowed me to browse to the relevant files (under the indicated directory tree). BROM-transport, however, is not with FABM and must be retrieved from a different repository, located at https://github.com/e-yakushev/BROM-transport, not mentioned in the paper.

I suggest that the authors give accurate and comprehensive instructions in the paper

about where the actual BROM source code files are located, both the biogeochemical ones and the main driver. And, please include also information about the license under which the code is distributed.

2.5.2 Code quality

The code is obviously "work in progress" and appears to undergo continuous changes. There are many lines of code that are commented out, some of them might be important. It is of not clear if they were also commented out when the results described in the paper were calculated.

I detected a few coding choices that put portability at risk. While `REAL`s in the three biogeochemistry related modules are declared in a portable way with `REAL(rk)`, where `rk` is an `INTEGER` parameter whose value gets derived from an appropriate `SELECTED_REAL_KIND(...)` call, there are some `INTEGER(4)` declarations that may lead to problems. In BROM-transport, there are numerous `REAL(8)` declarations, in different source code files. Kind type values – such as the '4' of the `INTEGER(4)` or the '8' of the `REAL(8)` declarations – are not standardized and may differ from one compiler to another. Programmers may not assume that they are equal to the expected byte length and for portability reasons kind type values must therefore not be hard-coded.[2] Portable and reliable code would consistently follow the FABM approach, with the `rk` parameter derived from `SELECTED_REAL_KIND(...)`

I have come across a few peculiarities or short-cuts in the code that may lead to serious confusion: e. g., in the subroutine `phIter` in `brom_carb.F90`, the `INTENT(IN)` argument `Sit_` (the total silicate concentration) is overridden by a local variable `Sit`,

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[2]I know of one compiler where `DOUBLE PRECISION` is not `REAL(8)` but `REAL(3)`.

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which is set to zero, thus making the code ignore silicate alkalinity. The paper does, however, not state that silicate alkalinity is ignored.

The pH calculation routine is neither safeguarded nor does it include diagnostics for possible convergence failures or for early convergence: it simply executes 100 Newton-Raphson iterations, starting from a preset fixed starting value, that furthermore seems to require manual modification from time to time. No diagnostic is included, neither for possible convergence failures nor for early convergence. (Why carry out 100 iterations if convergence is reached after five of them already?)

There are now reliable methods to solve the alkalinity-pH equation, which are guaranteed to converge under any physically meaningful conditions, howsoever exotic, and usually in less than six iterations (Munhoven, 2013). These would be particularly recommended in the environments that BROM has been developed for, with complex alkalinity compositions and unusual total concentrations.

Carbonate solubility constants do not take any pressure correction into account (the relevant lines are present, but commented out).

Finally, the comments in the code are not always correct, which also creates unnecessary confusion (e. g., the phosphoric alkalinity is not [H2PO4-] + 2.*[HPO4--] + 3.*[PO4---] as stated in a comment, but [HPO4--] + 2.*[PO4---] - [H3PO4]. Fortunately it is the latter that is implemented in the code.

2.5.3 Permanent access to the code for model version 1.0

As mentioned in the general appreciation, for model description papers there should exist a way to permanently access the precise model version described in the paper. The GitHub repository for BROM-transport includes a `Ver. 1.0` directory, so for the

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transport model, this seems to be conceivable. The biogeochemical modules that are hosted in the FABM repository are however not clearly tied to version 1.0 of BROM.

It would thus be necessary to provide somehow tagged versions of the source code files for the model version 1.0 described here, or to provide copies of those files as a supplement to the paper.

2.6 Tables

The tables contain a wealth of information and represent one of the most useful parts of the paper (with the exception of Table 6, which could be deleted without loss). Unfortunately, Tables 1 and 4 are nearly unreadable because of the small font size. They would clearly benefit from a reorganization of their contents. Table 2 currently spans eight pages, Table 3 six pages. It would be useful to split them into smaller parts, with dedicated captions. While Table 2 still contains extensive references, Table 3 does not contain a single one. Readers ought to know where the adopted parameter values come from or how they have been derived.

The second column of the row "Alkalinity changes" in Table 2 is completely overloaded. Please reorganize this information.

Table 6 is not essential for the paper and I suggest to delete it altogether. It also contains errors and except for Canfield et al. (2005), none of the references cited is in the reference list. A_{THF} is certainly not 68 μM, else it would not be negligible.

3 Technical comments

Throughout the paper: change "protolithic" to "protolitic" or "equilibrium" (depending on the context)

Throughout the paper: change "connected with" to "related to"

Throughout the paper: please check the usage of the word "parameterized" and "parameterization". For example, in Table 2, it is said that the carbonate system equilibration was parameterized. It were rather the stoichiometric constants that were parameterized, as a function of temperature, salinity and pressure, but the carbonate system equilibration (it would be more correct to say speciation) was calculated.

p. 4, l. 26: "death or flight"? "death or migration" would perhaps be more appropriate

p. 7, l. 15: "changeable" is not appropriate in this context. Perhaps "varying"?

p. 9, ll. 20–25: it is common usage to speak about bor*ate*, phosph*ate* and silic*ate* alkalinity (as with *carbonate alkalinity*) and to reserve the terms bor*ic*, phosphor*ic* and silic*ic* for the corresponding acids (as in *carbonic acid*).

p. 11, l. 20: change "Roy's constants" to "the set of constants of Roy et al." – the co-authors will appreciate

p. 16, ll. 4–5: change "FORTRAN" to "Fortran 2003" (spelling and standard) and change "Intel FORTRAN for Windows Compiler" to "Intel Fortran Compiler for Windows", which is the name of the product.

p. 16, l. 6: what is meant by "balanced distribution"?

pp. 21–26 (section 3.2.4 – section 3.4): please check for the English and rewrite where necessary.

p. 39, rows 10 and 11: "sulfatereduction" should read "sulfate reduction"

p. 40, second-last row, right-hand column: should the "$CaCO_3$" on the last linee not read "caco3_diss−caco3_prec"?

p. 41, row 7: there is probably some "NO_3"-"NH_3" mismatch here

p. 41, rows 7 and 8: the two trailing '2's in exponent seem to be misplaced (they probably belong to the second term in the denominator each time)

p. 46, in the first row relative to a half-saturation for OM denitrification, "NO_2" should probably read "NO_3"

Table 6: "$[PO_4^{2-}]$" should read "$[PO_4^{3-}]$"

References

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