Reviewer #2

Review of 'Ocean color algorithm for the retrieval of the particle size distribution and carbon-based phytoplankton size classes using a two-component coated-spheres backscattering model'. Reviewer: Emmanuel Boss, UMaine

This paper report on the design of a new model to invert remote-sensing inversion to size. Result suggest it is not ready to be implemented in its current form.

While we agree that the validation regression results are less than satisfactory (which has required the tuning implemented; in the case of the PSD validation regression we offer some reasons why the validation statistics are poor, in response to your comment to investigate the ξ to N_0 relationship), we respectfully disagree that the model and operational algorithm are "not ready to be implemented." The algorithm represents a substantial under-the-hood improvement of KSM09 (Kostadinov et al., 2009) – we now model phytoplankton cells and NAP as two separate particle populations, and phytoplankton are modeled as coated spheres to better represent their optical properties. Global patterns of PSD parameters and derived variables are meaningful in the sense that they correspond to current understanding of oceanic ecosystems. We acknowledge that this is an experimental satellite product, with relatively large uncertainties for some of the retrieved variables. Our goal is to have as mechanistic, first-principles based algorithm as feasible, while keeping it operational with current multispectral data. Naturally, also our goal is to push the boundaries of what's retrievable with such satellite data. We will add language to stress that this is an experimental satellite product, and not claiming to be a canonical, thoroughly validated product. Further validation and algorithm improvement is an ongoing and future work. Further relevant comments are provided below.

The algorithm also offers new (with respect to prior algorithm versions) and very useful ancillary retrievals – Chl from the PSD and bbp partitioned to Chl and NAP. These will be further analyzed and offer opportunities for further constraining and improving the algorithm. The Chl product is already used in the tuning. We believe that these results should be reported to the community now to move the science forward.

The paper is well written. It is of significant interest. It does represents a very significant effort.

Thank you!

However, my biggest fear is, as happened with the previous versions of this model, that it will be implemented by modelers of ocean BGC to make predictions on ecosystems, export etc' while not propagating the large biases observed in the validation of this paper. I do realize it is not my job to protect the community from poor use of biased models.

This is a very good point, and we agree – in the lead author's own experience, users of satellite data who are not experts in marine bio-optics and remote sensing tend to assume the satellite data is "perfect" and models need to be tuned to it. We emphasize that this is an experimental research product, and do not make claims that it is akin in validity and accuracy to the more established (and much more empirical!) algorithms for canonical products such as Chl and POC. We will add language to the manuscript to explicitly emphasize this and make it clear to potential users that they need to take into account product uncertainties, and algorithm assumptions. The products do come with (partial) propagated per-pixel uncertainties, which take a large effort to produce, but we consider them essential. These uncertainties should help guide users' understanding of product status. In an analogous fashion, over-trusting in-situ data when validating satellite data should be done with caution – see our comments below regarding the PSD parameters validation.

For it to be more useful it needs, in my mind, additional work.

See our reply above on your "not ready to be implemented" comment, as well as additional replies to your comments below. We agree that of course the algorithm needs more additional work – that is always the case (an algorithm of this nature, at this stage of the state-of-the-art, is never, in our mind, "finished") - but this step represents major changes and improvements with respect to prior versions. We believe publication of this novel algorithm at this stage will be useful also because the results (including and importantly "negative" ones such as relatively poor comparison with in-situ PSD data, continued need for tuning) will inform the team, and importantly the community for directions for further development – e.g., the phyto C:POC = 1/3 assumption, the PSD parameterization, how to deal with submicron particles, the globally used single set of Mie inputs, etc.

We do not realistically expect validation to be "perfect" or nearly so. In fact, we believe a major qualitative improvement to the approach is needed to make substantial further progress – we list some of those at the end of the paper, e.g. using phytoplankton absorption in the retrieval (blending our approach with that of Roy et al. (2017)). You also explicitly mention one such improvement – involving optical variables that are modeled by our algorithm, and are much more available globally. We thank you for this suggestion.

1. There is significantly more data for validation than suggested here. For example, there is LISST data from NAAMES and EXPORTS from my group on Seabass as well as direct observations of phytoplankton PSDs (reported in Haentjens et al., 2022).

