Biogeosciences Discuss., 12, C3888–C3892, 2015
www.biogeosciences-discuss.net/12/C3888/2015/

Biogeosciences
Discussions
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Interactive comment on "Parameterization of biogeochemical sediment–water fluxes using in-situ measurements and a steady-state diagenetic model" *by* A. Laurent et al.

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Received and published: 29 July 2015

In this manuscript a new meta-modelling approach is used to parameterize the sediment-water interactions in a coastal area. This is done so as to obtain a better, yet computationally effective representation of benthic-pelagic coupling in a 3-D biogeochemical circulation model. The metamodeling approach consists of using a calibrated 1-D resolved diagenetic model to generate multiple responses as a function of environmentally-realistic abiotic (water-column) conditions, and then statistically fitting fluxes of O2, NO3 and NH4. The method is not entirely novel, and akin to the procedure described in Soetaert et al., 2000 (hereafter referred to as S2000), with a

few exceptions.

As the method is of use for a broad audience, and it is suitable for the journal, I would recommend publication, albeit after major revision.

One of the flaws of the current manuscript is that the reasons and consequences of the deviations of the approach from S2000 are not at all discussed (see below-points 1 and 2).

Major comments:

1. One assumption is to make the return flux of oxygen and nutrients a function of the instantaneous organic matter (OM) deposition flux, whereas in reality nutrients are produced and oxygen consumed as a result of OM mineralization. Instantaneous deposition flux is a good proxy for mineralization only if the OM decay rate is very high. Yet the model settings are such that 26% of OM is rather refractory, which is inconsistent with this assumption. It also means that the time-lag induced between deposition and sediment-water nutrient and oxygen fluxes is not taken into account, i.e. the memory of the sediments is ignored. Hence it is not surprising that the modeled deposition fluxes are not well suited to reproduce the measured oxygen and nutrient fluxes. It is also the reason why the modeled O2 flux follows the POM deposition so closely (P16 L12). In the recommended procedure of S2000, the sediment model dynamically describes two OM fractions (vertically integrated), and the meta model therefore prescribes the dissolved fluxes are a function of OM mineralization. The reason for choosing a reflective boundary condition, and the implications, are however not discussed in this manuscript.

2. The 'novelty' of the method is that the meta model directly fits the oxygen, nitrate and ammonium fluxes as a function of the water-column conditions. In contrast, in the S2000 paper, the fraction nitrified, denitrified and anoxic mineralized is fitted instead, and the fluxes derived from the mineralization rates. The reason for this choice was that this is mass conservative. Deviating from this as in the current manuscript, it

is well possible that, due to statistical fitting, for instance more nitrogen is returned than is originally deposited in the sediment – which means that mass is numerically created. This may not be the case, but at least the authors should spend a paragraph as to why they decided to do the meta-modeling differently and whether or not mass is (numerically) created by doing this.

3. I have strong doubts on the statistical validity of the fitting procedure. In my experience, it is not possible to find robust estimates of the 20 parameters that were selected, given the small amount of data available. To be able to fit all these parameters, it is necessary that they are 'identifiable', i.e. the value of one parameter does not depend to a large extent on the values of (a set of) the other parameters. Parameters that are not identifiable by the data, have very large uncertainty. Unfortunately, the genetic algorithm does not return a measure of parameter uncertainty. A very old paper of mine deals with the identifiability of a diagenetic model (http://dx.doi.org/10.1357/002224098321822401) ; a more recent paper presents software to do more robust parameter fitting that includes a.o. estimating parameter identifiability, parameter sensitivity, and to evaluate the uncertainty of the derived parameters. (www.jstatsoft.org/v33/i03/paper). I realize that it would be too much of an effort to require all this now, but at least the lack of statistical rigor should be mentioned in the manuscript and the results discussed in section P12-L13 and on P18-L25 should be phrased less strongly.

4. From table 2, it is clear that the modeled sediment depth is only 10 cm. Given the boundary conditions that are imposed on the diagenetic model, this entails that gradients vanish at that depth (which is seen on the modeled ammonium profiles in Fig. 2). However, the observations, especially in April and one profile in September still show a large gradient at 8 cm; this makes me suspect that restricting the model to the upper 10 cm of sediment is not adequate for these data.

5. The OMEXDIA model would need a few other additions to make it better suitable for these high-flux sediments (e.g. a reaction of ODU and NO3).

Other comments:

Salinity is a parameter inputted to the meta-model, but it is unclear how it influences the diagenetic model.

Fig. 2. The original OMEXDIA model would never be able to generate the steady-state ammonium profiles from April. As ammonium peaks at 3 cm, it means that there is a sink of ammonium below that depth, although there is no oxygen. What causes this decline?

Fig. 9. The oxygen flux is negative everywhere except in this figure. Should be made consistent. Equation (1) Topt is not a good name for this parameter; the term 'optimal' suggest that the function peaks at the temperature, which it does not. Topt is the "base" temperature, i.e. the temperature for which the rate is defined. Usually the base temperature is taken as 0 degrees or 20 degrees. It would be easier to compare the derived rates with those from other models if using a more standard base temperature (rather than 30 degrees).

Equation (2). Give the units of I(z)

Equation (3):

*why is it sigma (s,i) and not sigma(s,t,i).

*I do not understand the meaning of 1/wi – this weighing is not standard and seemingly dependent on an –arbitrary- initial parameter set? Due to the division by the standard deviation, the fact that units are different is already taken into account, so I so not see the need to have an extra weighing term. *How does the variable cost in Table 3 relate to formula (3)-does it include the 1/wi term?

Table 2.

*Units of aNH3, aO2, etc.. and the unit of kinanox are wrong.

*Unit of Dbcoeff and PB is lacking; also the NC ratio has a unit: is it gram/gram or mol/mol?

*A lot of the optimized parameter values are rather round numbers, which make me assume that they are located somewhere near the edge of the allowed range? What was the range imposed?

Table 3. Why are FNO3 and FNH4 so high in comparison with the other data ?

Page4-Line7: ‘a proportion of the deposited nitrogen is lost as N2 gas’. If the denitrification would work like this, it would mean that the sediments would never be a sink of nitrogen, which is in contradiction with the previous sentence (P4-L6). ‘A proportion of organic matter is mineralized with nitrate’ is a correct description of denitrification.

P14-L14: what is RMSE ? How does this relate to the cost (equation 3)?

P20L22 What does the metamodel do when there is an O2-debt ? I assume this means that negative oxygen concentrations arise in the pelagic model – were negative oxygen concentrations used for fitting the metamodel?

Is the consumption of oxygen in the absence of a PON flux caused by the nitrification of ammonium that fluxes into the sediment or is it a statistical artifact (it appears to be quite high)?

Interactive comment on Biogeosciences Discuss., 12, 7537, 2015.