Review by Anonymus Referee #2

Review of "Deep chlorophyll maximum and nutricline in the Mediterranean Sea: emerging properties from a multi-platform assimilated biogeochemical model experiment" by Teruzzi et al.

The manuscript addresses the performance of a 3D-Var biogeochemical data assimilation system, constrained with both chlorophyll data from satellite and chlorophyll and nitrate data from BGC-Argo floats, that is applied to a realistic simulation of the Mediterranean Sea for the year 2015. After demonstrating the validity of the method, the authors use their product to investigate the spatial and seasonal variability in the vertical structure of chlorophyll and nitrate fields. The problem is introduced clearly, methodology appears sound, and results are compelling. I recommend the manuscript for publication in Biogeosciences after revisions. Below are a couple of important results that need to be clarified, a list of issues to be addressed, and some minor comments.

We thank the Anonymous Reviewer for the positive comment on our manuscript and the careful reading. All the points raised by the Reviewer are addressed in the following with replies in green italic.

1) Fig 2: With the exception of the "LEV" region, it seems that assimilating only float data yields a better fit with chl obs than assimilating floats + satellite. It seems like it would be best to ignore satellite data, even at the surface. On the other hand (Fig 3), assimilating satellite Chl yields a better fit with nitrate obs, which is counter intuitive, and assimilating float Chl barely has an impact. Please comment!

This Reviewer's comment will help us to clarify some aspects that in the current manuscript version are probably not appropriately presented and discussed:

In Fig. 2, RMSDs are calculated with respect to float chlorophyll. It is not obvious that satellite chlorophyll assimilation would positively affect metrics with respect to float chlorophyll because of erroneous propagation of surface information along the vertical by DA and because of potential inconsistency between satellite and float data. Indeed, we discussed the inconsistency between satellite and float chlorophyll in the Discussion section, where a comparison between values of chlorophyll concentration from satellite and float highlights their differences. Thus, since satellite and BGC-Argo float inconsistency at surface and because vertical covariance is a prescribed propriety, the change in chlorophyll profiles due to satellite assimilation is either to reduce and to increase the distance between modelled chlorophyll and BGC-Argo chlorophyll profiles (Fig. 2). On the other hand, considering RMSDs with respect to satellite chlorophyll (Fig.5), the effect of inconsistency between satellite and float chlorophyll is highlighted by the slight increase in RMSDs in simulations with float chlorophyll assimilation. Thus, we think that the model-assimilation can act as a filter solving inconsistency between sensors, meaning that even if the performance of the multi-platform assimilation is lower than anyone of the single assimilation, it produces a balanced solution with respect to all the available information.

Concerning Fig. 3:

- *With the exception of TYR, the assimilation of satellite chlorophyll reduces the RMSD of nitrate (computed on BGC-Argo data) with respect to REF simulation. This is because satellite assimilation correct surface modelled phytoplankton dynamics continuously during late winter/spring (i.e., reducing bloom maxima), and, as a results the entire profile of the phytoplankton is nearly uniformly modified (i.e., reduced) in the euphotic layer. In turn, by reacting to the new phytoplankton conditions, less nitrogen is eventually re-mineralized to nitrate and nitrate concentration is modified in the direction of reducing the REF overestimation in the upper layer. This mechanism has been investigated in previous applications of satellite chlorophyll assimilation (Teruzzi et al., 2018).*

- *In the case of BGC-Argo chlorophyll assimilation, the changes in the phytoplankton profiles are less uniform (Cossarini et al., 2019), often alternating positive and negative increments along the same profile. The effects on nitrate profiles (through new uptake or release after mortality and exudation) are non-linear and not uniform. It follows that also RMSDs with respect to float nitrate can both decrease or increase with respect to REF. Effects on non-assimilated biogeochemical variables are discussed in a number of works (e.g., Ciavatta et al., 2014; Ford, 2020; Mattern et al., 2017; Santana-Falcón et al., 2020; Simon et al., 2015; Teruzzi et al., 2018; Tsiaras et al., 2017; Yu et al., 2018), where the non-degradation of non-assimilated variables is considered a good result of the assimilation process. In the present manuscript, we briefly discussed the effects of satellite chlorophyll assimilation on nitrate RMSDs (L. 225-228) but we did not summarizes these effects in the Discussion.*

Considering the points highlighted above, we will modify the manuscript adding a paragraph dedicated to the effects on non-assimilated variables. In particular, we will focus on the mixed effects of satellite chlorophyll assimilation, which slightly degrade metrics with respect to float chlorophyll but improves those with respect to float nitrate. In perspective, when the inconsistency between satellite and float will be solved, the multi-platform assimilation will provide improvements over large areas thanks to the relevant spatial coverage of satellite observations. In the meantime, as discussed in the manuscript (and reinforced by new comments) the model, acting as a dynamical filter, effectively integrates both sources of information.

