Reviewer 3

We thank the reviewer for his suggestions, which helped making this version of the manuscript much clearer. Questions were clarified below, following the structure of the reviewer's reply, whereas the modifications of the manuscript can be tracked in **green**.

Major Comments

While this research is definitely useful, in many places I struggled to understand what exactly the authors were doing. In particular, in Section 2.3 they list 6 different models that they test, comparing measured downwelling irradiance with that derived from different models following Eq. 1-12. Their first model is pure water absorption and scattering, for which they test three different estimates of a_w (Fig. 3). It wasn't clear to me what downwelling irradiance observations they used to test the different a_w. From the text, it seems like they compared actual profiles of Ed to estimated profiles of Ed assuming clear water, but that doesn't make any sense. Did they only use BGC-Argo profiles in very clear waters, and if so, how did they define that? Or did they have a "basic" version of the other IOPs that they used in Eq. 1-12, in which case, what was it, and how does it differ from experiment 6? I have a similar question for experiments 2-5; from the text it seems like the authors assume the only constituents are those specifically tested, but that doesn't make sense unless you have measurement profiles for which that might be true. I'm sure I am missing something here.

The aim of this work , especially of the first part, i.e. when assessing each of the inherent optical properties (IOPs: absorption and scattering coefficients), was not to simulate reality, but rather to quantify the model performance with different configurations. When we test only pure water, that doesn't mean that we are implying that it's a scenario which is seen in nature. We are simply looking at the relative improvement/deterioration of the model performance. So, what happens if we include temperature and salinity? What happens if we update the pure water absorption model by more recent measurements? Same procedure with CDOM, NAP, phytoplankton, and particle (back)scattering. The scope of the chosen method, i.e. activating one IOP at the time, was twofold: first, as explained above, to choose a model which within that same optically significant material (OSM) gives you the highest skill (as well as assess the relative improvement/deterioration), and second, to quantify the impact each of the model range has at each of the tested wavelengths. It was therefore not aimed at saying that this is close to a realistic in-water propagation, but rather try to see how much does each of the OSM contribute to the relative improvement compared to the base. For example: how much only the inclusion of CDOM at specific wavelengths contributed to the light absorption versus NAP? What's the impact of different vertical shapes, e..g. Chl versus $b_{bp(700)}$ in case of NAP simulations? It enabled us to have a clearer picture on how much each of the OSMs absorbs/scatters light at a specific wavelength and their importance in terms of the relative contribution.

Another point of confusion was how the authors use estimates of Chl from BGC-Argo. BGC-Argo floats do not measure Chl, they measure fluorescence from Chl (fChl). During the daytime, near the surface fChl can be reduced even though Chl is still elevated because of non-photochemical quenching (NPQ). There are a number of methods to correct for this, including specifically for BGC-Argo (e.g., Xing et al., 2018). Was any sort of NPQ correction applied to the fChl data? If not, I would be worried that the authors' "Case I models" are tracking fChl and not Chl.

Indeed, you are right in underlining that the floats measure fluorescence, and this was properly accounted for by both converting it to Chl, as well as correcting the NPQ by following the official protocols. We clarified this point in the updated text (please see the 2.1 Section, 2nd paragraph - you can track the changes based on your suggestions in **green**). The protocols are available also online: `https://archimer.ifremer.fr/doc/00243/35385/`, and the official protocol follows the NPQ correction based on Xing et al. [2012] . The fluorescence-to-Chl conversion factor follows Roesler et al. [2017] and it's also written in the protocol (i.e. with an average value of 2). The values of the conversion factors for the the Mediterranean Sea are however between 1.6±0.3 and 1.7±0.2, thus we checked also the model sensitivity by modifying the obtained Chl accordingly. We achieved this by multiplying the profile by xCHL = $\frac{MeanF}{MedF}$, where $MeanF = 2$ and $MedF$ is between 1.3 and 1.9. This would result in xCHL range between 1.05 and 1.45. However, it didn't result in a major change in the simulation outputs and was hence not shown in the manuscript.

Finally, I was uncertain about how to interpret Figures 8-10 in light of the text on l. 254-256 and 332. Are the satellite values shown monthly climatological values? If so, I don't see how these can be compared with Argo considering the time frames and spatial locations are different (that is, Argo doesn't sample uniformly and because of cloud cover neither does the satellite, and they also have different temporal weights based on the different lifetimes of the satellites and Argo floats).

What you're saying would make perfect sense in case we compared radiometric measurements, i.e. irradiance values, which strongly depend on the external environment (solar zenith angle, also waves, wind, clouds of course.). We are, however, comparing apparent optical properties or AOPs (K_d and R_{rs}) which are related to absorption and scattering properties, and thus convey more about the biogeochemical state of the water column. By taking depth derivatives of irradiances, or their ratios, we are able to constrain the influence of the external environment and get a good link to IOPs. This was a justification to spatio-temporally aggregate values to monthly climatologies in terms of K_d and R_{rs}, divided to west and east, which as in published literature display different trophic regimes (e.g. see Terzić et al. [2019] and references therein or other papers). The number of floats in the Mediterranean Sea is clearly sufficient to be able to do this kind of aggregation.

Figures in general: I recommend removing Figures 1 and the top panel of 2 (see comment below), and moving the information in Figures 3-6 into a single Table, after removing experiments that don't make sense to include (see comments below). What would be more useful to see in a Figure would be some representative profiles of measured Chl, b_{bp}, E_d, and modeled E_d,. Instead of Figure 7, what would be more useful to see would be the regionality or where the measurements are close to or far away from the 1:1 line with the model.

