#### **Responses to Reviewer 3**

Below the complete reviewer comments are shown in black font along with detailed responses to each comment in blue font.

#### Review:

This study implements DEnKF-based data assimilation of satellite sea surface temperature, sea surface height and chlorophyll, and in situ temperature and salinity, with a physical-biogeochemical model of the Gulf of Mexico. The results are validated using the assimilated data plus profiles from five independent BGC-Argo floats, with a particular focus on subsurface biogeochemistry. Following the validation, a change was made to the light attenuation parameterisation to improve the fit to BGC-Argo chlorophyll.

The paper is well written and the experiments and results useful and well described. Subject to a few minor revisions, detailed below, I recommend publication in Ocean Science.

Response: We thank the reviewer for the constructive comments and suggestions which will be very helpful as we revise the manuscript.

P2 L41 - "discretion schemes" should presumably be "discretization schemes"? Response: We will correct it as suggested

P3 L65-70 - while less focus has definitely been given in the literature to validating the subsurface than the surface, it's not as rare as this paragraph would suggest. Some of the studies already referenced, and more besides, perform some validation of the subsurface, including on a point-to-point basis. See e.g. Fontana et al., 2013; Ford and Barciela, 2017; Mattern et al., 2017; Cossarini et al., 2019. The paragraph should be rephrased accordingly.

Response: We thank the reviewer to point out this. We will include these references and rephrase this paragraph into:

"The insufficient availability of subsurface and interior ocean biogeochemical observations is not only reflected in the immaturity of biogeochemical data assimilation but also its skill assessment. When compared with the surface, the subsurface has received less attention in skill assessments of biogeochemical data assimilation systems. Although there already have been studies which compared their vertical structures with in-situ observations and/or climatological datasets (e.g. Fontana et al., 2013; Ford and Barciela, 2017; Mattern et al., 2017; Ourmières et al., 2009; Teruzzi et al., 2014), these validations are often limited to low spatio-temporal resolution. The recent growth of autonomous observation systems, esp. BGC-Argo floats and gliders, make it possible to evaluate biogeochemical data assimilation systems below the surface in high resolution (e.g. Cossarini et al., 2019; Salon et al., 2019; Skákala et al., 2021; Verdy and Mazloff, 2017)."

#### P3 L74 - I think "Garcon" should be "Garcon".

Response: True. We will correct it in our revised manuscript.

# Is any transformation performed for chlorophyll to deal with non-Gaussianity?

Response: In this study, we assimilate the actual chlorophyll concentrations. Based on our prior tests, assimilating log-chlorophyll can yield more improvements of the surface chlorophyll in coastal regions but degrade it in the deep ocean (with depth>1,000m). In addition, assimilating log-chlorophyll results in less improvements of subsurface biological properties, including the chlorophyll, phytoplankton, and POC. As this study focused on the subsurface biological properties in the deep ocean of the Gulf of Mexico, we decided to assimilate the actual chlorophyll. Also, there already have been successful examples which assimilated or updated the actually chlorophyll (e.g. Hu et al., 2012; Yu et al., 2018). Nevertheless, we have to acknowledge that assimilating the actual chlorophyll is suboptimal because of its non-Gaussian nature and will state this more clearly in the revised manuscript.

### Do the observation errors used account for representation error? Is this likely to affect results?

Response: We didn't include representation errors in our study. It is also a common practice to only account for the instrument errors in data assimilation. The detailed influence of the representation errors need to be further investigated.

# P8 L04 - would additional metrics, even just bias and correlation coefficient, give additional information? Furthermore, chlorophyll and other biogeochemical variables are not normally distributed. Is RMSE appropriate here?

Response: We will also report bias and correlation coefficient in our revised manuscript. For the usage of RMSE, we understand the reviewer's concerns that the RMSE may skew to high values. In previous applications (e.g. Ford and Barciela, 2017; Pradhan et al., 2020, 2019), the RMSE of log-chlorophyll has been also applied to put a same weight on the low values. However, this study in particular focus on the subsurface biological properties in the deep ocean (with depth > 1,000m) of the Gulf of Mexico and the major subsurface features, e.g. the deep chlorophyll maximum, are relatively high in their order of magnitude (e.g.  $\sim o$  (1E-1 mg m<sup>-3</sup>) of chlorophyll). In addition, the low concentrations (e.g.  $\sim o$  (1E-2 mg m<sup>-3</sup>) chlorophyll) are less ecologically important than the high concentrations.

