Biogeosciences Discuss.,
https://doi.org/10.5194/bg-2017-122-AC2, 2017

Biogeosciences
Discussions

Interactive comment on "Inverse-model estimates of the ocean's coupled phosphorus, silicon, and iron cycles" *by* Benoît Pasquier and Mark Holzer

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Received and published: 7 July 2017

Reviewer 2 raises some interesting points (reproduced here in bold) to which we respond in detail below. The Reviewer also points out that our introduction did not explicitly articulate the main science questions addressed by our study, which can be easily remedied in the revised manuscript. Reviewer 2 then asks if our model can be used to constrain class-dependent Fe quotas and the scavenging efficiency of different particle types. However, these quantities are not robustly constrainable within our framework. Moreover, these questions are tangential to our study whose main goal is to obtain data-constrained estimates of the coupled iron–macronutrient cycles and to elucidate the relative importance of the different iron sources for supporting export production. The Reviewer also makes some "minor" points regarding detrital fractions

and a minimum iron quota. Thinking about these helped us deepen our understanding and improve our manuscript.

The submission by Pasquier and Holzer uses a new ocean biogeochemical and ecosystem model, embedded within a data-constrained steady-state circulation model, to explore linkages between the phosphorous, silicon, and iron cycles. The model uses interesting methods to represent nutrient uptake by multiple-species phytoplankton communities without explicitly resolving their biomass, allowing for efficient simulations and parameter optimization. Based on previous work, the authors understand that no single optimal solution for the Fe cycle can be obtained because certain source and sink processes have overlapping effects on the Fe distribution. They therefore explore a "family" of solutions with different source strengths, which are independently optimized and then compiled into a "typical" solution and uncertainty range. There are a number of interesting outcomes that are robust across the family of solutions, for example the patterns of phosphorous export supported by each iron source and the "efficiency" of each source at supporting export. Atmospheric Fe supports most export relative to the magnitude of its source, followed by benthic and then hydrothermal Fe.

We would like to point out that our work additionally shows that part of the uncertainty in the iron sources comes from the fact that, for very similar overall mismatch with observations, the three sources of iron can compensate for each other. We now explicitly make this point in the revised introduction.

I think this paper takes an interesting approach and has the potential to be a valuable contribution to the literature. Nevertheless, I have two main critiques of the paper in its current form. First, the paper lacks a clear direction from the

outset. The introduction does not lay out any specific questions or hypotheses that the new model is designed to address, nor does it identify the particular gaps in our understanding of the Fe cycle that the authors aim to close. Instead, the goal is simply states as “to constrain a model of the coupled nutrient cycles by optimizing the biogeochemical parameters against available observations”, which does not seem like a strong motivation. The purpose of an inverse model should be to extract new information from the available observations, not just to match the observations. The authors should begin by clearly stating what new information they aim to extract by explicitly simulating the coupling of Si, P and Fe, relative to their previous work.

We agree that the introduction could have more clearly articulated the key points of our paper. The purpose of the inverse model is definitely not to build a model and compare to observations. We have revised the introduction, which now clearly states that our paper makes the following advances:

A. We are building an inverse model of the coupled Fe, P, and Si cycles so that the macronutrients and organic matter export can respond to changes in the iron supply. This is a key advance over the work of *Frants et al*. [2016] where the phosphate cycle was prescribed. Our new inverse model provides, for the first time, a family of data-constrained state estimates of the coupled Fe-P-Si cycles for a wide range of not only aeolian, but also hydrothermal and sedimentary sources. Analysis of this family of estimates allows us to show that the uncertainty in the iron sources stems not only from compensation between sources and scavenging sinks, but also from the fact that the different types of iron sources (aeolian, hydrothermal, and sedimentary) can compensate each other.

