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To the
Editorial Office
Biogeosciences (BG)

Wilhelmshaven, June 16, 2010

Reviewer's comments to the manuscript
"On the origin of highly active biogeochemistry in deeper coastal sediments—inverse model studies" by J. M. Holstein & K. W. Wirtz

Thank you very much for your comments! Following your comments, we are thoroughly revising the entire manuscript with regard to readability and structure. Special emphasis is put on improving the scenario descriptions, the outline and justification of the model set-ups (see below), and on better presenting the general implications of our results (see Reply to review 1).

Please find brief responses to the specific comments below.

1. **Title:**
   Referee 2: *The title is very vague and does not properly reflect the content of the presented manuscript*

   Agreed. New title is: Organic matter accumulation and degradation in sub-surface coastal sediments: A model based comparison of rapid sedimentation and aquifer transport

2. **Introduction:**
   Referee 2: *The introduction is badly structured. The scientific question is not clearly defined and it is not put into a broader context. Single paragraphs or subsections are not clearly connected. For instance, the connection between tidal flat morphodynamics and organic matter degradation remains unclear. In addition, the introduction provides a lot of detailed information that is not directly relevant to the questions addressed in the manuscript. Therefore, the introduction needs to be rewritten.*

   The introduction is rewritten. The logical consistency will be made more transparent by improving the writing. Less relevant information is removed and the research questions are made more explicit: 1) to compare two different transport scenarios for the transfer of reactive organic matter into subsurface sediments in relation to data, 2) by that quantifying biogeochemical parameters for that specific site

3. **Modeling approach & model structure:**
   Referee 2: *These sections are not well organized and, therefore, hard to follow. For instance, the description of the two model scenarios provided in section 2.3 (p. 2074 16-22) should be moved to section 2.2. Furthermore, the general model description (section 2.3) should be provided before the two scenarios are described (section 2.2).*

   Both sections are reorganized/rewritten to improve conciseness and readability. The scenario- and general model descriptions swap positions.

4. **Modeling approach:**
Referee 2: *The two transport scenarios are not very well explained and their choice is not justified. The authors should provide a better justification for the choice of these two scenarios. Isnt it possible that other biogeochemical processes could cause the observed depth-profiles? And if not, why? In addition, the names "advection" and "burial" are not appropriate, since both processes are advective.*

We revise the scenario descriptions. To improve the justification of scenario choices we discuss the alternative cause of a deep intrusion of SO4 commonly used to explain sulfate occurrence below zones of sulfate depletion. In brief, the line of arguments goes as follows: 1) the NH4 peak at 1.5 mbsf and accompanying DOC bulge indicates massive and recent organic matter decay in that layer, by far exceeding the activity above and below. 2) If not injected, the organic matter to fuel this process originates from a (common) vertical or horizontal transport process. Translated to our scenarios, vertical means sedimentation, horizontal means lateral aquifer transport.

We clarify, that with "burial" we refer to "vertical transport" (sedimentation) and with "advection", we refer to "horizontal transport" (aquifer).

5. **Data:**
Referee 2: *The authors need to include a short description of the data collection and measurement methods. How critical is the time difference of 1 to 3 years between the core retrieval at site NN1 and NN2?*

We extend the description of coring methods (though, we already referred to the original publication on the pore water data which also contain a full rationale on pore water extraction and measurement techniques). The observed variability of the three subsequent cores shows no trend and is indicated by error bars (standard deviation). The measurement delay seems to be less critical. If the pore water situation is transient, the development is, also given our modeling study, very likely too slow to be noticed within 3 years.

6. **Model structure/ Transport:**
Referee 2: *I have doubts concerning the suitability of the model. I doubt that the one-dimensional model can be applied to the two-dimensional horizontal advection scenario (scenario B). The authors argue that this treatment is justified if horizontal gradients are negligible. However, the depth-pofiles from NN1 and NN2 show that there are strong horizontal gradients. The authors have to provide the comparison between their 1D approach and the 2D simulations they performed to verify this approach. The transport scheme has a comparably coarse resolution (10 cm). Yet, the model accounts for bioturbation and bioirrigation, which affect the uppermost centimeters (<10 cm) of the sediment. In addition, rapid sedimentation or erosion events will probably exert an important effect on the biogeochemical dynamics in the upper sediment. Therefore, the authors must provide a better justification of their model choice. They need to show that the model is suitable to address their questions in order to increase the confidence in their results*

The application of a one-dimensional (vertical) model to a two-dimensional horizontal advection scenario (scenario B) is to be understood as a Lagrangian approach, with an Eulerian 1D sediment column model embedded in a moving coordinate system. This will be explained with more clarity. Of course, the omission of horizontal exchange between neighboring columns requires negligible horizontal gradients. In our case, horizontal gradients remain always much smaller than vertical gradients: The difference in concentration from NN1 and NN2 in 1.5 mbsf is approx. 10 mmol/l at a distance of 40 m between the two locations yielding a gradient of 0.25 mmol/l/m. In the vertical, concentrations change per distance is much greater (20–40 mmol/l/m), as evident from SO4 profiles at NN1. From the gradients, horizontal diffusive SO4 transport can be expected to be relevant at time scales approx. 100 times greater than for vertical diffusive transport.