# P10 L56 - can the uncertainties be quantified?

Response: Yes. The uncertainty can be quantified by two methods, error propagation and validation with in-situ observations. The former method propagates errors from input to output with good knowledge of uncertainties from the input and model parameters. The latter one will calculate the root-mean-square difference (RMSD) and bias between the satellite estimates and match-up in-situ observations. Some satellite products (e.g. Ocean Colour CCI) can provide the pixel-by-pixel uncertainties. For this purpose, the uncertainty will be firstly calculated with respect to different optical water types and then extrapolated into each pixel as the weighted sum of uncertainties for each water type.

# P11 L87 - how was significance calculated?

Response: In this study, the significant improvement is referred as the reduction in RMSE larger than or equal to 10% (please see the caption of Table 2 in our original manuscript). We will clarify this in our revised manuscript.

# P11 L93-94 - what method was used to calculate the old and new parameterisations?

Response: Parameters of the original light attenuation scheme ( $Att=0.04+0.025 \times chl$ ) is based on previous studies (e.g. Fennel et al., 2011, 2006) and the alternative light attenuation parameterization ( $Att=0.027+0.075 \times chl^{1.2}$ ) is subjectively tuned based on the BGC-Argo floats. We will add some explanation for the two light parameterizations in our revised manuscript.

# Please comment further on why Fig. 9 shows limited improvement in the free run with the new parameterisation. Does this imply that the parameterisation is too tuned to the BGCArgo data, or that state-parameter estimation might be the best long-term approach?

Response: The over-tuning means that a model reproduces observations through wrong mechanisms. However, in the Free\_alt run of our study, the physical circulation features, e.g. the position of Loop Current eddy, are wrong. We cannot expect the alternative parameterization to improve chlorophyll by compensating errors from physical circulations, which otherwise is a symptom of the over-tuning. In the DAsat\_alt run, the chlorophyll is improved as the data assimilation corrects physical circulation features, which indicates that our alternative parameterization is well calibrated.

#### Fig. 1 - please state what the red square represents. Is this the model domain?

Response: Yes, the red rectangle represents our model domain. We will clarify it in our revised manuscript.

Fig. 3 - please include units where appropriate. (a-e) should probably be (a,b,d,e). Response: We will revise it as suggested

#### Fig. 7 - should the observations be included in a subplot here, as in Fig. 4?

Response: We didn't show NO3 observations because NO3 is not measured by the BGC-Argo floats in the Gulf of Mexico. In this study, we estimated NO3 based on its climatological relationship with temperature (Figure S1 of our original manuscript which is replot as Figure r1 here) and compared it with the model results. We will add the estimated NO3 distributions in our revised manuscript. However, the estimated NO3 tend to be overestimated in the high temperature regions (Figure r1), which typically occurs within the euphotic layer. Therefore we used the unbiased root-mean-square-error to quantify the model-data misfit of NO3.



Figure r1 Empirical relationship of temperature-NO3 derived from the World Ocean Atlas in the Gulf of Mexico. Colors indicate the number of observations within each bin.

# Fig. 10 - what is meant by DCM increment? DCM is not one of the state variables included in the assimilation.

Response: The definition of DCM increment is analogous to increment of other state variables. Specifically, we calculate the DCM depth based on chlorophyll profiles before (forecast) and after (analysis) update, and we define the changes due to update as the DCM increment. We will add a definition in our revised manuscript.

Fig. S3 does not appear to be referred to in the text. More generally, the figures in the supplement could reasonably be included in the main paper, but I appreciate the desire to limit the number of figures. Response: We will refer to this figure in our revised manuscript. In addition, as suggested by the reviewer 2, we will reorganize the manuscript to introduce the alternative light parameterization in a different way. We may include this figure into the manuscript.

### Reference

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