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Interactive comment

Interactive comment on "Use of remote-sensing reflectance to constrain a data assimilating marine biogeochemical model of the Great Barrier Reef" by Emlyn M. Jones et al.

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This work aims to demonstrate that assimilating satellite-derived remote sensing reflectance into biogeochemical-optical coastal models is better than assimilating empirical statistical products from satellite remote sensing, e.g. chlorophyll. To achieve this objective, the authors assimilate "super-observations" that were computed from remote sensing reflectance by using the OC3M algorithm and a set of empirically determined coefficients. The best model performance (i.e. OC3M forecasts) was obtained when assuming that observed OC3M represents a model OC3M diagnostic variable, rather than the sum of simulated chlorophyll. The assimilation system improved the simulation of independent in situ data (nitrate, ammonia, dissolved inorganic phosphorus

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and total suspended solids), as well as chlorophyll fluorescence from a glider, when compared to the model without assimilation (control).

Assimilation of remote sensing reflectance has the potential to be a crucial break-through in the area of marine ecosystem modelling. However, in my opinion, this work has some relevant issues and a major revision is needed before its publication. In addition, the editing of the manuscript definitively needs an improvement, though I am assuming that the numeration of the figures is missing because of the journal web system.

I feel that the methods and results are not supporting fully the objectives and conclusions of the present version of the work. The objective is to demonstrate that assimilating reflectance is better than assimilating empirical functions of reflectance (e.g. chlorophyll, Kd, PFTs). However, the authors assimilate OC3M, which is an empirical function of the reflectance ratios. I think they should have assimilated the reflectance directly. I acknowledge that the authors discuss this choice extensively, but I am not convinced by their arguments so far, for the following reasons.

A. Firstly, they assimilate OC3M, rather than reflectance, because "the relationship between individual state variables and remote-sensing reflectance is at time non-linear, thus violating the [sic] one of the underlying assumptions of the DEnKF." (page 45). If I am not missing something, the relationship between individual state variables and OC3M is also clearly non-linear, but still OC3M is assimilated. The authors add: "In contrast, the relationship between simulated and observed OC3M is linear": this is not "contrasting" or relevant, because the relationship between simulated and observed reflectance is also linear. Further doubts are casted by the conclusion (see point 8 below). I am not a DEnKF expert, but if it is based on the EnKF, the non-linear relationship between observed variable and other state variables is acceptable in practice, otherwise the authors could not have assimilated OC3M, and we could not even assimilate chlorophyll in models of normal complexity. Thus, direct assimilation of reflectance data should be possible.

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B. A second reason why the authors prefer assimilating OC3M rather than reflectance is the cross-correlation between observation errors of reflectance bands. However I think they should try to tackle this issue and assimilate reflectance bands. I fully acknowledge the importance and challenge of dealing with the above cross-correlations, which have not been addressed in biogeochemical assimilation so far. However, Numerical Weather Prediction systems (NWP, a point of reference for the authors) are tackling them, for example by inflating diagonal observational errors or by using more complex approaches (e.g. Weston et al., 2014 at UK Met Office). Tackling this issue is necessary in a work that advocates a "third novel approach to biogeochemical data assimilation, i.e. the assimilation of remote-sensed reflectance" (page 17).

C. Finally the authors motivate assimilation of O3CM rather than the 3 reflectance bands because of computational costs. They do not describe their computing facility and usage in the manuscript (not even which year(s) they have simulated), thus I cannot really comment on this point. In any case, I think spatial resolution or simulation window should be sacrificed if the objective is to propose a novel paradigm for biogeochemical data assimilation. Another option would be to use data assimilation approaches that are computationally cheaper, such as the SEEK the SEIK to stick on Kalman filtering (see e.g. Nerger et al., Tellus, 57a, 2005). Despite their limitations, such approaches have been proved useful in several applications with marine models (see e.g. the papers by Triantafyllou and colleagues).

In essence, I think that the authors should do a further effort and assimilate reflectance directly, rather than OC3M. I do recognise that this implies a lot of work, but I feel it is necessary given the objective of the work. Crucially, this would make the work a milestone in biogeochemical data assimilation.