We thank you for the suggestion and will add LISST data from EXPORTS and NAAMES to the PSD validation. We note that the validation is stated to be preliminary, and we do not make claims that the PSD data collected is comprehensive and includes every possible PSD measurement make globally. As you know, there's generally a dearth of PSD data, and importantly, lack of a one-stop-shop place where all such data is easily accessible in processed, merged if needed, and QCed form. As such, acquiring, quality controlling, processing and compiling PSD data for validation represents a large effort. The intention is to conduct further validations that should help inform further algorithm development in the future. This, importantly, includes not only PSD data, but validation with other variables as much as feasible, including phytoplankton C, HPLC, and optical variables as you have helpfully suggested. In short, validation effort will continue and does not stop with this manuscript.

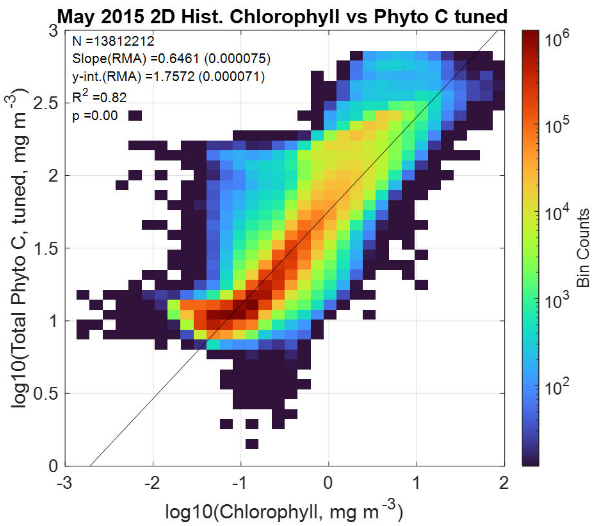
2. As Organelli et al., 2018 have shown, the same parameters retrieved here could be used to predict the beam attenuation measured by, for example, the LISST, C-star and AC-S instruments. We have many more data of all those from the whole ocean (e.g. Tara datasets on SeaBASS). Why not use them as part of your validation? It could help you to better constrain model parameters (particularly associated with NAP).

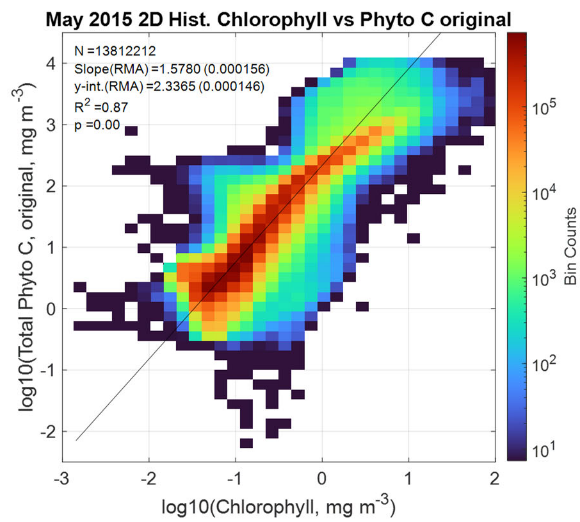
We thank you for this very helpful suggestion! In fact, as mentioned above, further validation is planned, and the full potential of all modeled variables by the novel algorithm has not been realized yet, it represents a large additional effort. For example, exploring bbp due to NAP. More importantly, we suggest as stated earlier that qualitative improvements in approach are needed in our opinion, and that importantly includes making more variables part of the retrieval, not just validation. For example, we've been strategizing the inclusion of phytoplankton and/or total particulate absorption in the inversion, rather than just bbp, i.e. a "blending" wit the approach of Roy et al. (2017).

3. Chlorophyll itself is a predictor of PFT, PCT and PSD. I would like to see, as I discussed with the lead author in the past, proof that the prediction of this model are significantly different than relationship with Chlorophyll itself or other current product from Rrs (e.g. bbp). Why go for a complicated model if a simple one is just as good (or just as bad, depending on your point of view)? I would love to see property-property plots involving C_phyto/POC, Chl, No and \xsi. In short, does the inclusion of all the model parameters into a novel model able to teach us about the ocean in ways [chl] does not (all the global maps presented seem highly correlated with [chl] and/or bbp distribution in the upper ocean)?