Thank you, this is indeed very helpful to visualize better the results. We added a chart, and kept the bar plots as well. We followed all suggestions relative to the plotting of one example, shown in Fig.1 and Fig.2 below. Both report modeled E_d values in red, whereas in-situ measured E_d profiles are in black.

As regards the suggestion to add more colors Figure 7 to account for the regionalization of the skill, we divided it into west and east and observed no different trends for any of the simulations. In Fig.3 we show the scatter plot of the final modelling configuration, i.e. the one comprised of all IOP groups: a_{NAP} with $b_{bp}(700)$ vertical shape, a_{CDOM} following fDOM, a_{ϕ} with Chl and b_p following $b_{bp}(700)$. The number of points is also too high as we plot all 150 meters (or less in case irradiance attenuates before) of all (more than) 1000 profiles.

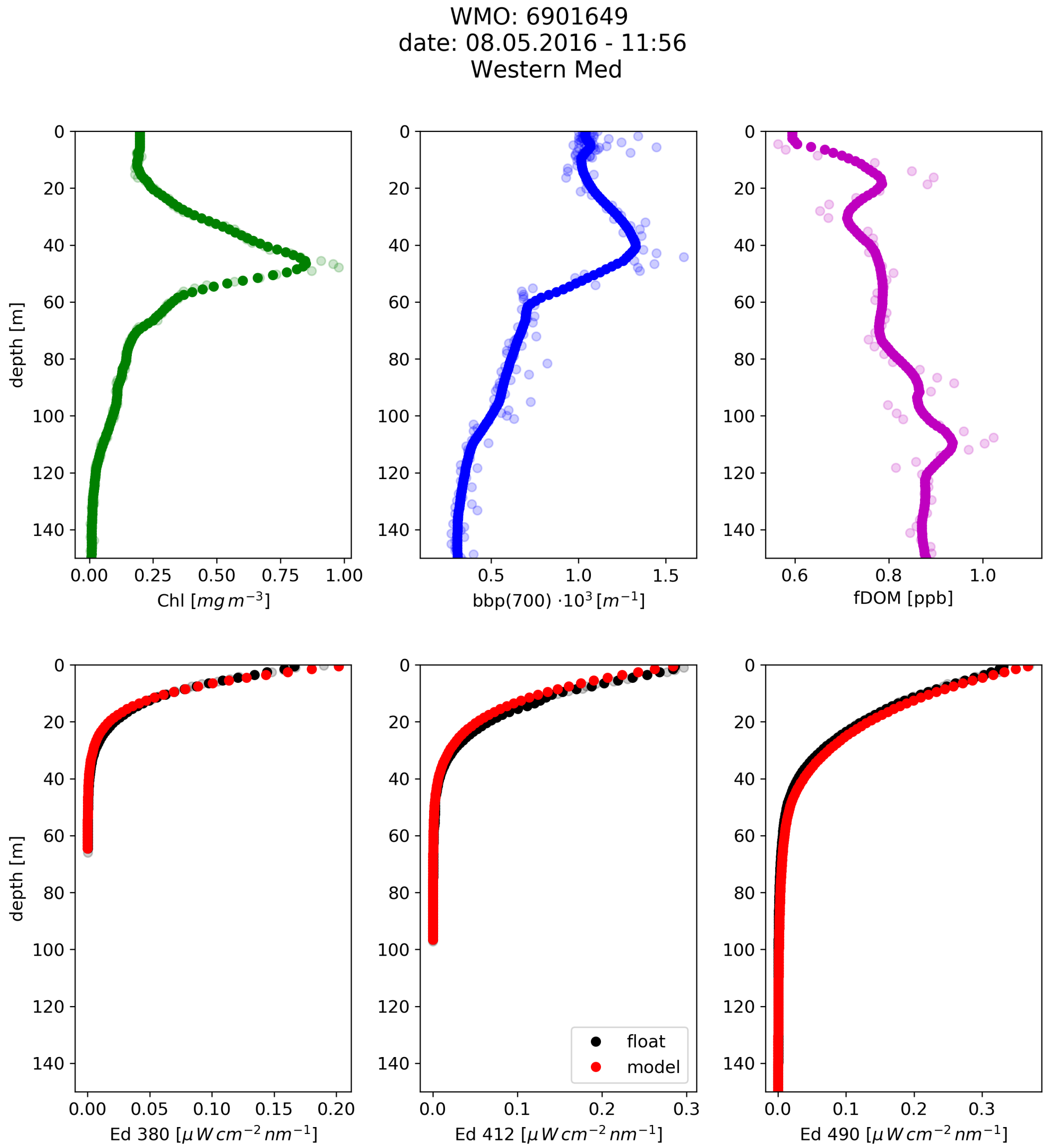

Figure 1: Example of a BGC-Argo profile in the Western Mediterranean with modelled and measured radiometric values. Pale dots are values prior the QC applied to this study (running mean and median filter).