2) L. 242-244, 260-261: In Fig 4 I don't see a reduction in RMSD, but instead an increase in levels 4-6. So data assimilation does reduce the model skill in fitting oxygen? It looks like the pink and red curves are on top of each other, suggesting that satellite Chl is responsible for degrading the O2 solution.

Thanks to this Reviewer's comment on the slight degradation of oxygen solution (Fig. 4), we went carefully through the oxygen validation results. Firstly, we considered a new recently updated dataset of BGC-Argo oxygen measurements available at the Coriolis/Ifremer data assembly centre (float trajectories are shown in Fig. R2). Using the updated oxygen dataset, the recalculated RMSD values (Fig. R3) are lower than in Fig. 4 of the original manuscript, indicating that the simulation better compares with respect to the more recent and possibly more reliable observations. At the same time, RMSDs very slightly differ among simulations, especially in the eastern sub-basins. Moreover, the effect of satellite chlorophyll assimilation is not univocal, since RMSDs are both slightly reduced (TYR) and increased (NWM) . On the other hand, the float assimilation has a very little effect on oxygen RMSDs. The limited and non-univocal effects of the assimilation on oxygen metrics are related to the interaction of a number of trophic processes (e.g., phytoplankton production and respiration, zooplankton and bacteria respiration) after the assimilation changes on phytoplankton biomass. We think that the non-degradation of the oxygen RMSDs is a good result of the assimilated simulations.

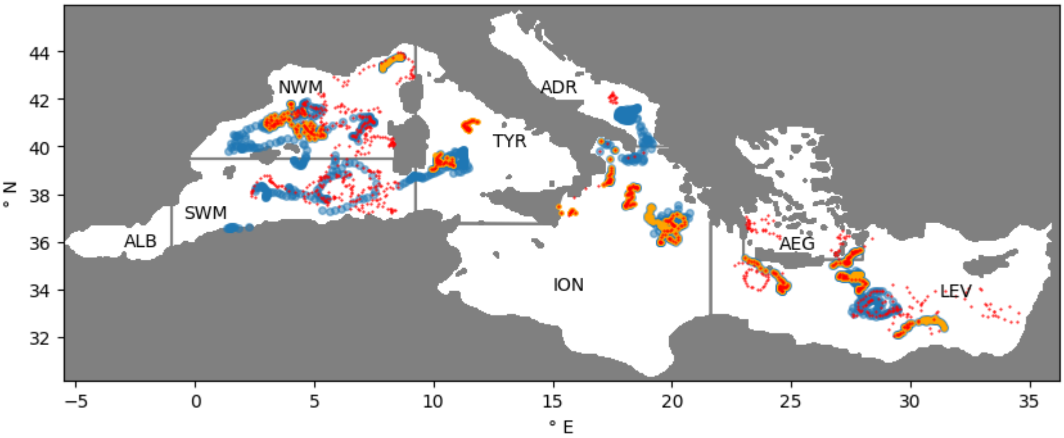

Fig. R2. Positions of BGC-Argo floats equipped with sensors to provide chlorophyll (blue), nitrate (orange) and oxygen (red) and limits of the subbasins.

