

OMEN-SED(-RCM) (v1.1): A pseudo reactive continuum representation of organic matter degradation dynamics for OMEN-SED

Author's Response

Philip Pika, Dominik Hülse, Sandra Arndt
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Dear Editor,
please find below our point to point listing of the changes made to the manuscript in response to the referees' comments and suggestions. A *latexdiff* version of the manuscript highlighting the insertions and deletions in the text has also been uploaded alongside the revised manuscript.
We hope the manuscript is now acceptable for publication.

Best regards,
Philip Pika

Revisions in response to comments by Anonymous Referee #1

General comments

The authors presented a multi-G approximation method, in which organic matter (OM) can be divided into a large number of classes with different degradation rate to represent a pseudo reactive continuum of OM, as an extension / further development of an existing analytical early diagenetic model (OMEN-SED) that is originally based on two reactive OM classes (2-G model). The approximation is based on two assumptions, namely (1) the distribution of reactivity/degradation rate of OM in marine sediments can be reasonably described by a gamma function, and (2) the vertical OM distribution in sediments is in an equilibrium status (i.e. the temporal gradient of OM is zero at any depth in sediments) so that an analytical solution of the transport-reaction equation of OM can be derived. Because the proposed multi-G approach is based on the analytical solution, which does not require solving the transport-reaction equation dynamically, therefore computational expense is not a hindering factor. This makes the proposed method appealing.

However, I have several major concerns:

Comment 1:

although the method seems to produce reasonable results, the authors did not provide convincing arguments that the proposed method outperforms the original 2-G model;

Response:

We would like to re-iterate again that the aim of the new model development is not to “outperform” the original version, but rather to offer a choice between two, equally valid OM degradation model formulations. Each of these formulations has specific advantages and disadvantages and we have added short discussion of the advantages and disadvantages of continuum and (multi-) 2-G models in the introduction (p. 4, l. 96-111). Furthermore, in the revised introduction, we also reference relevant papers that discuss this topic more extensively

(e.g., Manzoni and Porporato (2009); Forney and Rothman, 2012; Arndt et al., 2013; LaRowe et al., 2020).

Comment 2:

the method is described in an unclear manner;

Response:

- We clarified the methods section by removing unnecessary equations (eq. 4 and 8), adding further explanation (p. 8 l. 186-191) and/or rewriting parts of the methods (p. 7-8 l. 175-191). Please also see our detailed responses to the more specific comments 3, 6, 7, 8 and 9 (Reviewer 1) as well as our response to comment 1 (Reviewer 2) for more information.

Comment 3:

while the method tries to fit observational vertical profiles in sediments, the boundary conditions needed for the model-data fit at some places do not reflect reality and biophysical laws; and

Response:

- Please note that boundary conditions and model parameters are constrained as in Hülse et al. (2018). The only parameters that are tuned to fit the pore water profiles are the RCM parameters α and ν . In the revised manuscript, we clarified further which parameters we tune here and where we derive other constraints on boundary conditions and model parameters. Please also see our reply to comment 9 ‘specific comment on section 3.1’ (Reviewer 1) for a more details.

Comment 4:

the precondition for the validity of the approach, namely a zero temporal gradient of OM at any depth in sediments, can hardly be met in a dynamic environment. This makes the approach of limited use for coupling to dynamic models in which sedimentation of OM is variable, which is especially true for continental margins.

Response:

- OMEN-SED-(RCM) has been primarily designed for the coupling to Earth System models and to investigate long term sediment dynamics. In this context, the required assumption of steady-state is valid because the variability in boundary conditions and fluxes is generally longer than the characteristic timescales of the reaction–transport processes. However, the steady state assumption can be a limitation for the model’s applicability to shallow coastal environments. We added a paragraph addressing this limitation (p.6 l. 146-149) and also refer to the relevant section in Hülse et al., 2018, where additional model limitations are addressed.

Specific comments:

Comment 5:

** The method (section 2) is not described clearly.*

Response:

- We clarified the methods section by removing unnecessary equations (eq. 4 and 8), adding further explanation (p. 8 l. 185-191) and/or rewriting parts of the methods (p. 7-8 l. 175-191). Please also see our response to comments 6, 7, 8 and 9 as well as comment 1 (Reviewer 2).

