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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Initial response to RC2: Issue A

The authors would like to thank Dr Ciavatta for his thorough review of the manuscript. We’d like to apologize for the formatting errors that were present in the initial submission. A corrected manuscript can be found in the supplementary material in response to RC1.

We are currently working on a revised version of the manuscript where we address the issues raised by Dr Boss, Dr Ciavatta and Dr Ford. We’d like to take this opportunity to respond to a common criticism by both Dr Ciavatta and Dr Ford that relates to the title
and aims of the manuscript. More specifically there are concerns that perhaps we have overstated the findings of the study by saying we have assimilated reflectance (Rrs) data. We argue that we are assimilating reflectance data, however, we have chosen to apply some function f(Rrs), to avoid some problems associated with assimilating Rrs directly, as described in experiments (EXP1 – EXP4). With the exception of EXP1, we treat modelled Chl-a as an unobserved state variable, and assimilate the reflectances by using f(Rrs). To avoid difference in kind errors (see discussion below), f(Rrs) is applied to both modelled and observed Rrs.

We do agree with Dr Ciavatta and Dr Ford, that it would be a good idea to demonstrate the direct assimilation of Rrs, and we have accepted this advice and included an additional experiment (EXP5). In EXP5 we directly assimilate the reflectances used in the OC3M function. It was our intention to demonstrate this in a companion manuscript, and we currently have a number of experiments underway to refine this approach.

We’d like to point out that at this stage the assimilation of Rrs data leads to larger forecast errors than the assimilation of f(Rrs). We chose the function f(Rrs) to take the form of OC3M because it used band-ratios, which reduce the impact of cross-correlated observation errors between reflectance bands, in the observations being assimilated (e.g. the neglected off-diagonal elements of the observation error covariance matrix). Additionally, we suspect that if raw Rrs data is to be assimilated, then a much larger dynamic ensemble is required, and a likely reason for the high forecast errors in EXP5 is due to our small ensemble size. The reason for needing a larger ensemble arises from the need to essentially fit a multivariate surface in observation space when multiple reflectance bands are assimilated for a given model cell. Therefore, to address the concerns of Dr Ciavatta and Dr Ford, we have included the preliminary results of EXP5 in a second appendix (Appendix B), with the caveat that these results are preliminary and we expect to reduce the forecast error with a revised configuration of the assimilation system.

Below we have responded to the first issue raised in RC2:
"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. "

This was poor language on our behalf and needs clarification. We agree that there is likely going to be non-linear relationships between the observed and unobserved state variables, and the linear assumption is at best an approximation that is known introduce error. There have been various approaches to reduce errors associated with the linear Gaussian assumption (e.g. Gaussian anamorphosis; Simon and Bertino, 2009). The point we would like to make here is related to errors that arise due to what we are modelling (or including as an observed variable) is different to what we are observing. For instance, if we make the assumption that surface total Chl-a is equivalent to OCM3 Chl-a, then we have three sources of observational error ($E_{tot}$) that must be accounted for when relating these observation types to the modelled state variable:

1.) **Representation error** ($E_R$) – errors that arise due to the approximation that the modelled tracer quantities are an average over a whole model cell. This can be thought of as unresolved spatial variability.

2.) **Difference in kind error** ($E_D$) – these errors arise when the variables that are being modelled and included in the assimilation state vector differ from the observations. For
example, many studies have included surface Chl-a (or some optical depth weighted average) in the assimilation state vector, and assume there is a direct relationship with OC3M (or other quantities). OC3M is known to have typical errors of between 30-70 % in blue water domains, and errors that exceed 200 % in optically complex (or optically shallow) waters.

3.) Analytical/sensor/processing error \( (E_A) \) – Depending on the observational platform in use, then these errors can be small (e.g. ARGO float), or in the case Remote Sensing products then atmospheric correction can introduced errors as large as 25 % using the ANN method (see Schroeder et al., 2007).

The total observation error is then given by the sum of error types:

\[
E_{\text{tot}} = E_R + E_D + E_A
\]

The sum of these can be large and form the diagonal elements of the observation error covariance matrix. The larger \( E_{\text{tot}} \), the lower the impact of the observations. If we can remove the difference in kind error \( (E_D) \), then we only have representation error and analytical/sensor/processing error. Given that Level 3 ocean color remote sensing products rely on empirical/statistical relationships, \( E_D \) dominates, therefore if we can minimize \( E_D \) (or remove it entirely), then the information content of the observations increases. By simulating reflectances, we could directly assimilate a variety of level 3 products, or we have the flexibility of assimilating the Level 2 reflectances.

The approach that we are advocating for in this manuscript is not necessarily to assimilate the raw reflectances directly, but rather take an approach whereby the term \( E_D \) is eliminated, by assimilating like for like variables. To illustrate the possible effect of \( E_D \), simulated total surface Chl-a is plotted against simulated OC3M (derived using the EMS optics model), and it is clear that there is a non-linear relationship between surface Chl-a and OC3M in both normal and log-space (Fig 1). Therefore, if a linear relationship between surface Chl-a and OC3M is assumed, then there is a substantial risk of the assimilation system producing spuriously large positive and negative incre-
ments, if $E_D$ is not sufficiently large (to the point where most observations will have no impact in the assimilation system).

In the revised version of the manuscript we have expanded our discussion about error sources, clarified our language and included EXP5 as a preliminary experiment in assimilating raw reflectance data.

References:


Fig. 1. Scatter plot of simulated surface Chl-a concentration vs simulated OC3M (left) and on a log scale (right), for the 28/5/2013.