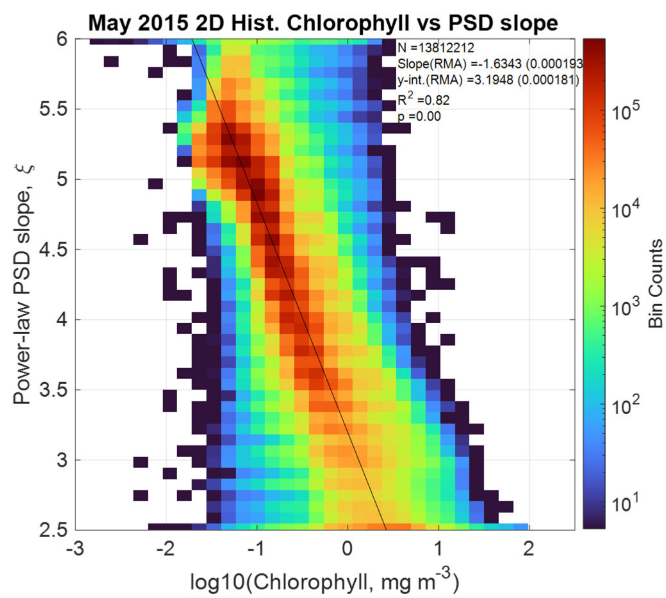
We recognize the fact that many variables in the ocean are correlated or strongly correlated with chlorophyll, especially the open ocean. This makes the issue of degrees of freedom and additional information content in more variables indeed an important one, especially in the context of many satellite variables being retrieved from a single multispectral spectrum. However, we also believe that it is not a good approach to push a more empirically oriented, reductionist agenda, where all things in the ocean are basically a function of Chl. While this is a very valid and practical approach, the overarching theme of this paper is to stay as mechanistic as possible (and push the envelope of what's possible to get from multispectral Rrs), even at the cost of a) degraded performance with respect to established, simpler, band-ratio algorithms or similar, b) the modeling and algorithm presented not being ideal for present-day multispectral data, i.e. its full potential is not realized with multispectral satellite data. We appreciate the fact that hyperspectral data is also only expected to have limited degrees of freedom, but even the ability to retrieve, say 2 or 3 more independent variables from hyperspectral Rrs will be a substantial improvement, i.e. perhaps we can model NAP and phyto PSD separately.

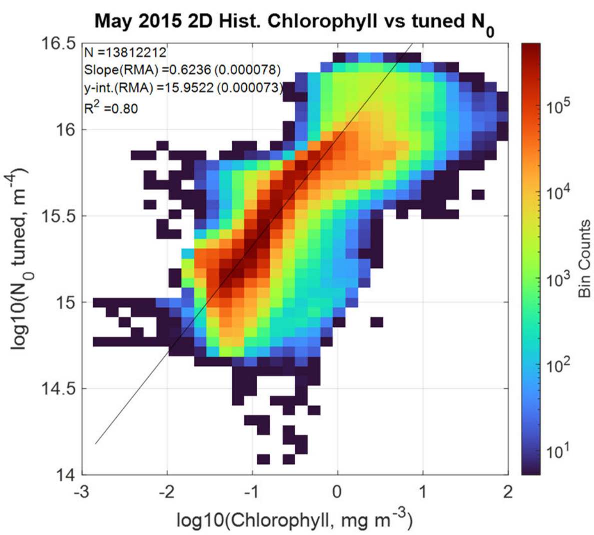
We also do not fully agree with everything is a function of chlorophyll approach for another reason, which is illustrated by the figures below (requested by the reviewer). While strong correlations with Chl do exist, there is substantial variability of the other parameters for a single Chl value. Brief discussion of these figures elaborating on this is given below. We will include some of these figures in the manuscript or its Supplementary material, and add a brief discussion of these figures to the main text.