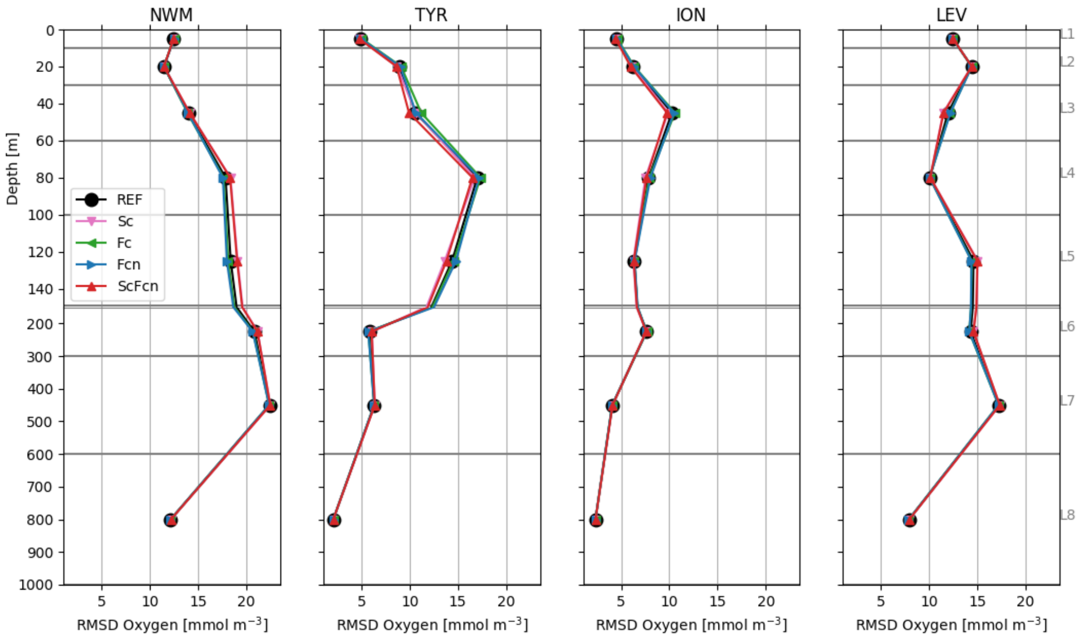

Fig. R3. RMSD between model simulations and BGC-Argo oxygen data in four sub-basins. Grey lines indicate the limits of layers L1-L8 used to calculate the RMSD. The depth scale is different above and below 150 m (double grey line).

We also calculated RMSDs using only oxygen profiles at locations where floats were assimilated (Fig. R4 and R5), thus excluding profiles far from float assimilations. While, oxygen RMSDs are further reduced in this case in the surface layer in NWM and in almost all layers of LEV, differences of RMSDs between simulations are very small also for this dataset and similar to those of Fig. R3.

According to the above considerations, we will update the manuscript introducing metrics based on the updated BGC-Argo oxygen dataset. In particular, Fig. 1 and Fig. 4 will be replaced by Fig. R2 and Fig. R3, respectively. Moreover, we will comment on the slight effect on oxygen in the assimilated simulations, which do not insert degradation on the non-assimilated variable .

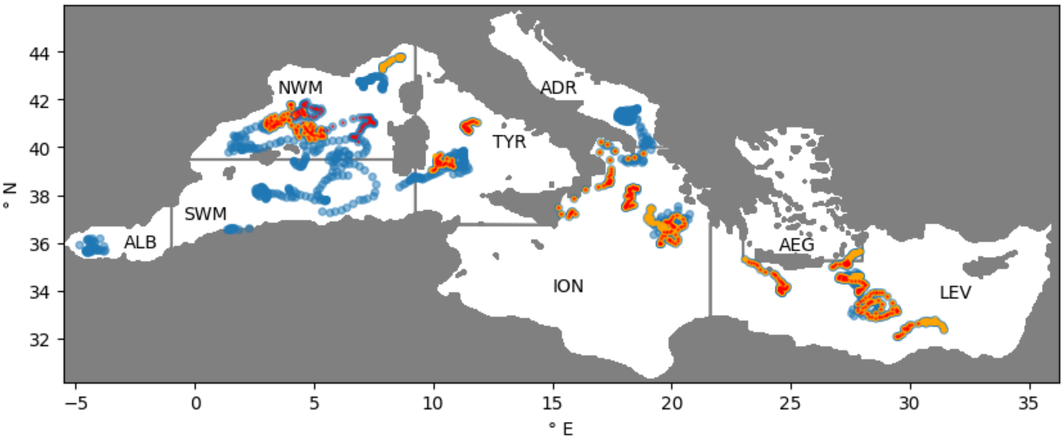

Fig. R4. Positions of BGC-Argo floats equipped with sensors to provide chlorophyll (blue), nitrate (orange) and oxygen (red) and limits of the subbasins. Only oxygen profiles where floats are assimilated are indicated.

