Review by Sarah Schlunegger

Referee comments on "Deep chlorophyll maximum and nutricline in the Mediterranean Sea: emerging properties from a multi-platform assimilated biogeochemical model experiment" by Teruzzi et al., currently in discussion at Biogeosciences.

Teruzzi et al presents the results from a data-assimilating biogeochemical model of the Mediterranean Sea. This work provides a novel case-study of the dual use of remotely-sensed (ocean color) and in situ (BGC-Argo) biogeochemical constraints in reconstruction of one year of the biogeochemical state of the Mediterranean Sea. Firstly, the data-informed model solution demonstrates fidelity with observations for a number of surface and depth-resolved biogeochemical metrics, such as the vertical position and longitudinal gradients of the deep chlorophyll maximum and its co-variance with the nutricline. Secondly, the study presents compelling evidence for the synergistic benefits of assimilating estimates of remotely-sensed chlorophyll concentrations in tandem with in situ, depth-resolved estimates of chlorophyll. Thirdly, the study discuses some of the nuanced differences between the impacts of assimilating satellite versus BGC-Argo chlorophyll upon the model solution. The most striking difference discussed is the strong seasonal signatures the different observational streams have upon the solution, with remotely-sensed chlorophyll providing stronger constraint during winter months, and in situ chlorophyll providing stronger constraint during summer months. Finally, implications for optimized sampling strategies, such as the recommendation that BGC-Argo increase sampling frequencies during the 'influential' summer season, are discussed.

This work represents a timely contribution to the underway community efforts towards optimizing the design of a global, autonomous biogeochemical observing network for use in constraining reconstructions of the evolving ocean state. I recommend this manuscript for publication after a few minor clarifications and elaborations are incorporated, as I outline below.

We thank Sarah Schlunegger for the positive and constructive comments on the manuscript. All the points raised in her review are addressed below with our replies in green italic.

Points of clarification:

The model setup describes the biogeochemical model as being coupled offline to the dynamical model. Coupled implies two-directional influence, i.e. that the biogeochemistry is both impacted by and impacts the dynamical fields. Is this the case?

If it is the case that the model set up is "coupled" in the true sense of the word, then the impact on the dynamical fields should also be presented.

If it is not the case, and in fact the biogeochemical model or assimilation of biogeochemical fields does not feed-back or modulate the underlying dynamical fields, then a more appropriate term to use is "forced" or "driven" – i.e. Line 135 should read "the MedBFM was forced or driven offline with output from MENO3.4-OceanVar…"

In MedBFM, the biogeochemical variables are tracers advected and diffused by ocean dynamics and transformed by biogeochemical processes, adopting a source splitting operator (Butenschön et al., 2012) without feed-back on the dynamical fields. In particular, transport and advection are driven by precomputed daily 3D fields of currents and diffusivity, while T and S are used in the biogeochemical module. We will modify the manuscript following the Reviewer's suggestion to better explain this aspect.

To improve accessibility, an additional paragraph of description or context of Eq. 1 should be included. This would involve, for instance, explanation of the "innovation" term (Line 159), and discussing the significance or intuitive purpose of the different covariance vectors.

In the new version of the manuscript we will add a clarification on the terms used in eq. (1):

"In 3DVarBio, assimilation is performed through the minimization of a cost function that is defined on the basis of Bayes' theorem (Lorenc, 1986) as a weighted sum of the square of the mismatches between the model background state x_b (the model state before the assimilation) and the analysis x_a (the assimilation result) and the observations y. Each square mismatch is weighted according to the respective accuracy estimation, meaning that $x_a - x_b$ is weighted by the background error covariance matrix $\mathbf{B}$ while $(y - H(x_b))$ by the observation error covariance matrix $\mathbf{R}$:

$$J(x_a) = (x_a - x_b)^T \mathbf{B}^{-1}(x_a - x_b) + (y - H(x_b))^T \mathbf{R}^{-1}(y - H(x_b)). \qquad (1)$$

In eq. (1) the term $y - H(x_b)$ is usually named innovation and H is the observational operator that provides the values of the model background state x_b in the observation space. In our application $H(x_b)$ are model concentrations of the variables observed by satellite or floats at observation locations. Through the minimization of the cost function (1), the assimilation provides the analysis x_a that minimizes its weighted distance from both y and x_b."