B. We use our state estimates to address an important open question about the marine iron cycle: What are the relative contributions of the different iron sources to supporting the world ocean’s export production? While there have been perturbation experiments

with forward models where one type of source (e.g., hydrothermal or sedimentary) was shut down to assess the importance of dFe from the missing source [e.g., *Tagliabue et al.* 2009, 2010, 2014], such experiments cannot quantify the true contribution of hydrothermal or sedimentary iron to biological production because of the nonlinearities of the iron cycle [*Holzer et al.*, 2016]. Moreover such experiments were conducted with definite but highly uncertain choices of the iron sources, and the models were not objectively constrained by the available observational data. Thus, in addition to presenting the first inverse model of the coupled Fe-P-Si cycle, the central scientific objectives of our study are to answer the following key questions:

1. How well can the observed dFe, PO_4, and $Si(OH)_4$ concentrations be fitted to observations for widely differing iron sources, and are there limits on the iron source strengths that are consistent with the observed dFe concentrations?
2. What are the limitation patterns that emerge from the data-constrained estimates of the coupled nutrient cycles, given that direct observational data on these patterns is very sparse?
3. How well constrained are the phosphorus and opal exports for optimized state estimates with widely different iron sources?
4. What fractions of phosphorus and opal export are supported by aeolian, hydrothermal, and sedimentary iron, and how do these fractions vary with the relative iron source strengths?

In addition, we have added a “road map” paragraph, so that the reader knows what to expect for the rest of the paper even without looking at the section headings. We think that the underlying theme and science objectives of our work should now be clear to the reader.

This same mentality extends throughout the paper, where numerous model-data comparisons are presented without properly highlighting what new has been learned in the process. For example, one of the key benefits of this coupled model is the ability to assess the relative Fe-scavenging efficiency of different particle types (organic, silica, dust), which remains an open question in Fe biogeochemistry. While this result is part of the model solution, it receives very little attention in the text — it is briefly noted that on a global basis, organic matter and silica are equally responsible for Fe removal from the ocean, and a figure is shown in the Appendix. But the authors should discuss which particle type is the stronger Fe scavenger on a per-gram basis, whether this is robust across the family of solutions. This would be a new interesting result of this study.

We would like to point out that we showed only three figures (joint pdfs, mean iron profiles, and phytoplankton concentrations) that compare model against observations, and we note that the Reviewer requests a yet more detailed comparison with GEOTRACES sections below. These comparisons are not made to answer new science questions per se, only to quantify the degree to which the dFe and macronutrient concentrations can be matched to the observations.

Regarding the suggestion to delve further into the scavenging efficiency of different types of particles (POP, opal, and dust), the partitioning of the scavenging among the different particle types is not something that can be constrained robustly from our inverse model. The scavenging by one particle type can be compensated by another particle type because of overlap in the spatial pattern of their fluxes. The nutrient and phytoplankton data used do not provide separate constraints on the scavenging by each particle type, only on the total amount of scavenging. For these reasons this aspect of our model is not a focus in our manuscript.

Nevertheless, one may of course ask how the partition among particles types varies across our family of estimates. We find that scavenging by dust is negligible for all our state estimates, while the fraction scavenged by POP ranges from $\sim$10% for the lowest iron source cases and saturates near $\sim$100% for the highest iron sources considered. (The remaining fraction is due to opal scavenging.)

In response to this comment, we will add to the manuscript a brief discussion that states that the partition among particle types is likely not robust, and that details the systematic dependence on the total iron source strength.

As another example, the new model seems to be the ideal tool for examining differences in Fe quotas among phytoplankton types — another open question in Fe cycle research. The authors briefly mention that they experimented with different Fe quotas, but abandoned the approach when the parameters converged to similar values. If the model selects similar Fe quotas for all plankton groups, and this is robust across the whole family of solutions, it would be an interesting result indeed and worth of some attention in the paper! Especially if the authors could demonstrate that there is no evidence for enhanced Fe quotas in subtropical gyres where diazotrophic plankton are common, given that there is ongoing debate about the relative Fe requirements of N-fixing and non-fixing plankton.

Reviewer 2 is correct that we do not distinguish the Fe:P parameters of different functional classes based on experiments where we optimized class-dependent Fe:P parameters. While we agree that establishing any differences in Fe quotas among N-fixing and non-fixing plankton is an interesting open question, we would like to remind the Reviewer that we do not model the nitrogen cycle at all so that this issue is beyond the scope of our paper.