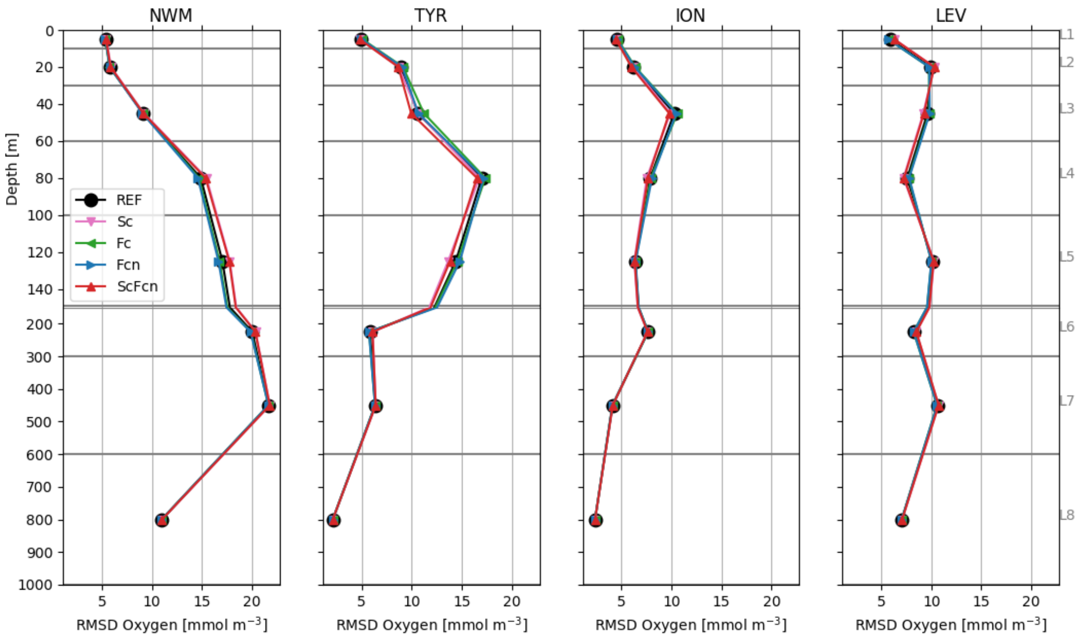

Fig. R5. RMSD between model simulations and BGC-Argo oxygen data in four sub-basins only at locations with float assimilation. Grey lines indicate the limits of layers L1-L8 used to calculate the RMSD. The depth scale is different above and below 150 m (double grey line).

Other comments:

3) Abstract and L. 68: is “semi-independent data” a common way to refer to observations used in model-data comparisons before and after assimilation? I suggest changing “semi-independent data (before assimilation)” to “assimilated data (before and after assimilation)”.

“Semi-independent data” refers to the use for validation of observations before the assimilation. We will change the term in “assimilated data (before the assimilation).

4) When data is excluded from assimilation based on a DA criterion, as stated in L. 98-100, is that a "quality check" on the data? Or is it removing observations that can't be fit because of model inadequacies? Is there a reference for the threshold values (5 mg/m3 for Chl and 1 or 2 mmol/m3 for NO3)? Similarly on L. 87-88 "A further quality check on satellite values before the assimilation resulted in the exclusion satellite chlorophyll observations whose mismatch value with respect to the model was higher than 10 mg m-3." - Is this a check of the quality of the data or a DA-based exclusion criterion?

5) L. 96-97: "chlorophyll profiles were checked for negative values (rejection)" - I imagine that a bias correction is applied to the Chl data, resulting in sometimes negative values at some depths. Does that necessarily mean the profile can't be used? Maybe negative values could be viewed as "zero"?

We thank the Reviewer for these comments . In the revised manuscript we will clarify that two levels of quality check are performed on both satellite and float observations. The first quality check is made on observations independently from data assimilation and is intended to the exclusion of spikes and possible unrealistic values. For satellites, this step consists in "removing observations whose anomalies were higher than 3 times the daily climatology standard deviation" (L. 85-86). Float observations were instead checked with a more complex (and somehow empirical) procedure, indeed, the relative novelty of BGC-Argo data sets release with respect to consolidated procedures adopted in ocean colour data processing may lead to a higher occurrence of poorly reliable observations. In particular: "nitrate profiles were rejected if the surface value was higher than 3 mmol m^{-3}, chlorophyll profiles were checked for negative values (rejection), and quenching correction was performed by imposing a constant chlorophyll value in the mixed layer" (L. 96-98). In this phase, the exclusion of negative values is thus based on the fact that negative concentrations cannot be accepted in the float dataset and on the choice to do not insert any artificial changes on concentrations.. The exclusion of nitrate values higher than 3 mmol m^{-3} in the surface layers is based on the analysis of climatological values provided in the EMODnet dataset (Buga et al., 2018).