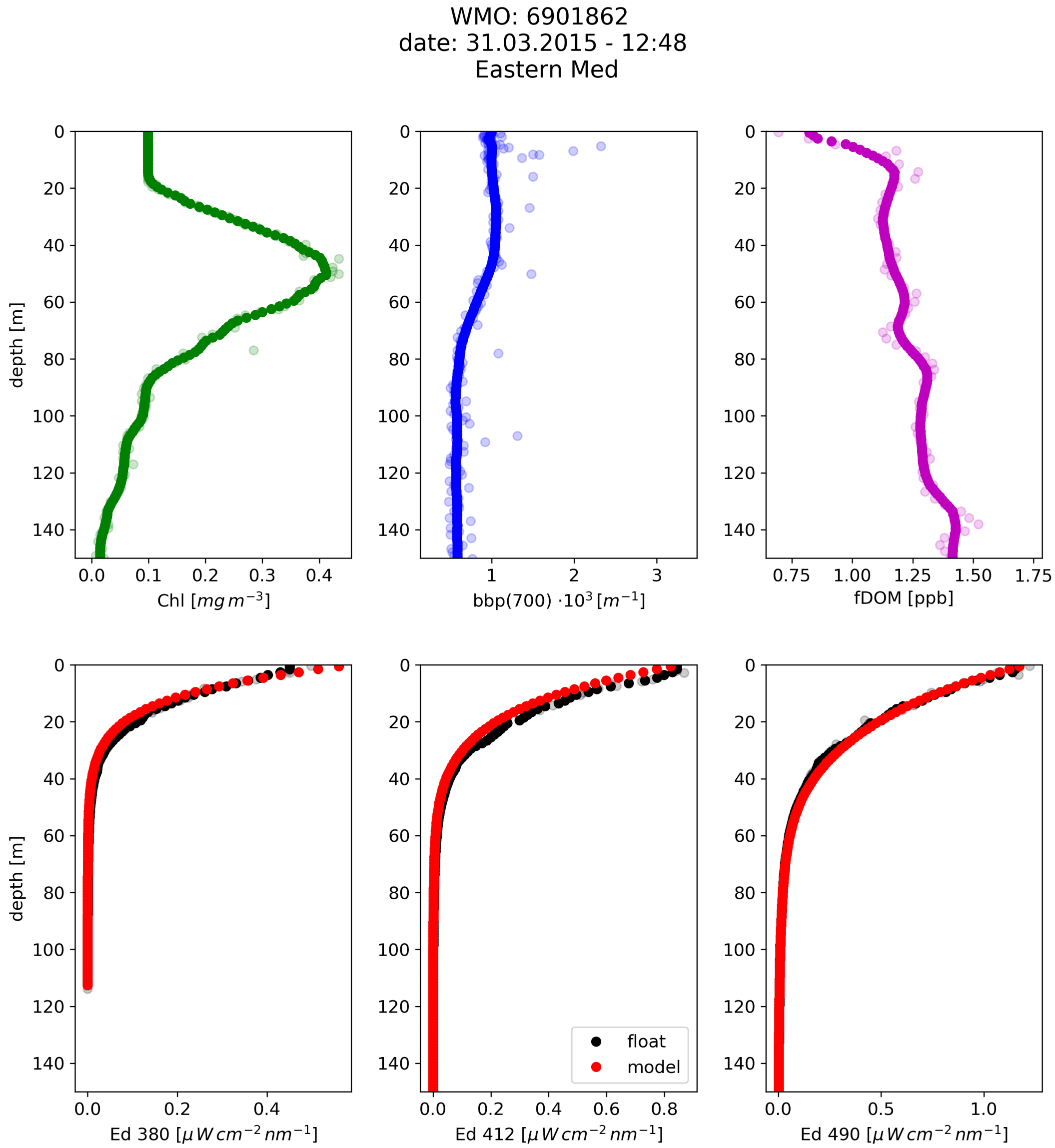

Figure 2: Example of a BGC-Argo profile in the Eastern Mediterranean with modelled and measured radiometric values. Pale dots are values prior the QC applied to this study (running mean and median filter).

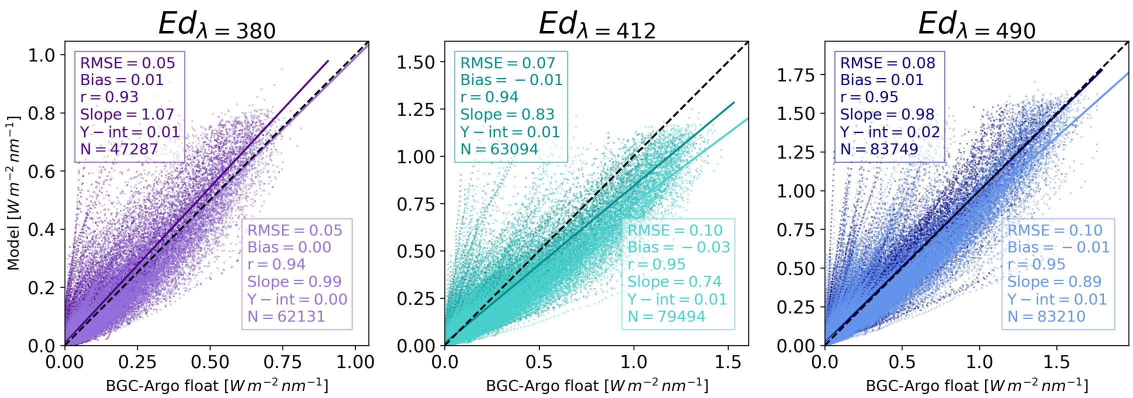

Figure 3: Scatter plot of the final modelling configuration, including all IOPs: within each panel, lighter colors represent Eastern and darker colors the Western Mediterranean.