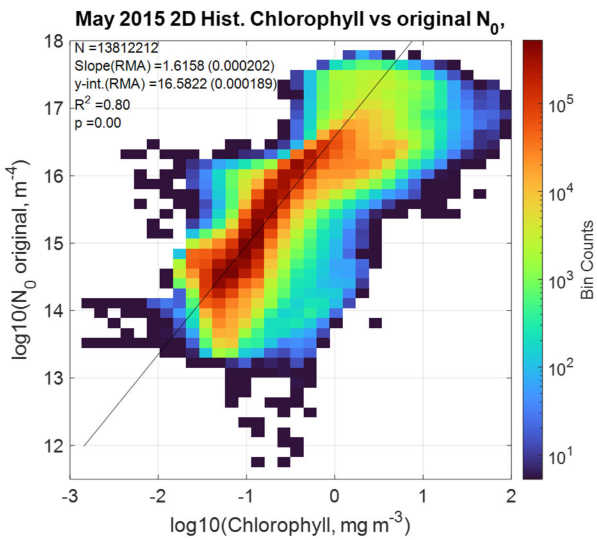




The Chl to phyto C bivariate histogram for May 2015 (the example image used in our manuscript), shown above, indeed illustrates that a strong correlation with Chl exists, and this is expected. However, substantial variability of Phyto C for a single Chl value also exists, albeit admittedly a lot of the variability falls within estimated error bounds. Regardless, the Phyto C to Chl ratio is expected to vary in nature, as a results of physiological adaptation of phytoplankton, and is itself a central parameter of ocean ecological and biogeochemical modeling (e.g. Geider et al., 1998; Behrenfeld et al., 2006; Sathyendranath et al., 2020). Therefore, investigating the Chl to phyto C ratio in our model is a very important next step of verification and improvement and we thank you for this comment, indirectly emphasizing that.