The second phase of observation checks is a pre-data-assimilation procedure, intended to exclude values not suitable for assimilation due to the range of variability model-observation differences to be consisted with the assumed uncertainties levels. For satellite, this check consists in the exclusion of "observations whose mismatch value with respect to the model was higher than 10 mg m^{-3}" (L. 89), while for floats the threshold values were set to 5 mg m^{-3} for and 1 or 2 mmol m^{-3} for chlorophyll and nitrate, respectively. These values have been calibrated after a statistical analysis of the distribution of the model-observations mismatches of the REF run. The exclusion based on DA criteria were of the order of 2%, <1% and 3% for satellite chlorophyll and float chlorophyll and nitrate, respectively. In the new version of the manuscript we will explain more clearly that the quality checks are sub-divided in two different phases and we will add information on exclusion occurrences and comment about them.

6) L. 115-116: "3DVarBio is the data assimilation scheme for the correction of phytoplankton functional type and nutrient variables (i.e., nitrate and phosphate)" - It sounds like phytoplankton type is a control variable, which to me suggests that the type can be changed by assimilation. However, I believe you mean that the biomass in each phytoplankton class can be optimized. It would be useful to know how many functional types there are (it's mentioned later, but at this point I was wondering). Also, this is one of a few places where phosphate is mentioned. Why control phosphate and not other bgc variables, like oxygen? Does the model include other nutrients?

The term "phytoplankton functional types" is usually used in multi-phytoplankton multi-nutrient complex model and satellite works (Butenschön et al., 2016; Nair et al., 2008) but we agree that in this contest can be misleading. For sake of clarity, we mention that BFM has 4 PFTs (diatom, picoplankton, nanoflagellates and *dinoflagellates; Lazzari et al., 2012). However, since this information is not relevant at this point, we will re-formulate the sentence: "3DVarBio is the data assimilation scheme for the correction of phytoplankton and nutrient variables (i.e., nitrate and phosphate)". Even if other nutrients are simulated in BFM model, the update of phosphate is a nutrient a key element in the Mediterranean basin, where both nutrients can act as limiting factors of phytoplankton growth (Lazzari et al., 2016) (L. 190). On the other hand, actual silicate concentrations in OGST-BFM applications in the Mediterranean Sea do no lead to limitation conditions, thus we did not applied assimilation update on this variable. Oxygen as well is not a limiting factor for plankton dynamics in our simulations of the Mediterranean Sea biogeochemistry, moreover, since the number of BGC-Argo floats equipped with oxygen sensors, it would be preferable to implement an assimilation scheme directly based on oxygen observations instead of on pre-computed covariance between oxygen and float chlorophyll or nitrate. Indeed, BGC-Argo oxygen assimilation is one of the foreseen update of the OGSTM-BFM system. Finally, it should be considered that the addition of variables in the assimilation scheme would increase its computational costs, compared to relatively small improvements in case of non-limiting nutrients or relatively high uncertainty in the definition of covariance between the assimilated and non-assimilated nutrients.*

In the new version of the manuscript, we will add details on the choice to apply assimilation updates based on nitrate observations to nitrate and phosphate only.

7) Section 2.2 is hard to follow, with so many models and acronyms. I would start by describing MedBFM, then OGSTM and BFM, then 3DVarBio. What does it mean that the transport model is "fully consistent with the off-line coupling of the NEMO3.6 vvl"? On L. 135 the "MENO3.4-OceanVar model" is mentioned: should it be NEMO? If so, why mention NEMO3.6 earlier when you're using version 3.4?

We will follow the Reviewer suggestions and we will modify Section 2.2. Concerning NEMO version we will correct the versioning: we used NEMO3.6 with the vvl configuration and z. Indeed the OGSTM transport model resolves the advection and diffusion of tracers and works with the same variable volume layer and z* configuration of NEMO conserving the continuity of the mass transport.*

8) L. 141-145: What does it mean for climatological profiles to "integrate" data? Is it different from initializing a model from data and spinning it up for a couple years? What is a "Newtonian dumping term"?

We were meaning that the initial conditions were calculated using data from EMODnet and those from Lazzari et al. (2016) and Cossarini et al. (2016). After initializing the model with these initial conditions, we let the model spin up for a couple of year, as the Reviewer pointed out. We will rephrase the sentence to make this point clearer.

The Newtonian dumping term is explained in Lazzari et al., 2010, and refers to the treatment of biogeochemical variable concentrations at boundaries. Since it is not relevant to detail this aspect in the manuscript, we will modify the sentence avoiding to refer to the Newtonian dumping: "In the Atlantic buffer zone (i.e., the area to the west of the Strait of Gibraltar) tracer concentrations were relaxed to climatological seasonally varying profiles. Seasonal profiles of phosphate, nitrate, silicate, and dissolved oxygen were derived from an analysis of the climatological World Ocean Atlas 2018 data (Garcia et al., 2019) and the EMODnet_int dataset".