Conclusions Section in general: A lot the text in the Conclusions does not logically follow from the results of this paper. For example, I don't see a clear path between this paper and combining oxygen, nitrate, and pH in numerical models (l. 412-417), and I'm not convinced that this paper in particular demonstrates the need for inclusion of multi-spectral measurements (l. 423-424) or hyperspectral models (425-427). To be clear, I don't necessarily disagree with any of these statements, I just don't think these are conclusions or logical next steps that one would arrive at from reading this paper. reply point-by-point.

Perhaps we weren't clear enough and will rewrite the text accordingly. The pattern between this paper and other biogeochemical variables lies in the fact that by coupling this kind of optical model with a proper biogeochemical modelling configuration could further support the use of additional variables, such as pH, oxygen, nitrates, as additional inputs and/or validation parameters. The advantage of multi- or even hyper-spectral measurements lies precisely in the findings of this work: the inclusion of light's spectral nature instead of working with PAR (photosynthetically available radiation - integrated light in the visible) enables to get a further grasp on the biogeochemical state of the water. Similarly as in remote sensing, exploiting different wavelengths or bands enables us to obtain more information on biogeochemical features, e.g. distinguishing different algal groups, obtaining more information on the dissolved organic matter pool, suspended matter etc.

Smaller Comments

I don't think it is useful to show how many BGC-Argo profiles didn't have the right set of measurements at the right depths to do this analysis. If profiles were discarded because of data quality (rather than data availability) that could be useful to know – e.g., "a condition of less than 30% difference between modelled and computed Ed values was thus added which resulted in 147 profiles less" (l. 77-78), although I don't quite understand what this means – but right now Figure 1 and the top panel of Figure 2 don't add anything to the paper.

Thank you for the suggestion, we removed the figures and modified the remaining one accordingly. As regards the additional conditions: the existent quality-control procedure for radiometric quantities still keeps noisy behaviour, which resulted in profiles for which it was difficult to obtain sensible values of K_d . For this reason we needed to discard them *a-posteriori* by adding a few criteria. One condition demanded values present also near the surface, and the other limited the maximum divergence of K_d-calculated and measured E_d values. The former was chosen for the main reason that we are mostly interested in profiles which have as many near-surface measurements, as we're later linking them with remote sensing quantities. If we saw that the profile had removed all 5 values in the first 1 m (Argo has a 0.20m frequency for the first 1 m in terms of radiometry), we got suspicious of the overall quality of the profile, even though it passed as "good" in terms of the standard QC. The latter criterion is on the other hand explained by the noisy profiles which generated dubious values of K_d. When calculating K_d values, the absence of a sufficient number of points close to surface depths resulted in a lower performance of the curve fit. For better clarity, we attach two examples of dubious profiles which passed the official radiometric QC procedure, Fig.4 and Fig.5. In the first figure, the shape of E_d at 412 nm caused problems in calculating K_d due to constant values from the surface to almost 10 m depth. The second plot has two different issues: a spike at 412 nm with increasing values, which was somewhat removed with an additional QC (running mean and median filters), whereas at 490 nm there seem to be constant values at the first 10 meters which like in the first example caused issues in computing the depth derivative.