Other issues:

1) The authors call OC3M in eq. 21 a super-observation, referring to the works of Cummings et al., 2005 and Oke et al., 2008. However, in those works, "super-observations"

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derive by super-obing, i.e. by spatially averaging observations to reduce their number, as wells as to deal with observation error correlations. In my opinion, the authors are doing something different. They are computing a nonlinear prognostic variable that is included in the augmented state vector and control variable space. This allows them to simplify the observation operator to a direct mapping of computed to observed OC3M (see Evensen2003, Ocean Dynamics 53, for such an approach with the EnKF). However, I was not any more sure after reading the conclusions (see my point 8 below). Can the authors clarify?

- 2) The current set-up of the assimilation experiments 1-4 does not provide a fair assessment of OC3M versus chlorophyll assimilation, in my opinion. It is known that OC3M may overestimate chlorophyll in coastal waters because of TSS and terrestrial CDOM. In experiment 1, observed OC3M is compared with simulated chlorophyll, and just chlorophyll classes are updated in the analysis: experiment 1 failed. In experiment 4 observed OC3M is compared with simulated OC3M and used to update chlorophyll classes as well TSS and nutrients. I suspect that experiment 4 outperformed experiment 1 because it had the chance to correct TSS. What if also TSS and nutrients were updated in the analysis in experiment 1? The authors should present such additional experiment, using the same observational error than in experiment 4.
- 3) Related to the above point: it is not clear how the authors computed the total chlorophyll that they compared to OC3M in experiment 1. Does it include only Trichodesmium, small and large chlorophyll? Can the author assume that benthic microalgae, corals, macrophytes do not contribute to ocean colour? Furthermore, TSS does not appear as a model variable in Figure 15: is it the sum of more than one model variable?
- 4) An appendix summarizing the bio-optical optical model should be included in the manuscript. In my opinion, the current appendix describing the biogeochemical model could be deleted because the scheme in Figure 15 is sufficient (but please renumber the figures in the order you cite them in the text). On the other hand, one needs to read

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Baird et al., 2016b to find crucial information to appreciate the current manuscript, e.g. on the representation of CDOM in the model.

- 5) The authors should include a larger number of critical variables in the control variable space, i.e. in the state vector that is updated in the analysis. In particular, the most important optically-active components in figure 15 should be included. I do appreciate that CDOM absorption is computed from a regression with salinity (Baird et al., 2016b), and salinity should not be updated by OC3M assimilation. However CDOM absorption dominates the signal in figure 2, as stated at page 9. I think it would it be worth to use a passive tracer instead of salinity in the regression for CDOM and exploit reflectance assimilation to correct the tracer. Furthermore, also organic components of NAP should be added in the control variable space. The authors justify the small number of control variables with computational costs, but see my comment C). In any case, it seems more sensible to include optically active compounds rather than nutrients in exp-4, if a selection is needed. I am rising this point because I think the strength of assimilating reflectances (and bulk optical properties in general) is their stronger covariance with a larger number of model variables, if compared to chlorophyll. Such strength is lost if most of the optically-active compounds are not included in the control variable space.
- 6) 36 members in the dynamic ensemble sounds a quite small number compared to 100 often used with the EnKF and marine models. I understood that such choice is related to the small number of control variables, and in turn to computational costs (but see my point C above). Can the author show the sensitivity of the results to the number of members, at least for one analysis cycle?
- 7) The dataset used for the assessment of the simulation skill is relatively small: e.g. 3 or maximum 4 data of nutrients at each station and depth (why so few if the IMOS sampling is monthly?). With such a low number of data in time, there is the risk that improvements are not statistically significant. This doubt must be avoided in a work that presents a new paradigm. Can the simulation be extended, or performed for a different period that is covered better by data?

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8) In the conclusion, the authors wrote "The non-linear observation operator in the assimilation system subsequently converted remote-sensing reflectance into a simulated OC3M approximation of Chl-a". This contradicts what stated in the Methods and reported in the above point A), where OC3M is described as a prognostic variable computed in the model and included in the augmented state vector and control variable space. If a non-linear operator was used in the analysis instead, several issues would arise. Please clarify what has been done in this work.

I have added further comments in the pdf of the manuscript, but I neglected the typos, letting their correction to the copy-editing office. I am now realizing that my review is extremely lengthy and I will be happy to elucidate the points where I was unclear. I stress that I really appreciate the novelty of the work and I believe that its eventual publication will represent a crucial contribution to marine system modelling and prediction.

Kind regards,

Stefano Ciavatta

Please also note the supplement to this comment: http://www.biogeosciences-discuss.net/bg-2016-168/bg-2016-168-RC2-supplement.pdf

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