Comment 6:

(a) From eq.6, it is stated that $om(k,t)$ represents the probability density function that determines the amount of bulk OM with a reactivity between k and $k+dk$ at time t . As $om(k,t)$ is a probability density function, the sum of $om(k,t)$ across all k at any specific t should always be 1. However, this is not satisfied in eq.7, in which $om(k,0)$ is dependent on $OM(0)$. Please clarify this.

Response:

- We removed the term “probability density function”, as it is indeed confusing.

Comment 7:

(b) I am confused by the definition and use of k . k is supposed to indicate the reactivity of OM, which is a variable. So what is the justification of eq.8 that k is determined by a , v and sediment age? I understand that the latter three parameters at any specific depth are either pre-described (e.g. $v=0.15$ in case studies) or derived by model-data fitting. This means that k is also fixed by these values, which is not variable any more. Further, how is the age of sediment layer at depth z derived? It seems that this quantity is another variable which needs to be solved in the method, in addition to a and v . This contradicts the statement and conclusion that only a and v need to be solved. Please clarify.

Response:

In this case, k represents the apparent OM reactivity of the bulk OM mixture. It is indeed a function of a and v , as well as $age(z)$ (or burial time) and thus varies with depth, z . The $age(z)$, in turn is a function of sedimentation rate, porosity (and bioturbation intensity). We carefully revised these parts. More specifically:

- We omitted eq. 4 and 8 as they are not relevant for our model approach
- We added a new equation for the bulk OM reactivity $k(z)$ (i.e. Eq. 6), and a better explanation of our RCM approximation (p. 8 l. 175-191).

Comment 8:

(c) Another parameterization of k using eq. 16 clearly violates the original relationship as mentioned in (b). Please justify the validity of the method if a different parameterization of k is used.

Response:

This part of the manuscript describes the parametrization of Thullner et al. (2009) and Hülse et al. (2018). They apply equation 16 to derive the first-order OM degradation rate constant for their 1G model approach. We, in contrast, use a previously published $a=f(w)$ relationship (Equation 15) to calculate the sedimentation rate dependent apparent initial age of the OM mixture (parameter a). We recognize that this part of our manuscript might be confusing and, therefore, removed Eq. 16.

Comment 9:

** In the case study 3.1, although the free variables a , v are tuned that the model produces results close to observed sediment profiles, their setting has no mechanistic connection with other environmental variables, e.g. in Table 1, it is not clear why z_{bio} is set to 0.01 cm at depth 585m, which means that there is no bioturbation at all, but then why $Dbio$ has a non-zero value and how these parameters are related to the setting of a and v ? Also it is not clear why a has a very small value (corresponding to very small lifetime of OM, therefore quite labile component) for depth 2213 m. Compared to a very confusing setting in this case study, the setting in 3.2 (Table 2) seems more reasonable and respects reality.*

Response:

- Corrected typo in table 1. For the site at 585 m depth, Db is set to $1e-20$ and not 0.02.

Comment 10:

** There is hardly justification for the validity of the approach in global application in section 3.3, as shown in Fig.6. In particular, the part that simulated OPD exceeds 10^3 mm is not supported by any observation.*

Response:

In section 3.3, we aim to illustrate the model's ability to simulate diagenetic dynamics on the global scale. However, as pointed out in the manuscript itself, application of diagenetic models in data-poor areas, such as the global-scale, are currently limited by the lack of a general framework that would allow constraining OM degradation model parameters (e.g. see also Arndt et al., 2013). In addition, biases in observational data sets such as the bias towards settings with shallow OPD pointed out in our reply further affect global simulations.

- We now discuss the mismatch between observed and simulated OPD and DOU values
- We added new simulation results from an OMEN-SED-RCM run with a re-scaled version of the $a-w$ relationship that accounts for the overprediction of a in shallower areas, see figures 5 b, d, f) and 6 b)
- Updated section's methods accordingly (p. 20 l. 375-382)
- Expanded results/discussion according to the new results (p. 20 l. 384-419)

Revisions in response to comments by Bernard Boudreau

This paper reports a means by which the OMEN-SED diagenesis program (Hülse et al., 2018, GMD 11), which uses 2-G organic matter (OM) decay kinetics, can be altered to approximate a reactive continuum decay model, instead. The interest in this modification lies in better approximating the observed decrease in OM reactivity with depth in sediments, which is a desirable goal. I do have four comments on the execution of this paper, one of which reflects one that I made on a recent related submission by some of these authors, i.e., Freitas et al. (2020, BG-2020-435).