9) L. 145: Tracer concentrations need to be relaxed to climatology even though the simulation is only 1-year long? Is that typical for the Med Sea?

Any relaxation of tracer concentration is done in the model domain. This refer only on the Atlantic boundary, that has a buffer zone of 2 degrees in longitude (between 9W to 7W) to have stable boundary effects. Thus, *tracer concentrations are relaxed in the Atlantic buffer zone only, as the change proposed in the answer 8 will clarify.*

10) Comment on the fact that RMSD increases at the surface in TYR when only satellite chlorophyll is assimilated?

Manuscript changes according to your comment 1) will add comments also on this aspect.

11) L. 281: What is the significance of the 0.3 value?

We decided on this threshold after testing on other values, since it highlights the effect on the vertical profile in Fig. 7. Moreover, using other threshold values would not relevantly modify the shape of profiles of Fig. 7 but only intensify or weaken the differences between REF and ScFcn simulation profiles.

12) Fig 7: Why does the y-axis stop at 300m? There is a large change at 300m in summer, TYR. Caption: “5 left panels” should be “5 right panels”. It would be helpful to label figures panels “a”, “b”, “c”, etc. Why are some panels empty?

We decided to limit the profiles to 300 m to better focus on the assimilation impact in the euphotic zone were biogeochemical processes are more rapid and intense. Moreover, differences between REF and ScFcn of Fig. 7 propagate nearly constantly until 500 m and then tend to vanish between 500 and 600 m (Fig. R#). We will add a comment on the impact below 300 m in the next version of the manuscript but we prefer to keep the limit to 300 m in the manuscript Fig. 7 to highlight the assimilation effects in the euphotic zone.

We will correct “5 left panels” to “5 right panels” and add label to figures.

Some panels are empty since not all the sub-basins have areas with I(t) higher than 0.3 during winter.

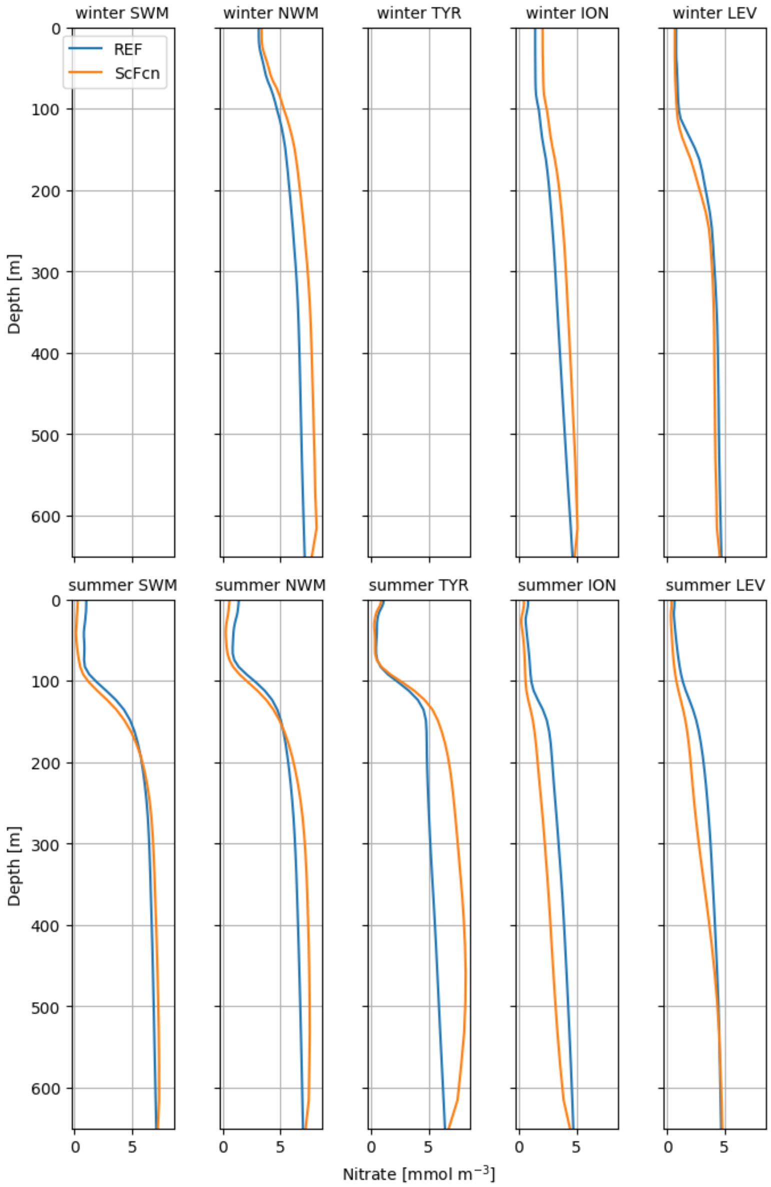

Fig. R#. Mean profiles at time and location with $I(t)$ higher than 0.3 in five sub-basins for the ScFcn and REF simulations in winter (top panels) and summer (bottom panels).