We cannot use our inverse model to robustly constrain different values of $R_0^{\text{Fe:P}}$ and

$k_{\mathrm{Fe:P}}$ for each class because these six parameters (two per class) would directly compensate for one another in the global Fe export. We therefore decided to use only the two class-independent parameters, $R_0^{\mathrm{Fe:P}}$ and $k_{\mathrm{Fe:P}}$, and optimized them sequentially. Constraining class-dependent Fe quota is beyond the scope of what is possible with our inverse model, which we will explicitly point out in the revised manuscript.

My second main critique of the paper is that it doesn't present the model-data comparisons for Fe that would be best suited to support the conclusions. If one of the main goals of the paper is to understand the relative contribution of each Fe source to organic matter export, one would want to show that the model accurately reproduces the locations and transport trajectories of the sources. By design, many of the GEOTRACES transects sampled different source regions of Fe, and show clear signatures of these sources and their transport across basins. For example, GA03 and GP16 both traverse benthic and hydrothermal source regions. Plotting cross-sections of modeled and observed Fe along these transects would give a clearer visual impression of the model's performance than the summary statistics and basin-wide profiles that are presented. The reader would want to ensure that these source signatures and transport trajectories are well reproduced, before considering the export contribution analysis.

The Reviewer is correct that a key point of our analysis is to quantify the relative contribution of each iron type to organic matter export and to explore the systematics of these contributions over a wide range of iron source strengths. While source patterns and transport are important for this, we do not think one can reasonably expect our model to reproduce the GEOTRACES transects with complete fidelity. First, we use a coarse-resolution, steady-state inverse model, while the GEOTRACES sections provide snapshots in space and time. Therefore, as we point out in our manuscript, our model cannot capture any transient plumes (e.g., from an African dust event) that are highly localized and episodic. Our state estimates can only capture the long-term average concentration, coarse-grained to 2°×2° resolution. Second, we had only the Intermediate Data Product available when developing this model. Pacific features are therefore only constrained from the older data compilation by *Tagliabue et al.* [2012]. In terms of capturing hydrothermal plumes, we note that our model uses a data-assimilated circulation, but this circulation only assimilated T, S, PO_4, and ^{14}C but not ^{3}He. Therefore, there are likely still some biases in the abyssal circulation, which contribute to the fact that we do not perfectly match the observed hydrothermal iron plumes. However, what matters for our analysis is the large-scale transport into the euphotic zone, particularly the transport into iron-limited regions such as the Southern Ocean. We have no reason to think that this large-scale transport is suspect as evidenced by realistic large-scale patterns of production that are robust across a family of states with widely varying iron source strengths. We emphasize that production in our inverse model is mechanistically driven by dFe and macronutrient availability.

Of course, we are happy to show a direct comparison with the GEOTRACES sections subject to the caveats discussed above. Figure 1 herein compares the main transects included in the Intermediate Data Product with our typical state estimate. The coarse resolution model does capture the large-scale features, but localized high concentrations cannot be captured at our resolution.

We respectfully disagree that we did not present the model–data comparison best suited to supporting our conclusions. We think that Figures 1d, 2c, and 3 of our manuscript are the most relevant and appropriate *quantitative* comparisons between estimated and observed dFe, given that essentially raw bottle data is compared with a coarse-resolution steady-state model. Figure 1d plots the RMS cost-weighted mismatch for the whole family of estimates. This shows how varying iron source strengths affects our ability to match dFe observations. Figure 2c plots the cost-weighted joint distribution of modelled and observed dFe for our typical estimate. This shows just how difficult it is to match the sparse dFe observations, at least compared to the macronutrients for which gridded climatologies are available. Figure 3 shows the basin dFe profiles of each family member. Because these profiles average a large number of observations, they provide a robust metric for assessing the model's ability to capture the large-scale vertical gradients and a realistic nutricline.

In response, we will add an appendix showing the GEOTRACES comparison of Figure 1 herein, plus a brief discussion on what features one should not expected to be captured by our coarse-resolution steady-state estimates.

