# Comment on gmd-2022-84

Anonymous Referee #1

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Referee comment on "FESDIA (v1.0): exploring temporal variations of sediment biogeochemistry under the influence of flood events using numerical modelling" by Stanley I. Nmor et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2022-84-RC1, 2022

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Review of "FESDIA (v1.0): Exploring temporal variations of sediment biogeochemistry under the influence of flood events using numerical modelling" by Stanley I. Nmor et al.

--- General comments ---

The authors provided a model (FESDIA) that facilitates examination of the effect of a flood event on early diagenesis based on the published model OMEXDIA. The data-model comparison was carefully made and relaxation to pre-flood profile was examined as an application example. While the validity of the model looks sufficiently examined, I cannot say the manuscript is carefully written, and more clearance may be desired as a model development paper. Below are my comments that I hope can be of some use to the authors.

(1) Model description

It would be helpful if the authors can provide a short overview of model development relative to the previous and already published works/models. Current manuscript referred to these works, but what is exactly new is kind of obscure. Also, brief summary of the capacity/features of previous models from which the current model has been developed will be useful, including programing language, governing equations, and algorithms utilized for numerical solutions (finite difference/volume/element method for equation differencing and Newton iteration if adopted for solution seeking etc.). The current manuscript provides some of above information, but some information is still missing. And it is not 100% clear which part is new to the current model and which part is not new.

(2) Definition of relaxation time

Eq. 22 describes the change rate of species concentration within sediment profile but does not necessarily define deviation from the pre-flood profile. Also, current manuscript lacks figures that directly compare the solute profile development relative to the pre-event profile. I think Figs. 4-8 need to be improved so that profile development relative to the pre-event profile is more visually obvious.

(3) Description of model limitations and future development

Relevant to the above point, but limitations of model should be discussed more. There are several simplifying assumptions in the model but its influences on e.g., model validation, comparison with observation and estimation for relaxation time are not discussed. For instance, the authors assume that burial rate/porosity does not change with the flooding, but it is not discussed whether this assumption is defendable or close to what we observe. Model validation or comparison with the observed data is essentially based on solute profiles, which likely resulted from a good fit of TOC and may be achievable under different assumptions (those that allow changes of burial rate, porosity, bio-mixing and irrigation etc.). If this is the case, the relaxation time is likely quite different under different assumptions. While most of manuscript discussed how relaxation time is calculated under the specific assumption adopted for this study, it is not discussed how the relaxation time is affected by adopted assumptions.

--- Specific comments ---

In model description, it may be better if you say what programing language you are using earlier on (even in abstract).

L134. Three OM fractions? Thought the authors are using two.

L138. Froelich et al. (1979) rather than Froelich (1988) according to Bethke et al. (2011, AJS 311, 183)?

L166. What does 'a coupled reaction formulation' mean?

Eqs. 6, 7. It does not make any sense to use/define 'maximum rates' when one is not using Monod or Michaelis-Menten type of equation.

Eq. 7. What is the definition of ð□□□ð□□»2ð□□□ð□□□ð□□¥ð□□□ð□□□?

Eqs. 8, 9. What is the assumption behind the formulation of these equations? For instance, how do you obtain Eq. 9 for aqueous $NH_4^+$ with accounting for adsorbed $NH_4^+$? Can you track $NH_4^+$ adsorbed onto solid species along with OM and other solids or do you have to simplify that adsorption is depth-independent and/or time-independent? This can be important if solid materials with unoccupied exchange sites are flooded to sediment depocenter in a short period of time. If such case is possible, one would expect a large sink of $NH_4^+$ to the exchange sites? Related to this, do you model $PO_4$ adsorption onto Fe hydroxides or you do not have to do this?

L205. Does porosity 'decay'?

L209. According to Eq. 10, the authors seem to assume intraphase biodiffusion (Meysman et al., 2005, GCA 69, 3601). The statement here mentioning an interphase biodiffusion is inconsistent with Eq. 10.

Eq. 14. Irrigation term is not found in the governing equation. Is it included as a reaction term?

Section 2.2.5 & Section 2.2.6. More details are desirable as adding grid for implementing a deposition event must be an important addition to the previous modeling framework. For instance, how you define Zpert, e.g., number of grids and their geometry etc. Some examples, not only schematics may also be useful.

L276. 'maximum in the spring and minimum in fall and winter'. This line does not make sense to me.

Eq. 21. What is the units of TOC? Also, how do you derive Eq. 21? Is this simply analytical solution of the governing equation? In any case, it would be helpful if the authors can provide the procedure to obtain Eq. 21 somewhere.

L321. 'were utilizes the R programming language'. Correct English?

Section 2.2.9. It would be helpful if the authors can make a short description of what part of "deSolve package" they used, not only directing the reader to the R-forge webpage. More specifically, how the authors numerically solve the governing equations, apart from "method-of-lines" methods? Use of any finite difference/volume/element method? How is

the time-integration of governing equations made (time-implicitly or -explicitly)?

L331. What is a "slow" stationary state?

Eq. 22. Not quite sure this is a legit mathematical expression. phi(tau) < threshold is what I thought is consistent with what the authors described.

L334. "threshold (i.e given by the median over the entire time duration)." Do you mean that the run is finished when difference becomes less than the median value throughout the simulation and then tau is defined as the model time required for this?

L340. I probably do not fully understand the ensemble of simulations here to estimate the uncertainty in tau. What parameter do you randomly re-sampled exactly? Median of the reference run through time? If so, the runs for determining the uncertainty in tau is conducted until (randomly-chosen) prescribed median is crossed? But this does not necessitate re-running of the model as the boundary conditions are not changed?

L383. "a thickness scale of 1 cm to 30 cm in 5 cm increments". This line does not make sense to me. What exactly did you use for thickness in sensitivity analysis?

Section 2.2.11.2. If the tested values are not too many, it would be better to list exact values you used for sensitivity analysis.

L507. Please specify what "RiOmar" stands for.

L621. above à below?

--- Technical comments ---

Table 1. What does unequal mark on Fe(OH)3 mean? Is this typo? At least notion should be consistent with that in main text.

L139. Eq. 3 à Eq. 2?

L165. Typo in the second line of Eq. 5.

L168. Right parenthesis in the last line of Eq. 6 is missing.

L212. Where à where?

L214. specify à specified?

L230. i.e à i.e.?

L232. occur à occurs?

L246. Figure. 2 à Fig. 2 or Figure 2?

L318. "method-on-lines" à "method-of-lines"?

L409. dissolved DIC à DIC?

L415. as thus à as follows?

L418. Table. 3 à Table 3

L433. "Solid" should not be superscript

L434. "Solid" should not be superscript

L535. Improve à improved

L581. introduction à introduction of or introducing

L660. thickness. à thickness

L694. design à designed