13) L. 429-430: The results are consistent with previous studies. Can you elaborate on whether the results are quantitatively different? Or do they simply agree with previously known features of the Med Sea?

Our results on DCM features are quantitatively consistent with previous studies as discussed at L. 322-324 ("Consistent with previous findings (Lavigne et al., 2013; Lazzari et al., 2012; Mignot et al., 2014), the simulated DCM depth exhibited a west-east gradient (Fig. 8) ranging from nearly 80 m in the western basins to values higher than 100 m in the eastern basins"). Moreover, we discussed differences of nutricline depth with respect to the findings of Barbieux et al. (2019). The added values of our results consists mainly in the capability to provide a full 3D validated descriptions of a number of features of the Mediterranean Sea DCM. We will further stress on this aspect in the new version of the manuscript.

Minor comments:

- L. 84-86: “Original products […] were reviewed for spikes excluding observations whose anomalies were higher than 3 times the daily climatology standard deviation” - The sentence is not clear. Maybe rephrase to “In the original products […] observations whose anomalies were higher than 3 times the daily climatology standard deviation were excluded in order to remove spikes”.

We will rephrase the sentence according to the Reviewer’s suggestion.

- L. 122-123: Is it only the optical model this is not included in the present application (but the other 2 are)? Why isn’t it included?

Among the improvements listed at L. 122-123, the optical model only is not included in the present application since the development of BGC-Argo assimilation was carried out in a separated branch of the model. However, it is foreseen that the two model branches will converge in the near future. We will remove the reference to the optical model from the sentence since it is not applied in this work.

- Fig 2: The gray lines hard to see; I suggest removing other grid lines.

We will remove the other horizontal grid lines in the figure (as in Fig. R3).

- L. 286 p5th = 95th?

- L. 384-385: “Maintaining the diagonal the observation error covariance matrix” - remove second “the”?

- L. 393: “Thus, while it is desirable an increase of nitrate sensors number” - should be “while it is desirable to increase the number of nitrate sensors”?

- The Verdy and Mazloff reference is missing from the bibliography.

We will correct all the four previous typos as suggested by the Reviewer.

References

Barbieux, M., Uitz, J., Gentili, B., Pasqueron de Fommervault, O., Mignot, A., Poteau, A., Schmechtig, C., Taillandier, V., Leymarie, E., Penkerc’h, C., D’Ortenzio, F., Claustre, H., Bricaud, A., 2019. Bio-optical characterization of subsurface chlorophyll maxima in the Mediterranean Sea from a Biogeochemical-Argo float database. Biogeosciences 16, 1321–1342. https://doi.org/10.5194/bg-16-1321-2019

Buga, L., Sarbu, G., Fryberg, L., Magnus, W., Wesslander, K., Gatti, J., Leroy, D., Iona, S., Larsen, M., Koefoed Rømer, J., Østrem, A.K., Lipizer, M., Giorgietti, A., 2018. EMODnet Chemistry Eutrophication and Acidity aggregated datasets v2018. https://doi.org/10.6092/EC8207EF-ED81-4EE5-BF48-E26FF16BF02E

Butenschön, M., Clark, J., Aldridge, J.N., Allen, J.I., Artioli, Y., Blackford, J., Bruggeman, J., Cazenave, P., Ciavatta, S., Kay, S., Lessin, G., van Leeuwen, S., van der Molen, J., de Mora, L., Polimene, L., Sailley, S., Stephens, N., Torres, R., 2016. ERSEM 15.06: a generic model for marine biogeochemistry and the ecosystem dynamics of the lower trophic levels. Geosci. Model Dev. 9, 1293–1339. https://doi.org/10.5194/gmd-9-1293-2016

Ciavatta, S., Torres, R., Martinez-Vicente, V., Smyth, T., Dall’Olmo, G., Polimene, L., Allen, J.I., 2014. Assimilation of remotely-sensed optical properties to improve marine biogeochemistry modelling. Prog. Oceanogr. 127, 74–95. https://doi.org/10.1016/j.pocean.2014.06.002