In addition, I have the following minor comments:

1. I agree with Reviewer #1 that caveats of neglecting DOP cycling need to be more carefully considered. Ignoring DOP will not only bias the total estimated export, but also its pattern and therefore potentially the contribution of different Fe sources to export. Particularly, DOP convergence is thought to provide a significant P supply to subtropical gyres, and essentially "relocates" export downstream, from tropical and coastal upwelling zones into the gyres. Given that benthic Fe supports most export in upwelling zones and atmospheric Fe supports most export in gyres, relocating exporting between those two regimes seems important.

We agree that not carrying DOP has (minor) implications for converting our phosphorous (P) export to carbon export as discussed in response to Reviewer 1. However, our optimized P export effectively includes DOP effects in spite of DOP not being explicitly represented. The optimization of the P-cycle parameters implicitly accounts for all P

export by minimizing the mismatch with the observed distribution of PO_4, which in the real ocean is determined by the remineralization of DOP (and possibly also of POP directly). We are therefore not concerned about missing or "relocated" export due to lateral transport and utilization of DOP. This reasoning is supported by the fact that our POP export averaged over the subtropical gyres matches the estimates of *Letscher et al.* [Nature Geoscience, 2016] when we use the same masks (interpolated to our grid) to define the subtropical gyres. *Letscher et al.* [2016] explicitly model DOP transport and utilization and find a mean subtropical-gyre POP export of 10±2 mmol P m^{-2} yr^{-1}, which agrees with our corresponding export of 10±1 mmol P m^{-2} yr^{-1} (mean and standard deviation across our family of estimates). Our estimates agree with *Letscher et al.*'s despite the fact that we do not have DOP contributing to biological production, which underscores that our estimates of POP export implicitly account for DOP effects.

Regarding the patterns of dFe-supported P export, it is true that aeolian dFe support is more important than sedimentary dFe support in the subtropical gyres, although both aeolian and benthic dFe are important in upwelling regions (Figure 9 of our manuscript). However, as discussed above, we capture effects due to DOP implicitly and there is no reason to think that export has been relocated out of the subtropical gyres. Our estimates of the Fe-type-supported export patterns are by construction consistent with the available nutrient data and we showed that they are robust for a range of Fe sources with widely different ratios of the benthic to aeolian source strengths.

In response to this comment, and in addition to our edits in response to Referee 1, we will add some discussion to the manuscript about the agreement with the subtropical POP exports of *Letscher et al.* [2016] when we more fully discuss our choice of omitting an explicit representation of DOP.

2. What is the justification for choosing such widely different export ratios between plankton types (page 5, line 13)? The authors cite Dunne 2005, but there have been other studies since (e.g., Richardson 2007) that suggest small

plankton contribute as much export, relative to their NPP, as large plankton.

Reviewer 2 is correct that the values of our detrital fractions, f_c, are the optimized values from the work of *Dunne et al.* [2005], that is, $f_{\mathsf{sml}} = 0.14$ and $f_{\mathsf{lrg}} = f_{\mathsf{dia}} = 0.74$. This means that export due to large phytoplankton is $\sim$5 times larger than export due to small phytoplankton for the same amount of production. We prescribed the f_c parameters because they are not constrainable from the nutrient and plankton concentration data alone. The f_c values set the fractional export of each phytoplankton class. However, the nutrient observations constrain only the total export of all classes, while the phytoplankton data [*Kostadinov et al.*, 2016] constrain only the concentration of the different functional classes and thus their respective *uptake*, but not their respective *export*. We think that prescribing f_c to take the values from the study of *Dunne et al.* [2005] was an appropriate choice, and we will argue below that this is not contradicted by the findings of *Richardson and Jackson* [2007], although we acknowledge that the precise f_c values are uncertain.