Regarding the "Impact indicator" metric:

(a) It needs to be explained that the impact indicator given by Eq 2, although it does not contain an explicit 'directionality' of the impact (i.e. towards better or worse agreement with the data-constraints), that the assimilation methodology works to push the model solution towards the data, therefore any non-zero value of I(t) represents a nominal improvement in model-data fit. From the equation alone, and without sufficient prior understanding of the methodology, this is not obvious, making it difficult to interpret if the additional streams of assimilated data are merely influencing or in fact improving the solution.

Thank you for the very constructive comments about the Impact Indicator. Concerning the first comment (a), it is true that the impact is in the direction of the assimilated observations for grid-points corresponding to observation locations. On the other hand, grid-points without observations are corrected consistently with the solution of the DA scheme (e.g., the effects of surface chlorophyll assimilation on the water column profiles) with impacts vanishing for grid-points far from any observation locations. Thus, the impact indicator is higher where the assimilation brings the simulation toward the observations and this can be considered an improvement of the simulation with respect to nearby assimilated observation. As suggested by the Reviewer, we will modify the description of the impact indicator in order to highlight this aspect:

"[...] The subscript 200 represents the integral over the 0-200 m layer, while the overbar represents the average over the whole Mediterranean and over seasonal periods. The impact indicator $I(t)$ was calculated for each assimilation date and each grid point, then, statistically analysed and summarized on a seasonal base. The indicator I(t) quantifies how much an assimilated run deviates from the REF simulation, thus it is higher where and when a simulation is closer than REF to the assimilated observations."

(b) The maps of Fig. 6 and Fig. 7 present a very derived / abstract metric. These figures present the 50th and 90th percentile 'impact' of assimilated the given field during the given season. Interpretability of this abstracted metric would improve if an additional subpanel was included in each figure which showed a representative distribution of the impact-indicator for a single grid-cell (or averaged over a region), with markings at the 50th and 90th percentile. This could also provide opportunity to contrast the summer vs. winter distributions of the indicator. For instance, for chlorophyll, the winter distribution of the indicator would be shifted toward "1" while the summer distribution would be closer to "zero". See a mock-up below. This will help orient the reader as to what the maps are presenting.

We thank the Reviewer for this constructive comment about the Impact Indicator. Following the Reviewer's suggestion, we investigated the distribution of the Impact Indicator over winter and summer. In particular, we analysed frequency distributions of the impact indicator at some locations, and we provide in Fig. R1 two examples. The histograms confirm results shown in Fig. 6 and 7, with higher Impact factor percentiles in winter with respect to summer for chlorophyll and the opposite for nitrate (since the impact of sparse float observations is negligible at the simulation beginning). Further, the histograms are quite scattered since they depend on a number of factors (e.g., the number of observations in the area and assimilation changes during subsequent dates). Therefore, we think that the non-parametric statistics (percentiles) shown in the manuscript are a sound choice to quantify the impact of the assimilation on model solution and we prefer to avoid to insert the grid-point histograms.