Comment:

1) Equations (4) and (8) in the Introduction and on page 7 are strictly valid only in non-bioturbated sediments, where there is a simple relationship between time and depth, a point that is only briefly mentioned in the present manuscript. These equations are stated and applied without any serious caveat. The correct expression with bioturbation is given in Boudreau and Ruddick (1991), their Equation (49), and it is not in an easily implemented form, as needed here.

No one has adequately explored the effects of applying Equation (8) to a bioturbated sediment. In Table 1 of Boudreau and Ruddick (1991), there are 6 applications of Equation (8) to non-bioturbated or negligibly bioturbated sediments. These generate v values between 0.05 and 0.3; the Peru Margin sediments in that same table are almost certainly bioturbated and have associated v values closer to unity (0.8 and 0.91). This dichotomy of results may indicate the effects of improperly dealing with bioturbation, but I really cannot affirm this. I also recognize that the actual calculations are made with a discrete numerical approximation, which removes much of the mathematical challenge, but also assumes a v characteristic of a non-mixed sediment; this may create unintentional modifications to the calculated “ a ” value.

Further to this point, $om(k,0)$ in Equation (7) is said to be the initial distribution of reactivities. In a non-mixed sediment, that distribution is exclusively altered by the decay of components with time. In a bioturbated sediment, “older” and “newer” organic matter components are mixed together, so that in leaving the mixed layer, the organic matter reactivity distribution is different than $om(k,0)$ at the SWI. Thus, the mathematics get even more demanding.

Progress in global modelling is needed to meet the challenges of global change; I appreciate that; corners will be cut by necessity. However, explicitly recognizing and stating those shortcuts is not only desirable, but is essential.

Response:

We carefully revised the following aspects of the methods section:

- Revised the equations stated in our Introduction and Model Description (removed Eq. 4 and 8)
- Adapted text in Methods to clarify the discrete approximation of the continuum model (p.8 l. 175-191)

Comment:

2) The methodology of this paper and of Hülse et al. (2018) is to create a diagenetic module that can be solved analytically and to calculate the resulting integration constants by fast linear matrix methods (see section 2.3.1 of Hülse et al., 2018). I am confused about this second part, as there is insufficient detail in either paper to see how the latter can be accomplished. Take sulfate in its reduction zone. The analytical solution will be a sum of exponentials, two of which will be multiplied by unknown integration constants. Boundary conditions at the top of the zone and at the base of the zone will allow calculation of the two constants, and these resulting equations will indeed be linear in the two integration constants. However, the position of the base of the sulfate reduction zone is a further unknown, a point that was extensively discussed in Boudreau and Westrich (1984, GCA 48, 2503-2516). A third boundary condition is needed to determine the unknown zSO_4 .

Hülse et al. (2018) do supply a third equation, and so it should be in the present paper too. What puzzles me is that this third equation, as in Boudreau and Westrich (1984), is a nonlinear function of zSO_4 . Thus, linear matrix methods cannot be employed to arrive at a solution. What have the authors done to avoid this problem, which seems fundamental to their paper?

Response:

Hülse et al. (2018) provides an explanation for how to solve the dynamically changing penetration depth problem in the subsections for the specific terminal electron rather than in section 2.3.1. We included a specific reference to the relevant section of the original OMEN-SED publication in the revised manuscript (p. 6, l. 145-149).

Comment:

3) I fail to agree that the model predictions and observations provided in Figure 6 “generally agree well with observations and capture also the widely observed increase in OPD with water depths (see Fig. 6).” The model in this paper generally overpredicts the OPD, more often by far more than an order of magnitude. The data appear to have an upper limit of 1000 mm with ocean depth, which is not present in the model predictions. The obvious discrepancies are not discussed in the paper. They really need to be. Is the “observed” 1000 mm limit an artifact or real? Why the common overprediction of the OPD? There is something valuable to be learned from negative results!

Response:

Also see response to Reviewer 1. To clarify these points we:

- Discussed mismatch between observed and modelled OPD and DOU values
- Added new simulation results from an OMEN-SED-RCM run with a re-scaled version of the a - w relationship that accounts for the overprediction of a in shallower areas, see figures 5 b, d, f) and 6 b)
- Updated section’s methods accordingly
- Expanded results/discussion according to the new results

Comment:

4) Finally, as much as Equation (15) might prove valuable, it is repeated as Equation (17) with a discussion that is similar. Is this duplication needed or am I missing something?

Response:

- Removed Eq. 17