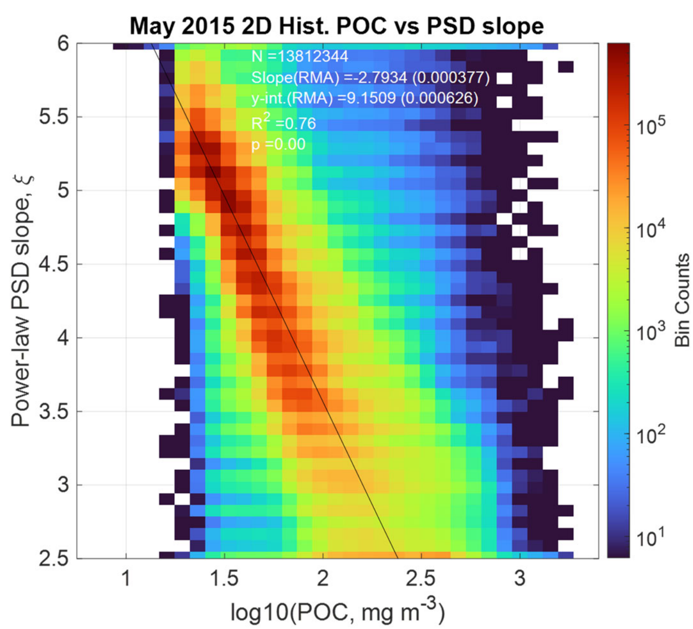


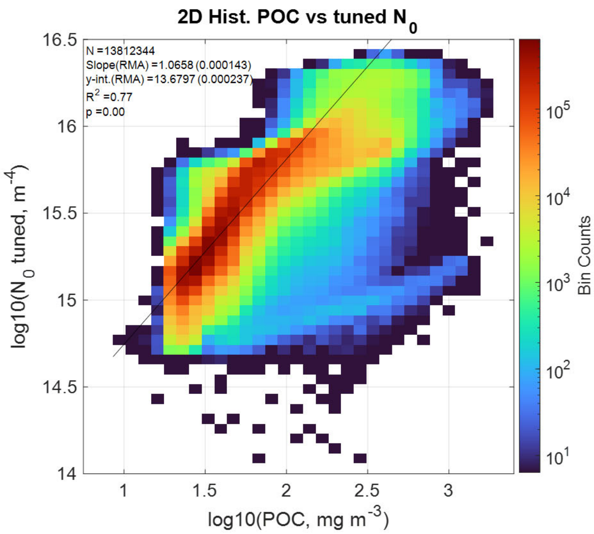


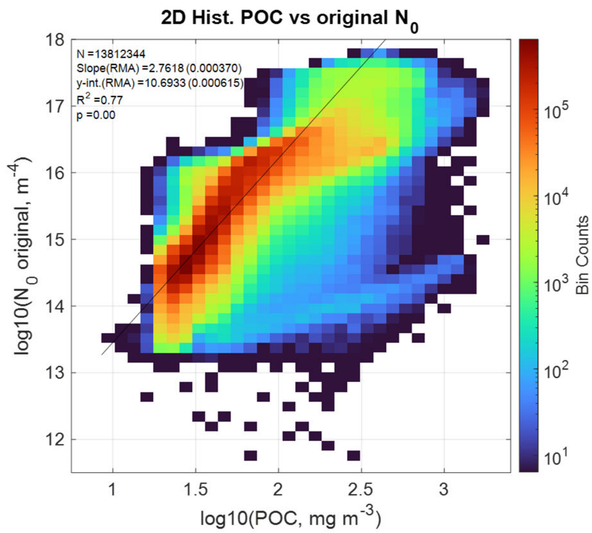


The Chl to PSD parameters bivariate histograms are shown above. They illustrate that while a relationship obviously exists (with relatively high linear R^2 of about 0.8), substantial variability of the PSD parameters exists for a single value of Chl, especially so for the PSD slope. This illustrates that the PSD parameters and Chl are not "one and the same thing", and we do not advocate for juts retrieving the PSD via Chl. See also Brewin et al. (2012), their Fig. 6.

Below, we also show the relationship of the Stramski et al. (2008) POC retrievals vs. the PSD parameters, also illustrating the same conclusion – strong correlations with POC do exist, but substantial variability of the PSD parameters for a fixed POC value is present as well, especially for the PSD slope.

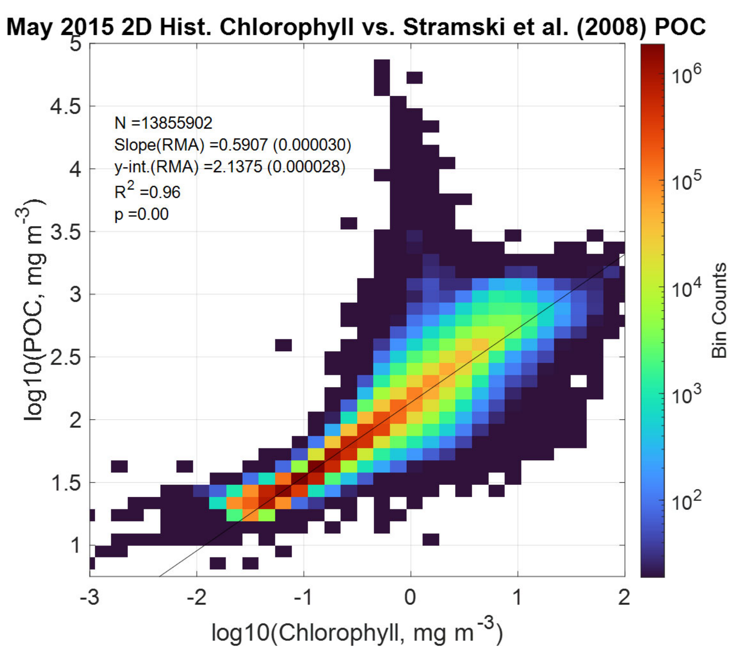






We of course do not claim that the x and y axes on these bivariate histograms are fully independent measurements. They are not because they both come from one set of Rrs spectra, and because they're not fully independent in oceanic ecosystems as well.