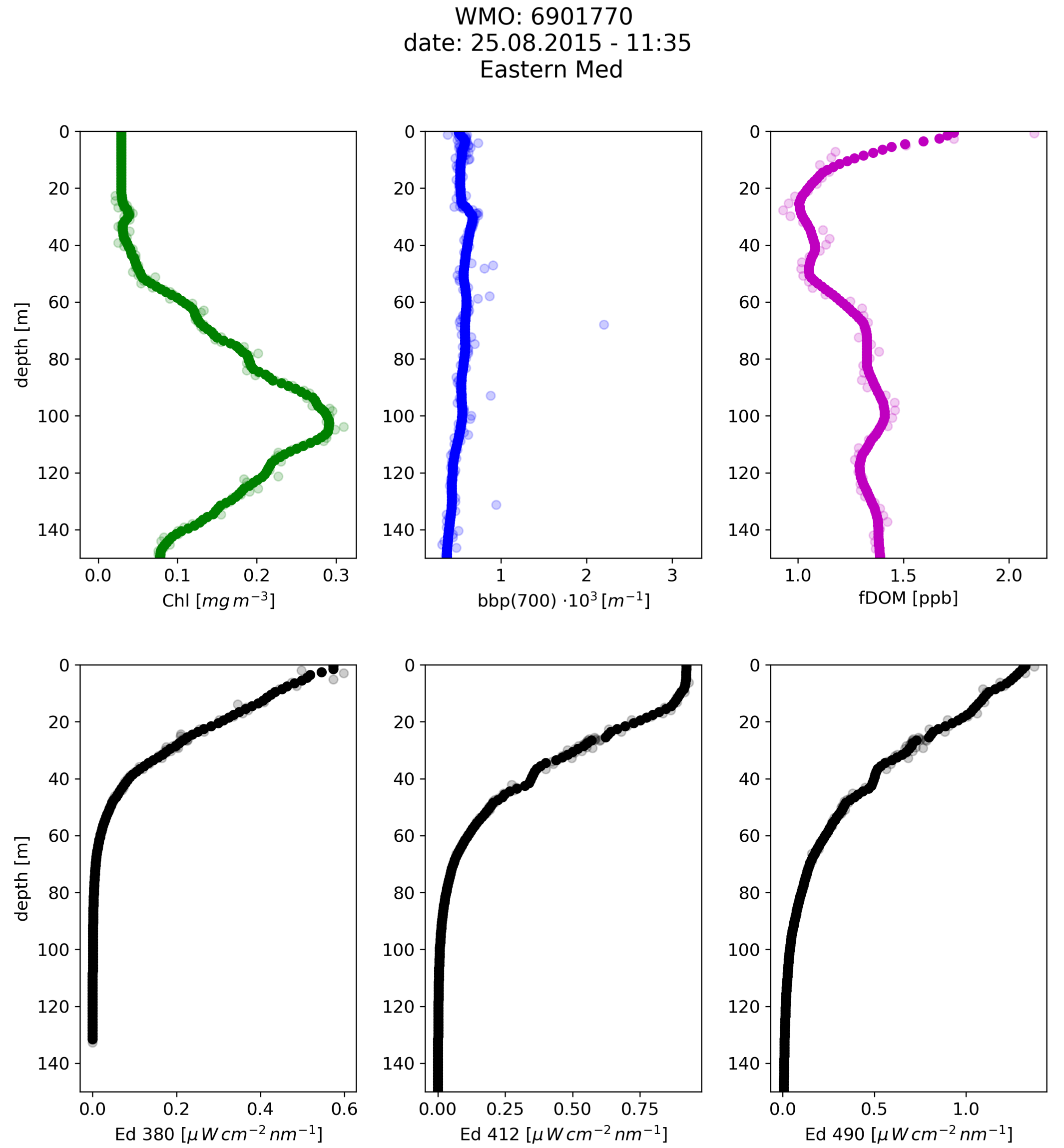

Figure 4: Example of a BGC-Argo profile in the Eastern Mediterranean with radiometric values that caused issues in obtaining K_d and was therefore discarded. Pale dots are values prior the QC applied to this study (running mean and median filter).

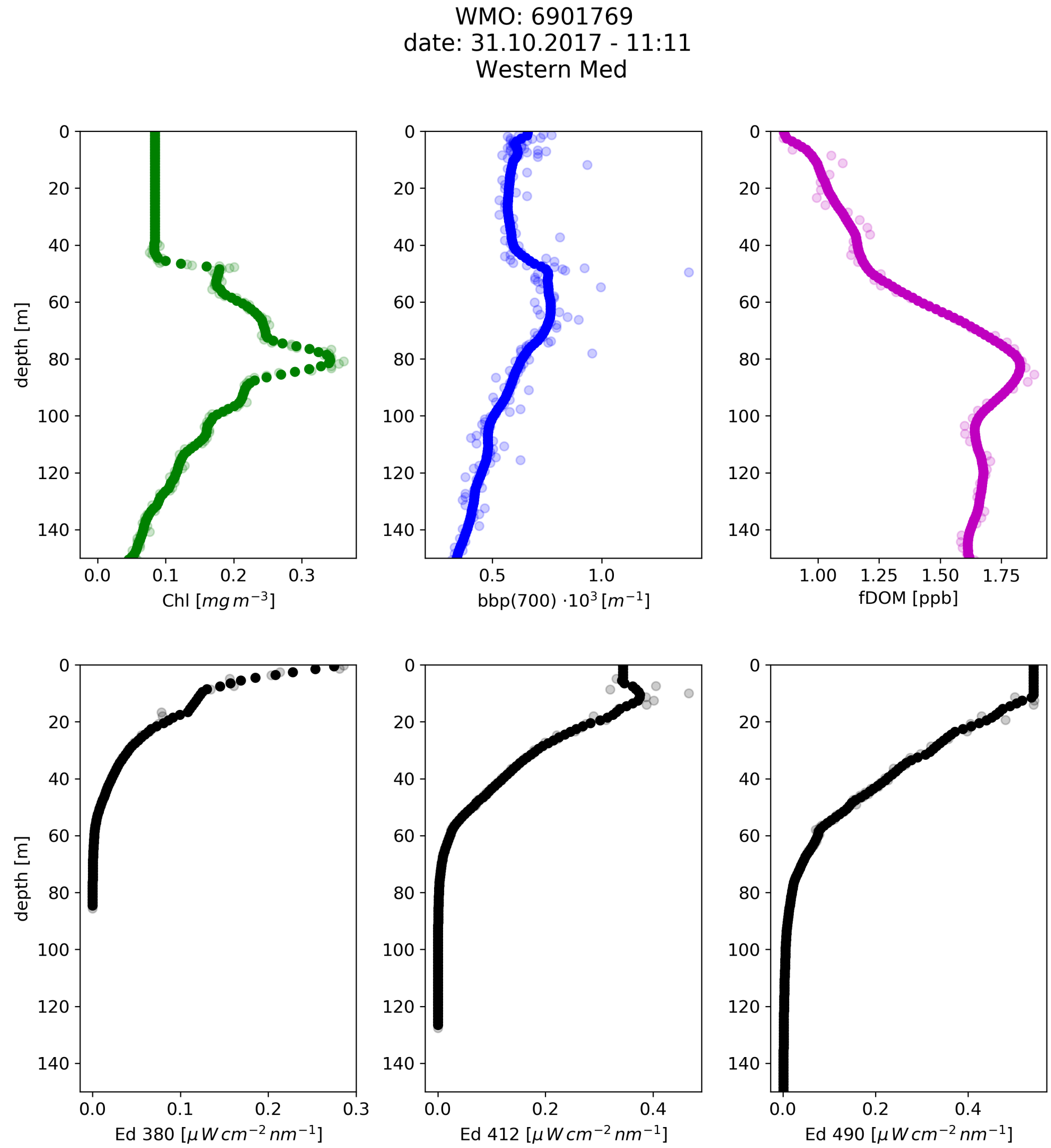

Figure 5: Example of a BGC-Argo profile in the Western Mediterranean with radiometric values that caused issues in obtaining K_d and was therefore discarded. Pale dots are values prior the QC applied to this study (running mean and median filter).