We clarify that Fig. 9 already shows the result of the 2D simulation. We will explain in more detail, that due to the coarse vertical resolution (16 unevenly sized boxes) of the 2D setup, RMSE calculations (of pore water profiles) are done with the 1D model results to obtain optimal OM degradation rates and pore water age (Fig. 8).

The choice for the vertical resolution of 10 cm reflects a tradeoff between number of evenly-spaced boxes (to prevent numeric diffusion) and numeric efficiency (i.e. the ability to vary a large array of parameters many times). Pre-examinations showed no significant improvement of having thinner boxes in general. We agree that the model resolution is at the edge of being too coarse for processes like bioturbation and bioirrigation. However, these processes usually affect the surface sediment (<10 cm) which is not the focus of our study.

7. **Model structure/ Organic Matter Model:**
   Referee 2: *The parametrisation of the organic matter model and in particular of the quality classes exerts an important influence on the results since the amount of reactive or intermediately reactive organic matter that reaches the deeper sediments drives the biogeochemical dynamics at these depths. Yet, the authors do not provide any explanation for the distribution of bulk organic matter into different quality classes. I am surprised that critical parameters, such as the distribution among the quality classes are not included in the inverse modeling approach. In addition, the initial conditions for scenario A and B are very different. Why? And how are they chosen?*

   We clarify that organic matter important for both model scenarios solely consists of quality class 2 (intermediate), for which the decay rate is inversely calculated. Organic matter of class 1 and 3 is either extremely short lived, affecting surface processes which are less important here, or extremely long lived constituting the TOC content of the basal organic rich clay.

   The differences between the initial conditions for scenario A and B derive from the fact, that only in scenario A 140 cm of sediment are deposited on top during the scenario (and removed from the bottom). Therefore, concentration that we initially assume in 5 mbsf in scenario B are found in 3.6 mbsf in scenario A. Likewise, the depth of SO4 being used up is 3.9 mbsf in scenario B and 2.5 mbsf. Consequently, linear gradients in scenario A turn out to be slightly steeper due to the need to meet bottom water concentrations at the upper boundary

8. **Inverse Modeling:**
   Referee 2: *The inverse modeling is only based on two profiles (SO4 and NH4). How confident are the authors in their results? Why did they not include other depth-profiles?*

   There have been additional measurements only of CH4, Cl and Delta13C. The latter two are no model parameters, Cl is inconspicuous and Delta13C is discussed. CH4 poses a problem as it is extremely sensitive to the POC decay constant. Since SO4 and NH4 profiles are largely insensitive to the methanogenesis rate this is not a problem for the model calibration (the SO4 and also NH4 profiles are controlled by sulfate reducers. Not until sulfate is used up by them, methanogens get relevant. However, on the relatively short timescale examined, methane does not effectively move up and down the sulfate front since measured methane gradients are of the order of only 0.1 mmol/l/m). A post examination was performed showing that for the calibration found, the methanogenesis rate can in principle be calibrated to fit the methane profile.

The results presented in Fig.7 (and, in part, also Fig.8) directly reveal the degree of confidence on inversely estimated model parameters (here sedimentation rate and degradation rate). We will extend the analysis and discussion of the calibration results to elucidate their implication for the confidence intervals in parameter estimates. In particular we will stress that in the total of Monte Carlo simulations no indications for several minima were found. The calibrated values, albeit their scatter, should represent/approximate a unique solution.

9. **Results:**
   Referee 2: *The authors should also provide the complete set of simulated depth-profiles for their most plausible burial scenario to increase the confidence in their results. I would like to see the simulated methane, sulfide, oxygen, nitrate and rate profiles. They could compare these results with available field data or published data from similar sites.*

   Due to the lack of additional, model-related field data (see above), further model results (other chemical species) would not help to distinguish the validity of each scenario. Nevertheless, we understand that the reader is interested to see that the model as a whole produces sensible results. A discussion on this topic is included and reference is given to the CH4 and bacterial abundances published in Holstein and Wirtz (2009).