Richardson and Jackson [2007] suggest that export efficiencies of large and small phytoplankton should be closer to each other, specifically that “the relative contributions of various phytoplankton size classes to carbon export are proportional to their contributions to total net primary production”. However, their data is consistent with f_c having different values for different classes. Figure 2 herein shows the local fractional uptake plotted versus the corresponding fractional export of each phytoplankton class for our typical estimate. The small class collapses to a compact curve because $f_{\mathsf{dia}} = f_{\mathsf{lrg}}$. If we chose different “detrital” fractions for the Diatoms and Large class, then the “small” curve would become a cloud of points whose boundaries are determined by the ratios $f_{\mathsf{lrg}}/f_{\mathsf{sml}}$ and $f_{\mathsf{dia}}/f_{\mathsf{sml}}$. Specifically, if one of these ratios were reduced to 4 or 3, the “small” points would spread out somewhat toward the 1:1 line. *Richardson and Jackson* [2007] show that the export through mezozooplankton dominates the purely detrital export by about an order of magnitude so that our “detrital” fraction pertains to

the export through the mezozooplankton pathway. Therefore, Figure 2 should be compared to Fig. 1B of *Richardson and Jackson* [2007] for mezozooplankton-driven export. Note that our Diatom and Large points in Figure 2 are broadly consistent with the measurements plotted by *Richardson and Jackson* [2007], while our compact curve for the Small class is very close to two of the Arabian-Sea picoplankton measurements. Given the extreme sparseness of the measurements and the fact that they are presented without error bars, we think the *Richardson and Jackson* [2007] paper provides no strong evidence that our f_c values should be drastically different from those of *Dunne et al.* [2005]. We acknowledge however that there is significant uncertainty in the precise values of the f_c parameters and that the small-to-large ratio may well be smaller than 5, although the *Richardson and Jackson* [2007] data certainly does not suggest that it should be unity.

In response, we will relegate Figure 7 of the manuscript, which shows the export production of each functional class, to an appendix because the partition of the export among functional classes depends strongly on our choice of the prescribed, somewhat uncertain f_c parameters. In addition, this appendix will briefly discuss the uncertainty in the f_c values.

3. What is the justification for not prescribing a minimum Fe:P quota in equation 14? It is impossible to sustain phytoplankton growth with no Fe, so if the model is optimizing towards zero it means that model is straying into unrealistic parameter space, not that this parameter can be neglected. The authors should set a reasonable lower limit during the optimization (e.g. low end of the range shown in Moore et al 2013), rather than allowing the Fe quota to approach zero at low [Fe].

The justification for not prescribing a minimum Fe:P quota in Equation (14) is that it turns out that none is required to obtain realistic state estimates for the following reasons: For very low dFe concentrations, our Fe:P cellular ratio would fall below a realistic cell quota, but this has no mechanistic consequence because for such low dFe concentrations there is essentially no uptake in our formulation. This is because our Fe:P ratio is proportional to a dFe Monod term, while phosphate uptake is proportional to the square of a dFe Monod term. Thus, as dFe becomes small, the uptake goes to zero faster than the Fe:P quota itself. Simply put, this means that when Fe:P is unrealistically small, it does not matter because there is no P or Fe uptake.

One should therefore regard our formulation to have a minimum Fe:P quota of zero, and we should not have stated on page 8 that we “ignored it for simplicity”. The fact that optimizing a minimum quota (constrained to be non-negative) resulted in an optimized minimum quota of zero means that a simple Monod factor suffices to capture the dFe dependence of the Fe:P ratio where there is significant uptake. In response, we will reword these passages in the manuscript to make these points explicit.

We thank Reviewer 2 for making us revisit our formulation of the Fe:P ratio, which made us realize that there was an issue not with the minimum Fe:P ratio, but with the parameter $R_0^{\text{Fe:P}}$. $R_0^{\text{Fe:P}}$ multiplies the dFe Monod term in the Fe:P ratio and is thus the maximum attainable Fe:P ratio at high dFe. For a small fraction of our state estimates, the optimization pushed $R_0^{\text{Fe:P}}$ to near-zero values. This is very unrealistic as it means significant P uptake and export are maintained without Fe uptake. We have now corrected this by excluding cases for which the optimized $R_0^{\text{Fe:P}} < 0.5\,\text{mmol Fe (mol P)}^{-1}$ from our family of state estimates. We have updated all our figures accordingly and note that removing these unphysical outliers makes no visual difference, although it narrows the range of Fe export across our family of estimates to 0.87–5.6 Gmol Fe yr^{-1}. Where we discuss our family of solutions (Sec. 3.4), we will add a brief discussion on the fact that we excluded state estimates with $R_0^{\text{Fe:P}} < 0.5\,\text{mmol Fe (mol P)}^{-1}$ because they are unrealistic.