Cossarini, G., Mariotti, L., Feudale, L., Mignot, A., Salon, S., Taillandier, V., Teruzzi, A., D’Ortenzio, F., 2019. Towards operational 3D-Var assimilation of chlorophyll Biogeochemical-Argo float data into a

biogeochemical model of the Mediterranean Sea. Ocean Model. 133, 112–128. https://doi.org/10.1016/j.ocemod.2018.11.005
Ford, D.A., 2020. Assessing the role and consistency of satellite observation products in global physical–biogeochemical ocean reanalysis. Ocean Sci. 16, 875–893. https://doi.org/10.5194/os-16-875-2020
Lavigne, H., D'Ortenzio, F., Migon, C., Claustre, H., Testor, P., d'Alcalà, M.R., Lavezza, R., Houpert, L., Prieur, L., 2013. Enhancing the comprehension of mixed layer depth control on the Mediterranean phytoplankton phenology. J. Geophys. Res. Oceans 118, 3416–3430. https://doi.org/10.1002/jgrc.20251
Lazzari, P., Solidoro, C., Ibello, V., Salon, S., Teruzzi, A., Béranger, K., Colella, S., Crise, A., 2012. Seasonal and inter-annual variability of plankton chlorophyll and primary production in the Mediterranean Sea: a modelling approach. Biogeosciences 9, 217–233. https://doi.org/10.5194/bg-9-217-2012
Lazzari, P., Solidoro, C., Salon, S., Bolzon, G., 2016. Spatial variability of phosphate and nitrate in the Mediterranean Sea: A modeling approach. Deep Sea Res. Part Oceanogr. Res. 108, 39–52. https://doi.org/10.1016/j.dsr.2015.12.006
Mattern, J.P., Song, H., Edwards, C.A., Moore, A.M., Fiechter, J., 2017. Data assimilation of physical and chlorophyll a observations in the California Current System using two biogeochemical models. Ocean Model. 109, 55–71. https://doi.org/10.1016/j.ocemod.2016.12.002
Mignot, A., Claustre, H., Uitz, J., Poteau, A., D'Ortenzio, F., Xing, X., 2014. Understanding the seasonal dynamics of phytoplankton biomass and the deep chlorophyll maximum in oligotrophic environments: A Bio-Argo float investigation. Glob. Biogeochem. Cycles 28, 856–876. https://doi.org/10.1002/2013GB004781
Nair, A., Sathyendranath, S., Platt, T., Morales, J., Stuart, V., Forget, M.-H., Devred, E., Bouman, H., 2008. Remote sensing of phytoplankton functional types. Remote Sens. Environ., Earth Observations for Marine and Coastal Biodiversity and Ecosystems Special Issue 112, 3366–3375. https://doi.org/10.1016/j.rse.2008.01.021
Santana-Falcón, Y., Brasseur, P., Brankart, J.M., Garnier, F., 2020. Assimilation of chlorophyll data into a stochastic ensemble simulation for the North Atlantic Ocean. Ocean Sci. 16, 1297–1315. https://doi.org/10.5194/os-16-1297-2020
Simon, E., Samuelsen, A., Bertino, L., Mouysset, S., 2015. Experiences in multiyear combined state–parameter estimation with an ecosystem model of the North Atlantic and Arctic Oceans using the Ensemble Kalman Filter. J. Mar. Syst. 152, 1–17. https://doi.org/10.1016/j.jmarsys.2015.07.004
Teruzzi, A., Bolzon, G., Salon, S., Lazzari, P., Solidoro, C., Cossarini, G., 2018. Assimilation of coastal and open sea biogeochemical data to improve phytoplankton simulation in the Mediterranean Sea. Ocean Model. 132, 46–60. https://doi.org/10.1016/j.ocemod.2018.09.007
Tsiaras, K.P., Hoteit, I., Kalaroni, S., Petihakis, G., Triantafyllou, G., 2017. A hybrid ensemble-OI Kalman filter for efficient data assimilation into a 3-D biogeochemical model of the Mediterranean. Ocean Dyn. 67, 673–690. https://doi.org/10.1007/s10236-017-1050-7
Yu, L., Fennel, K., Bertino, L., Gharamti, M.E., Thompson, K.R., 2018. Insights on multivariate updates of physical and biogeochemical ocean variables using an Ensemble Kalman Filter and an idealized model of upwelling. Ocean Model. 126, 13–28. https://doi.org/10.1016/j.ocemod.2018.04.005