10. **Technical comments:**
    Referee 2: *p.2066, l. 3: SO4 and NH4 are not defined*

    sulfate (SO4) and ammonium (NH4)

11. **Referee 2:** *p.2066, l. 6: the authors refer to organic matter as OM, TOC, POC or POM throughout the manuscript. They need to be more consistent.*

    TOC, POC and DOC are measured quantities and commonly used as proxies for the respective organic matter species OM, POM and DOM. The ..C species are also model state variables. We check for consistency.

12. **Referee 2:** *p.2066, l. 9: Capital S*

    Ok.

13. **Referee 2:** *p.2066, l.17: The term "specific assumptions" is unclear.*

    Rephrased.

14. **Referee 2:** *p.2066, l.22: propagation*

    To our knowledge, progradation is the correct sedimentological expression for the seaward oriented growth of a sediment body

15. **Referee 2:** *p.2067, l. 1-11: This paragraph is obsolete.*

    The introduction is rewritten. Less relevant information is removed (cmp Comment 2).

16. **Referee 2:** *p.2067, l. 19-24: What is the connection to the scientific questions addressed in this study?*

    The introduction is rewritten. Less relevant information is removed and the research questions are made more explicit (cmp Comment 2).

17. **Referee 2:** *p.2067, l.25: unusually*

    Ok

18. **Referee 2:** *p.2068, l.2-3: The term "relevant estimates for local deposition" is unclear.*

    Reworded

19. **Referee 2:** *p.2068, l.22: replace "chiefly" by "mainly"*

    Ok

20. **Referee 2:** *p.2068, l.24: longterm*

    Yes

21. **Referee 2:** *p.2069, l.13-24: This paragraph has nothing to do with "the fate of oragnic matter". The introduction needs a better structure.*

    The introduction is rewritten. The logical consistency will be made more transparent by improving the writing. Less relevant information is removed and the research questions are made more explicit (cmp Comment 2).

22. **Referee 2:** *p.2069, l.27-29: Sentence unclear.*

    Reworded

23. **Referee 2:** *p.2070, l. 7: Capital S in "sedimentary"*

    Yes

24. **Referee 2:** *p.2070, l.13: Rephrase. Dont start sentence with "40 m".*

    Yes

25. **Referee 2:** *p.2071, l.1: remove "is"*

    Ok

26. **Referee 2:** *p.2071, l.10-12: Move this paragraph to the introduction.*

    Ok

27. **Referee 2:** *p.2071, 17: differentiating*

    Sure! (probably p.2072, 17:)

28. **Referee 2:** *p.2073, l.2: replace "diffusion acting on" by "a diffusive processes for both"*

    Gladly.

29. **Referee 2:** *p.2073, l.4: Add reference for "with exponent 2/3".*

    It is according to simple geometric calculations, that surface area scales approximatly with volume$^{2/3}$. We clarifiy that.

30. **Referee 2:** *p.2073, l.16-22: Move paragraph to section 2.2.*

    Yes

31. **Referee 2:** *p.2074, l.4-12: Move paragraph to section 2.2.*

    Ok

32. **Referee 2:** *p.2075, l.11: "accurately fitting" is very vague.*

    We specify that in terms of standard deviation.

33. **Referee 2:** *p.2077, l.8: Why do the authors include bioturbation if there are no bioturbation structures?*

    Reworded to clarify that bioturbation structures are lost (due to resuspension and deposition events)

34. **Referee 2:** *p.2077, l.15-16: Sentence unclear.*

    Reworded

35. **Referee 2:** *p.2077, l.29: What is a soft peak?*

    Reworded

36. **Referee 2:** *p.2078, l.19-20: Sentence unclear.*

    Reworded

37. **Referee 2:** *p.2080, l.16: Sentence unclear.*

    Reworded

38. **Referee 2:** *p.2089, Fig.1: Increase size, show zoom into study area and indicate site location*

    We add to the caption that the locations of cores NN1 and NN2 are 10 and 50 m from the charted low water line (LWL)respectively. They lie on a transect perpendicular to the LWL. An extreme zoom level at which the two core positions separate and their relative distance to the LWL would be visible seems unfavorable.

39. **Referee 2:** *p.2091, Fig.3: Scenario A is unclear.*

    We include to the caption that "bedding planes" indicate former surface planes and that excessive sediment supply causes the tidal flat to vertically grow and laterally prograde into the channel by that burying the "labile POM" deposit.

40. **Referee 2:** *p.2096, Fig.8: Increase size.*

    We could split Figure 8 into 2 figures by moving Fig. 8a into a seperate Figure.

On behalf of all authors

Jan Holstein