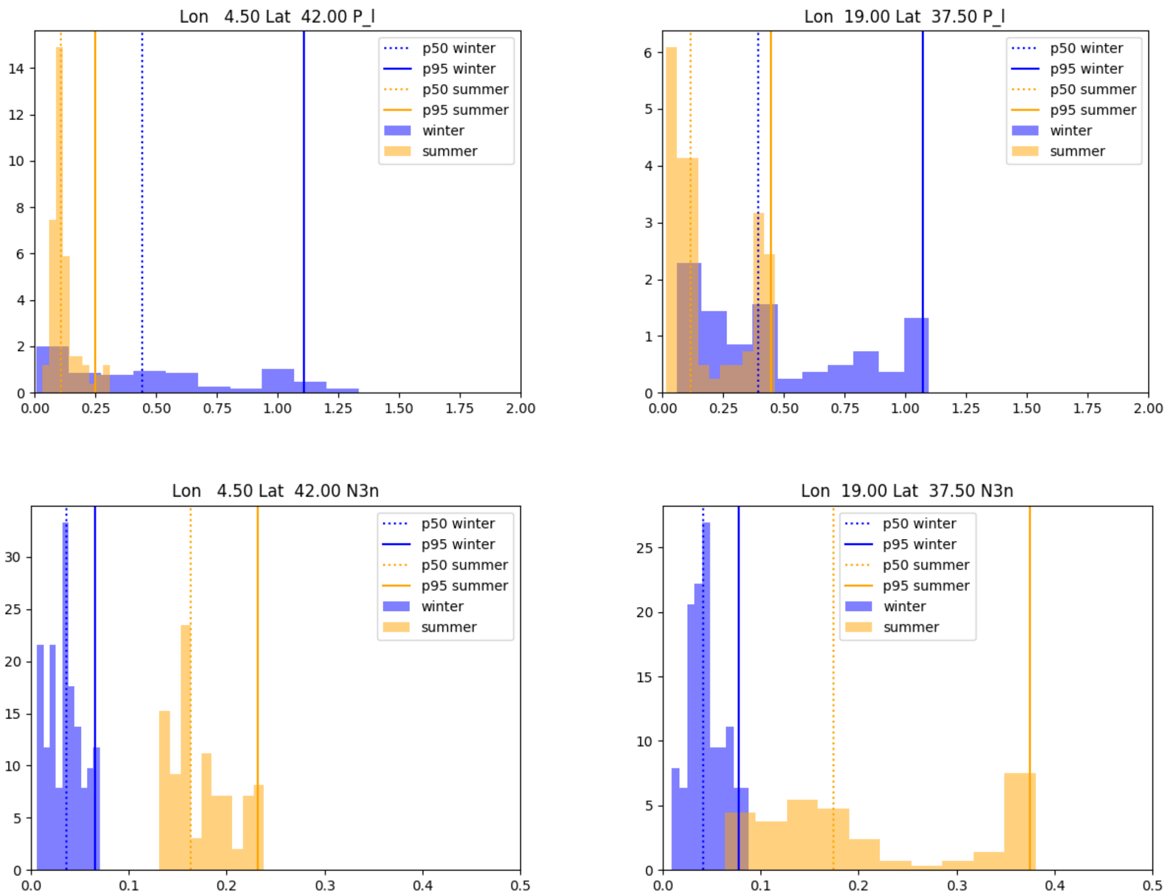

Fig. R1. Frequency histograms of the Impact Indicator at two locations for chlorophyll (top) and nitrate (bottom) in winter (blue) and summer (orange). Vertical lines indicates the values of the 50^{th} (p50, dashed line) and 95^{th} (p95, continuous line) percentiles.

The conclusions section would benefit from a final sentence that poses the significance of the study within the context of future advances in biogeochemical data assimilation within basin and global domains, i.e. something like " The multi-platform assimilation yielded improvements in model representation of large-scale (hundreds to thousands of kilometers) bio-dynamical features and is suggestive of the applicability of this advancement to reconstructions of other ocean regions and the global domain."

We thank the reviewer for this suggestion that helps to enlarge the perspective of our manuscript. We will add a comment about the applicability of multi-platform DA to other domains:

"The impacts of multi-variate profile assimilation are directly linked to the sampling frequency and dimension of the BGC-Argo network, which should increase to match the consolidated importance and relevance of satellite observation assimilation. Thus, in a perspective view, the multi-platform assimilation can improve model representation of both large-scale (hundreds to thousands of kilometres) to mesoscale features and be beneficial for robust reconstruction in global and regional reanalysis."