Sec. 2.2 could use more textual help for the equations – make sure to define variables in the same paragraph where they first appear and provide text to explain the equations. Also, when denoting variables associated with direct downward irradiance sometimes a subscript of "dir" is used (e.g., E_{dir}) and sometimes "d" (e.g., C_d); please pick one. Similarly for "dif" and "s". Please also check in this section and throughout to make sure b and b_p mean scattering, and b_b and b_{bp} mean backscattering, and that variable dependencies are correct (e.g., a_w doesn't depend on z).

We made sure to follow all suggestions in the updated version of the manuscript. Thank you.

l. 125: Define PFT.

We renamed it simply to phytoplankton and described PFT in Section 2.3.4.

The text around Eq. 13 is confusing; I don't think this equation is actually helpful. The authors can just say in the text in Sections 2.3.3 and 2.3.4 that profiles either follow Chl, b_bp, or fDOM.

Thank you, we will modify the part accordingly.

l. 141-142: I am confused by the statement that AOPs "to a certain extent remove the impact of the external environment's variability"; by definition, AOPs are properties that depend on these external parameters.

They do, but they are able to convey more the biogeochemical properties of a water body. By taking depth derivatives or ratios, we get properties which can **limit** the influence of the external environment. For example, in the Ocean Optics Web Book, chapter Apparent Optical Properties [1] : "Apparent optical properties are those properties that (1) depend both on the medium (the IOPs) and on the geometric (directional) structure of the radiance distribution, and that (2) display enough regular features and stability to be useful descriptors of a water body." By being ratios or depth derivatives (R_{rs} and K_d respectively), the discussion that follows in the text demonstrates that the influence of the external environment is limited, thus justifying their use to link them with IOPs with great confidence.

Sec. 2.3: I found some of this section backwards – the text in l. 194-195 would be nice to have before the authors explain the text around Eq. 16. Also, considering the authors have chosen to use Mason et al. [2016] instead of Pope and Fry [1997], why show the test with the Pope and Fry-derived values at all? Similarly, in Fig. 5, why show the values without the T/S correction for a_w?

Pope and Fry [1997] still remains the most widely used pure water absorption model. We kept both to assess the difference in the models' performances. We are not trying to suggest that one is "better" than the other. As already discussed with one of the reviewers, in the IOCCG protocol on IOP measurements [2], the Addendum on page 3 on top says that "A recent study by Mason et al. [2016] includes measurements of absorption in this spectral range". We chose this one as a reference in subsequent simulations due to the fact that is more recent, assuming that the latest technology development enabled more accurate spectral measurements.

l. 229-230: If the estimated variability in this backscattering spectral power-law slope parameter is from 0-4, using a constant value of 2 seems overly simplistic. Some discussion about error and uncertainty as a result of this would be good to include.

Of course, you're right in saying that taking a constant value is overly simplistic, but at present we don't have a sophisticated scattering model, which would link the slope values with a biogeochemical configuration that would account for varying particle size distributions (PSD), be it for phytoplankton or inorganic matter. The chosen configuration with a slope of 3 is however consistent with the range of values from reaching best agreement for the Eastern Mediterranean. Exceptions are seen during summer months, when the most adequate slope amounts to 4, and for the west, where modelled and observed values align better with a slope of 2. This result suggests that there are different scattering regimes in play in the two basins, most likely stemming from a different particle size distribution. Lower slope values imply larger particles, which is consistent with the results in the west during usual spring bloom events with larger, microphytoplankton assemblages. On the other hand, higher slope values could suggest smaller particles, consistent with the pico- or nanophytoplankton assemblages usually predominant at the basin level, with

[1] `https://www.oceanopticsbook.info/view/overview-optical-oceanography/apparent-optical-properties`

[2] `https://ioccg.org/wp-content/uploads/2020/09/absorption_protocol_final-incl-cover_rev.pdf`

the former prevailing especially during spring/summer and the latter during winter. Such conclusions are in line with the literature, as shown in Section 3.2. Still, the authors are aware that the selection of the proper scattering model proves to be the weakest point of the paper. As already pointed out in the text, with the lack of in-situ L_u measurements we are certainly not in the position to quantify the skill of different scattering models as thoroughly as we could assess the skill of absorption models that were evaluated both in terms of in-situ E_d and in-situ and remote sensing K_d values. Changing b_{bp} models didn't result in major changes in K_d values, so R_{rs} was the only AOP available for the model skill validation. This could be properly tackled by including instruments with radiometric upgrades, such as ProVal, and also by upgrading the three-stream radiative transfer model to a full one as Hydrolight.

l. 233: What final value of the backscattering ratio was used? What error and uncertainty is the result?

We tested the range of values as reported in the manuscript that followed the range in the literature, i.e. between 0.2 and 1.5% (see 2.3.5., last sentence).

As explained above, the choice of the proper backscattering ratio was more qualitative rather than quantitative, as the only metric left for assessing the model performance in terms of scattering models was R_{rs}.

l. 336-337: The authors could be more explicit about what the two K_d estimates actually are here (both are float-derived). There should also be more discussion somewhere – why might IOPs be overestimated?

