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Biogeosciences Discussions

Interactive comment on "Towards accounting for dissolved iron speciation in global ocean models" *by* A. Tagliabue and C. Völker

Anonymous Referee #1

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The authors present a computationally-efficient parameterization of complex iron speciation chemistry, suitable for use in global ocean-biogeochemistry models. I think this is a paper worthy of publication, in principle, and my comments here are intended to help the authors improve the manuscript.

As I understand it, there are two reasons why speciation of iron could be important for global biogeochemistry. First, it affects the rate at which iron is scavenged onto sinking particles and thus removed from the water column. Second, it somehow affects the bioavailability of iron to microorganisms. Developing a mechanistic, quantitative understanding or iron speciation and its effects in the marine environment is certainly a worthy goal, and a significant challenge.

My primary suggestion for the paper is that the authors emphasize more strongly that

this is a case in which model complexity is running up against the limit of sparse observational data. The model is introducing a new level of complexity into what are already fairly complex parameterizations (I would disagree with the authors' characterizations of other iron models as 'simple'), and there are scant data with which to judge whether or not these new aspects truly capture reality. For example, there are only a few limited observations of the apparently highly-variable Fe(II) concentrations, and despite significant effort, our understanding and quantification of ligand dynamics is still in its infancy. I would say that this work should be presented as fairly hypothetical, and is most useful to highlight the aspects of iron speciation that need to be better constrained by observations.

The study also presents an illustration of how dissolved iron speciation might respond to future environmental changes. The main conclusion here is that the presumably highly-bioavailable Fe(II) will become more abundant as the ocean acidifies, which the authors claim will provide more iron to phytoplankton. I am somewhat confused by this, in that I would have thought that this would also increase the scavenging rate by sinking particles as the Fe(II) is re-oxidized to non-ligand bound Fe(III), which might lead to less total dFe in the water column, and in fact reduce the availability of Fe, particularly if ligand-bound Fe is in fact fairly accessible to phytoplankton? Whether this is correct or not, I think it deserves comment.

In general, I would think that the authors should not present the speciation model here as a necessary, or even generally-desirable inclusion for ocean biogeochemistry models at this point, as it seems to me that the parameterization still needs better observations in order to verify its applicability. As such, I feel the most important part of the paper is section 5, which could be expanded to more explicitly emphasize the observations needed to improve our understanding of speciation and bioavailability. This is not meant to take away from the value of the work, which is certainly a useful contribution and one which I would hope will spur further quantitative investigation into iron speciation.

Some specific comments.

- Abstract, Line 6: I would suggest adding text to the effect of: ...simplified in such OGCBMs 'due to gaps in understanding and' to avoid high computational cost...

- Abstract, Lines 9-11: The model makes predictions based on the assumptions which go in. I would suggest rewriting the sentence here as something like: We construct an Fe speciation model based on hypothesized relationships to environmental parameters (temperature, light, oxygen and pH) and some assumptions regarding Fe binding ligand strengths and distributions.

- I think the abstract should also include a list of the most significant hurdles to improving the parameterization, according to the authors - what data are most needed, given their insight into the sensitivities of iron speciation?

- Page 2777: Given the importance of bioavailability to the entire premise here, I would personally appreciate a bit more background on what is known, and how important this might really be (or not). What lines of evidence are available to show that iron speciation impacts its uptake by phytoplankton? How well has this been generalized across phytoplankton groups?

- I would find it helpful to have a table listing all the variables and their full names, and a flow-chart figure showing the various iron pools and the flow between them.

- I had a hard time understanding the description of model experiments (3.4). Perhaps it would be clearer if the experiments were simply listed in terms of their initial conditions, boundary conditions, and integration time. If the authors are mixing initial conditions of physical circulations and biogeochemistry from different spinups, this should be explained clearly. As it stands I have a hard time figuring out exactly what the simulations were.

- Page 2777. The main paragraph discusses how Fe bioavailabiilty depends on iron speciation. As a non-expert in this, I would really appreciate some more detail on

the observational background for what forms of iron are accessible and which are not. Also, I would not say that dFe treatments are very simple (line 27) in other models - they often have a number of ad hoc equations and arbitrary functions to achieve the desired result.

- Page 2779. Methodologically, the comparison to the calculation of inorganic carbon speciation is reasonable. However, there's a big difference with iron speciation: DIC speciation is very well understood, whereas iron speciation remains full of mysteries.

- Equation 3. k_ok should be k_ox.

- Page 2782, line 13. How 'identical'? Bitwise reproduction? Or just very similar? Also, I am confused about the terminology 'analytically' vs 'iteratively' on this and the next page, which appears to be inconsistent. By iteratively, you mean a numerical solution? If so, what does 'the analytical solution ...was solved iteratively' mean? (p 2782, line 20)

- Equation 17. It looks like this equation might have a typo - the coefficient for Tk seems too large?

- Bioavailable Fe (p 2786, line 23). I think it should be explained why Fe(III)Ls is bioavailable, but the more weakly bound Fe(III)WLw is not. Presumably you are assuming that Ls are siderophiles of microbial origin, designed to facilitate uptake?

- I would recommend changing the notation of 'proportion' of Fe(II), and similar, from pFe(II) to perhaps the 'fraction' fFe(II). Calling it pFe(II) could make a reader expect that this is the negative log of the Fe(II) concentration, analogous to pH.

- Importance of seasonality, p 2787. The modelled seasonal changes are interesting, but are they real? Can they be backed up with some observations?

- Page 2788. Lines 15-16. This does not sound like particularly good agreement to me, given that even the ranges differ by a factor of more than two. I would suggest that comparisons such as these (and other locations in the text citing unquantified 'good agreement') be removed. I would suggest figures, tables, or correlation coefficients between observed and modeled values be provided instead.

- Figure 4a shows only minor departures from 1, except in coastal regions. Does this mean this is actually a very small effect, except in the green coastal regions?

- Figure 5. Do the authors really think it's likely that the ligand-bound iron is not accessible? I think it's fine to show this, but if so perhaps the authors could explain more thoroughly why.

- Figure 7. Are these measured profiles in the same place as the model profile? Why is there so much variability in measured Fe(II) over such a short distance? Is this typical? Some comment about this would be helpful.

- The references by Boye seem to be missing.

Interactive comment on Biogeosciences Discuss., 8, 2775, 2011.