Minor editorial and stylistic suggestions:

L7-10: Rewrite to something like: "Data assimilation has lead to advancements in biogeochemical modelling and scientific understanding of the ocean. The recent operational availability of data from BGC-Argo floats, which provide valuable insights into key vertical biogeochemical processes, stands to further improve biogeochemical modelling through assimilation schemes that include observations from floats in addition to traditionally assimilated satellite data." (bold is new)

Thank you for the suggestion. We will include it in the revised manuscript.

L16: "maximum depth, intensity and nutricline depth" (added a comma and removed the first 'and')

We will change the sentence accordingly.

L39: Add the following reference, which also provides motivaiton for the direct use of optical properties in data assimilation:

Dutkiewicz, Stephanie, Anna E. Hickman, Oliver Jahn, Stephanie Henson, Claudie Beaulieu, and Erwan Monier. 2019. "Ocean Colour Signature of Climate Change." Nature Communications. 10 (1). https://doi.org/10.1038/s41467-019-08457-x.

We will inserted the reference.

L40: Ocean-colour observation assimilation takes advantage of the frequent, large-scale satellite observations of ocean properties related to the microbial biology of the upper ocean.

L42: "deeper ocean layers requires approximations and assumptions."

We will change the manuscript according to the two previous Reviewer's suggestions.

L45: "localization" – what does this mean?

In Ensemble Kalman filter (EnKF)-like data assimilation, "localization" is a method applied to limit the impact of the assimilation (increments) to areas relatively close to the observations. In particular, localization is applied when knowledge of spatial covariance is relevantly approximated due to the limited ensemble size. In this sense, localization avoid to insert spurious and non-realistic effects and can be applied not only to limit the spatial covariance but also on covariance among variables or on the time dimension. Concerning the use of "localization" in the sentence at L. 45, we are referring to vertical localization applied in some DA application of satellite ocean colour, meaning that the assimilation impacts are limited to a portion of the *water column through localization. We will modify the sentence as follows to make it more clear about "localization" in EnKF-like data assimilation:*

"Vertical covariance must be parameterized by synthetic pre-calculated vertical profiles in variational schemes (Teruzzi et al., 2018), while EnKF-like (ensemble Kalman filter) schemes may have limitations in effectively impacting deeper ocean layers (Fontana et al., 2013; Hu et al., 2012). Indeed, some EnKF-like applications introduce limitation to the increments in subsurface layers through localization in the vertical direction to address spurious correlations (Goodliff et al., 2019; Pradhan et al., 2019)."

L66: "ideal" – replace with "suitable" or "appropriate" – as it could be easily argued that a region with less coastal margins and more open-ocean conditons, where ocean color is more reliable, would be a more 'ideal' location to do a multi-platform assimilation.

We will replace "ideal" with "suitable".

L348: "In our results, this hypothesis was supported by higher nutrient uptakes in the western…"

We will replace "scenario" with "hypothesis".

L409: Remind readers of what Vv means, i.e. " Vv (vertical co-varience error)"

L415: Remind readers of what Vb means, i.e. " Vb (biogeochemical co-varience error)"

We will add a remind of what Vv and Vb mean into brackets as suggested by the Reviewer.

References

Butenschön, M., Zavatarelli, M., Vichi, M., 2012. Sensitivity of a marine coupled physical biogeochemical model to time resolution, integration scheme and time splitting method. Ocean Model. 52–53, 36–53. https://doi.org/10.1016/j.ocemod.2012.04.008

Goodliff, M., Bruening, T., Schwichtenberg, F., Li, X., Lindenthal, A., Lorkowski, I., Nerger, L., 2019. Temperature assimilation into a coastal ocean-biogeochemical model: assessment of weakly and strongly coupled data assimilation. Ocean Dyn. https://doi.org/10.1007/s10236-019-01299-7

Pradhan, H.K., Völker, C., Losa, S.N., Bracher, A., Nerger, L., 2019. Assimilation of Global Total Chlorophyll OC-CCI Data and Its Impact on Individual Phytoplankton Fields. J. Geophys. Res. Oceans 124, 470–490. https://doi.org/10.1029/2018JC014329