K_d values from the model are the depth derivatives of E_d profiles obtained from the radiative transfer model, depending on the choice of IOPs. K_d from floats are the only ones that are actually float-derived, i.e. derived from radiometry itself. In the model we use only Chl, fDOM or $b_{bp}(700)$ data for IOP parameterization, so there is no variable overlapping in terms of different metrics, be it for initialization (Chl, fDOM or $b_{bp}(700)$ for IOPs) or model validation (irradiance profiles and irradiance-derived AOPs). As regards the overestimations of certain IOPs, it is indeed a very good point, which raised some doubts also among the authors, especially in terms of using $K_{bio}(380)$ as a proxy for CDOM absorption. In the first version of the manuscript we assumed that the contributions of NAP and phytoplankton are much smaller. As discussed in Organelli and Claustre [2019], there are some previous studies in the clearest oligotrophic world oceans that have shown that CDOM dominates the light absorption budget at 380 nm (pg. 6 of the paper). In the absence of coincident light absorption data to prove this statement, other possible sources that affect light attenuation in the UVs, such as light absorption by mycosporine-like amino acids and NAP, can be excluded or considered negligible. NAP light absorption at 380 nm contributes less than 20% to total non-water absorption in clear oligotrophic waters [Bricaud et al., 2010]. As we are aware that this is not at all correct, it's the best shot in the absence of a_{CDOM} from fDOM data which do not exist for the current sensor configuration as far as we know.

We decided to run an additional set of simulations by changing the relative contribution of $K_{bio}(380)$, i.e. by assigning a factor ranging between 0.5 and 1 and thus assessing the relative contribution of such a model, thus leaving some uncertainty in the method to use $K_{bio}(380)$ as a proxy for a_{CDOM} only. Results show that in terms of E_d, the impact is negligible (the performance increases a bit at 412 nm at the expense of 380 nm), however by looking at the monthly climatological scatter plots in terms of K_d, modelled values approach much more closely the measured ones. We are more confident in this result also due to the fact that we are comparing our results with remote sensing products as well, and achieve the greatest 3-platform consistency when halving $K_{bio}(380)$, i.e. using the factor 0.5 instead of one, Fig.6 - right. We will add this part in the updated text, hoping to make it clearer to the readers as well.

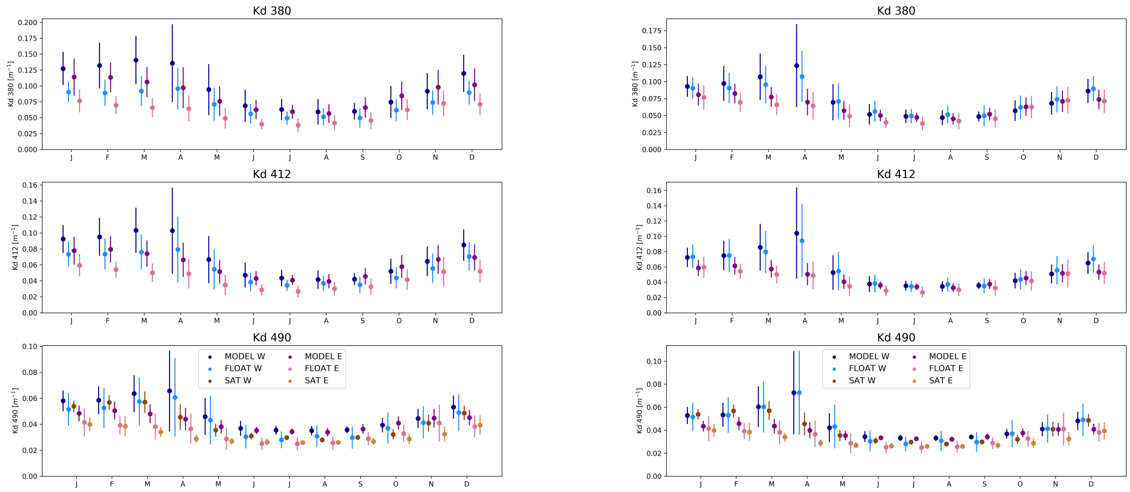

Figure 6: Monthly climatology of K_d values with $a_{CDOM}(380) = K_{bio}(380) * f$, where f=1.0 (left) and f=0.5 (right).

Need a statement about data availability somewhere (typically in Acknowledgements). Also, should specifically list which BGC-Argo floats were used.

Data supporting the conclusions are freely available at `https://doi.org/10.17882/42182`, however without the additional quality control procedures for radiometry, Chl etc. QC-ed radiometry data is not available online as the procedure is not officially accepted. The table of all floats was also created, with start and end dates, start and end positions and WMO codes.