Interactive comment on Biogeosciences Discuss., https://doi.org/10.5194/bg-2017-122, 2017.

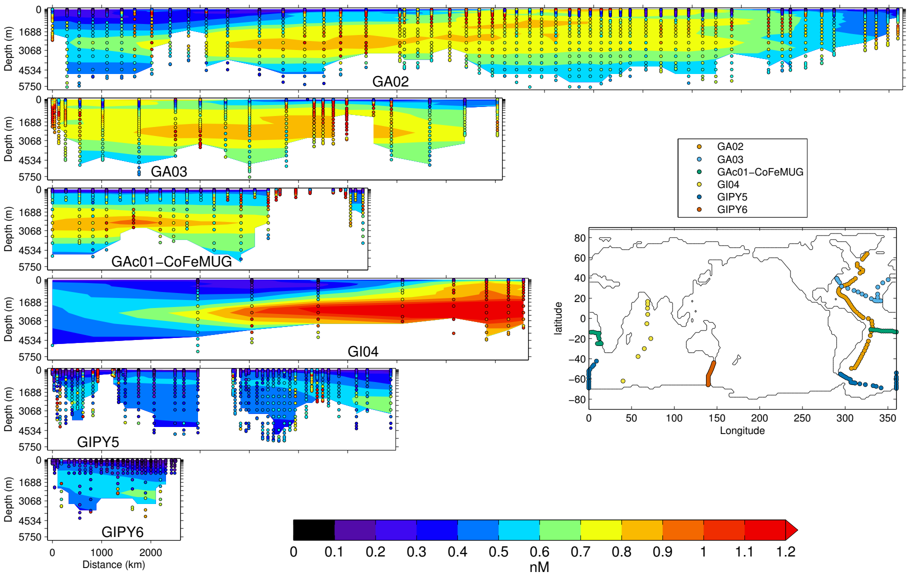

Fig. 1. dFe concentrations of the typical state estimate (contours) compared to the GEOTRACES Intermediate Data Product (dots). The abscissa runs south to north or west to east along the transects (map).

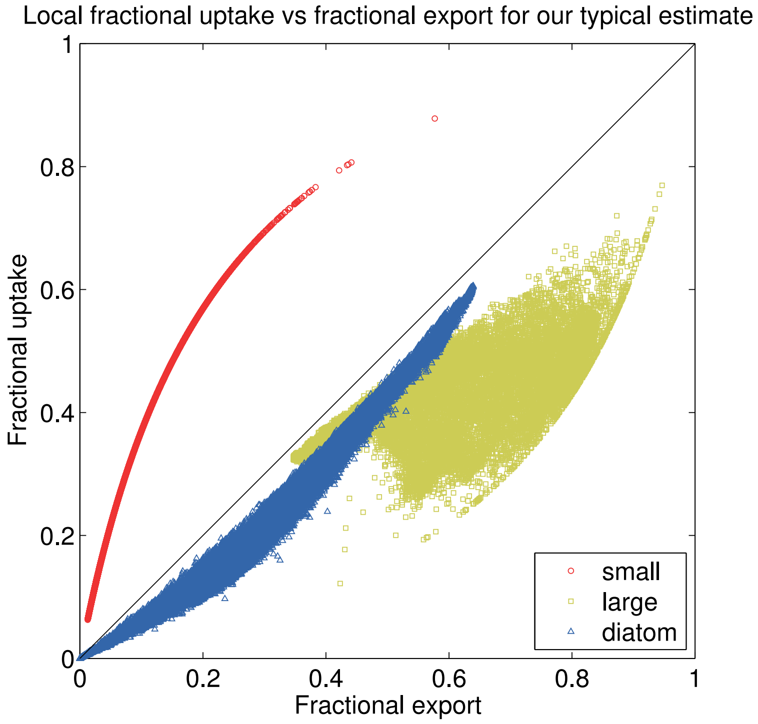

Fig. 2. Fractional uptake versus fractional export of phosphorus at each grid cell of our typical state estimate for the three phytoplankton classes considered.