WMO	start date	end date	lat start [°]	lon start [°]	lat end [°]	lon end [°]
6901032	25.11.2012	24.01.2013	43.38	7.90	42.51	6.33
6901483	30.11.2013	21.03.2014	38.63	11.88	38.43	13.09
6901490	17.06.2013	22.06.2013	39.74	11.94	39.65	11.99
6901491	19.06.2013	27.05.2015	39.69	11.98	39.23	11.00
6901496	02.12.2013	12.03.2014	43.25	9.03	43.27	7.76
6901510	26.05.2013	23.05.2015	37.71	18.54	36.67	20.11
6901511	19.02.2013	31.08.2014	42.15	4.71	36.19	-2.27
6901512	10.04.2013	04.05.2014	41.87	4.85	41.43	3.52
6901513	10.05.2013	07.04.2015	38.43	5.54	39.14	6.12
6901528	17.05.2013	15.05.2015	33.58	28.02	32.72	30.83
6901529	29.05.2013	31.01.2015	37.74	18.52	40.05	17.37
6901600	24.08.2014	04.11.2015	37.78	6.55	38.28	2.59
6901605	12.02.2014	01.07.2014	37.04	20.54	36.52	22.34
6901648	11.07.2014	13.05.2016	41.93	4.60	40.89	4.66
6901649	16.07.2014	23.05.2016	40.71	5.97	40.83	3.21
6901653	29.03.2015	22.12.2015	40.01	1.60	39.44	4.13
6901655	20.12.2014	20.05.2015	34.87	27.75	33.57	28.46
6901766	09.06.2015	24.12.2017	34.52	27.12	31.61	27.13
6901768	20.05.2015	11.11.2017	38.30	18.52	37.19	19.52
6901769	31.05.2015	19.12.2017	39.22	10.84	37.97	8.96
6901770	21.05.2015	26.12.2017	35.67	27.91	34.38	26.53
6901771	27.05.2015	20.05.2017	36.69	20.10	37.85	17.67
6901776	17.03.2014	30.04.2014	43.12	7.40	42.51	7.27
6901861	27.05.2014	17.02.2015	36.91	-0.69	36.59	1.39
6901862	30.03.2015	24.12.2017	41.56	18.39	37.86	16.19
6901863	27.05.2015	07.05.2017	36.69	20.09	36.96	17.98
6901864	01.07.2015	13.12.2017	39.62	10.75	40.60	5.95
6901865	19.02.2014	20.03.2015	41.84	17.74	38.54	17.40
6902700	13.11.2015	13.01.2016	43.76	8.58	43.26	8.56
6902732	29.05.2016	27.11.2017	41.31	5.16	38.78	3.20
6902733	28.05.2016	22.12.2017	40.93	5.94	42.97	9.17
6902826	27.05.2017	07.11.2017	37.76	17.66	39.21	17.88
6902828	27.05.2017	27.05.2017	35.41	19.87	35.41	19.87
6902879	06.12.2017	27.12.2017	43.38	7.77	43.09	7.08
6903197	19.04.2016	05.02.2017	41.66	17.72	41.37	17.92

Minor Edits

l. 157-158: I think it is more correct to say that the absorption spectrum is often modeled (not “follows”) as an exponentially decreasing shape despite its heterogeneous biogeochemical composition.

Thank you, we modified the sentence accordingly.

l. 173: “expressed” should be “parameterized”? Similarly, in l. 225 “obtained” should be “estimated”.

Thank you, we modified the sentence accordingly.

l. 201-202: Organelli et al. (2017c) doesn't provide spectra for wavelengths shorter than 400 nm; how do you get data at 380 nm? Also, how representative are these of Mediterranean waters? And finally, some explicit response should be given to that paper's caveat that their results "were not intended for any algorithm development and/or validation" (to quote from their Conclusions).

Yes, indeed, in the paper you mention they used from 400 nm for the analysis. However, the original data set provided to us by dr. Organelli himself has measurements from 350 nm. The species are representative of Mediterranean waters for a few reasons:

1. They were isolated from samples collected in the Mediterranean Sea.
2. The cultures were grown in an ambient based on the Mediterranean Sea.
3. In the Section B.1 of the results in the paper, it is said that the taxonomic composition, as well as the optical properties of the mixed populations are similar to the ones found in natural waters (including the Mediterranean Sea)

Regarding the remark from the Conclusions: "were not intended for any algorithm development and/or validation", the analyses made by Organelli et al. [2017] were done with the aim to deepen certain aspects/limitations from the optical discrimination of the PFTs, and not with the scope to propose a new algorithm (nor was this proposed in the present study). The methods used in this work were not aimed at developing an algorithm, still, the spectra can be utilized as a model parameter, i.e. an IOP for the radiative transfer model, describing phytoplankton absorption.

l. 213-214: How many data points have Chl outside of these bounds? Would it not be preferable to just omit those profiles? If the authors keep them in, some discussion should be present about what error this introduces.

We checked the range of Chl values in our data set. Only 5 profiles out of 1126 had values with maximum Chl values above the range (i.e. 5.71, 5.77, 5.82, 5.96, 5.53 $mg\,m^{-3}$ in the North-Western Mediterranean during spring blooms), thus we simply followed the limits of the algorithm by correcting minimum and maximum values in such way that were in the range of acceptable values. We plotted outputs and haven't observed any features. We thought of underlining this range of values to name one of the inherent limitations of this algorithm, although it seems to correspond rather well to the range observed from BGC-Argo measurements

Eq. 21: negative sign missing in the exponent?

Of course, thank you!

Fig. 5: Is it still considered Case I if the CDOM profile follows fDOM and not Chl?

In theory no. But Case I refers to the model used, i.e. describing CDOM absorption with Chl, such as in Morel and Gentili [2009]. We separated the model type from the shape for the sake of clarity when describing simulations. We added a table in this version to make things clearer.

l. 368: It should be noted that satellite-derived Rrs(412) is prone to large uncertainty, especially in optically complex waters; see e.g. Wei et al. (2020) and references therein.

Thank you for the reference. Indeed, the authors are well aware of that fact. Due to this uncertainty, and due to the lack of in-situ upwelling measurements, we preferred to keep this part of the study in a more qualitative rather than trying to make quantitative assessment out if it, as also underlined in the last section of the results.

Fig. 7: I don't think the word BIOPTIMOD was anywhere in the main text

Thank you, that was corrected as well, we changed BIOPTIMOD simply to "model".

References

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