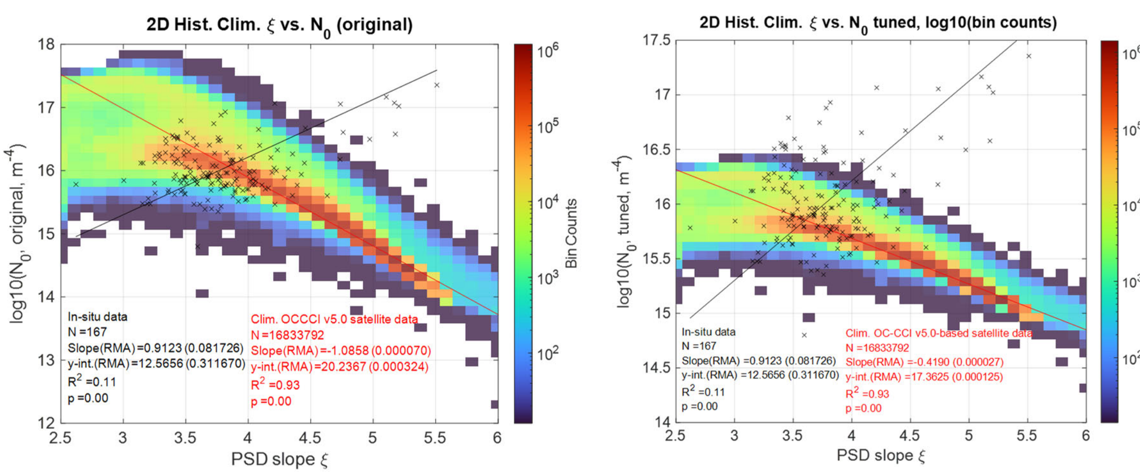
Finally, below we show the Stramski et al. (2008) POC vs. OC-CCI v. 5.0 Chl relationship. The relationship is stronger (R^2 = 0.96) that those shown above, showing the high predictability of POC from Chl. Yet, the community finds POC retrievals valuable as well, and both are considered standard OC products.



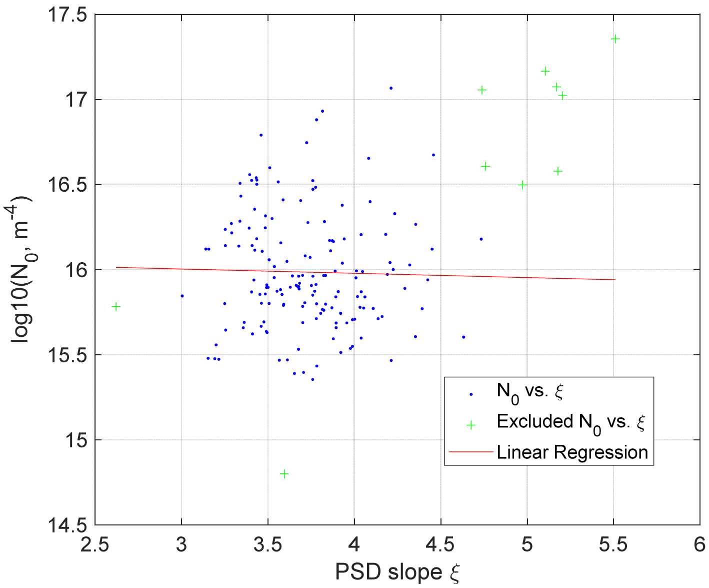
See also the similar bivariate histograms in Kostadinov et al. (2016). In conclusion, we agree that there is correlation with Chl, but we do not agree that there is no added value to our products. We do agree that there is a need for further investigation to avoid uniqueness of retrieval issues and degrees of freedom/independence issues, more comprehensive and complete error propagation, and very clear communication to the community about the status of the algorithm. It is to be expected for many variables we retrieve from ocean color data to be correlated – after all they all come from one Rrs spectrum with 5 or 6 data points. We will add language in the manuscript to emphasize the points discussed above.

4. It is obvious that No and \xsi are correlated. Why not show their relationship? Is it consistent with in-situ data?

Thank you for suggesting this plot and analysis, it is informative, see below. Bivariate histograms of ξ vs. N_0 are shown below (using the climatological OC-CCI v5.0-based sinusoidal projection image), with overlaid linear regressions for both the satellite (red) and the in-situ data (black crosses & regression line). The in-situ data is show after the duplicates averaging you suggested in your later comment, which is why the number of match-ups (N=167) is slightly lower than the one in the original manuscript.



When only a few outliers are removed, the in-situ data exhibit no significant linear relationship (slope 95% confidence interval crosses zero, $R^2 << 0.01$) between the two PSD parameters. See the figure below with outliers removed. We conclude that the subset of in-situ data matched with satellite data do not exhibit a significant relationship between x and N0, much unlike the satellite data, which do exhibit a strong negative correlation.



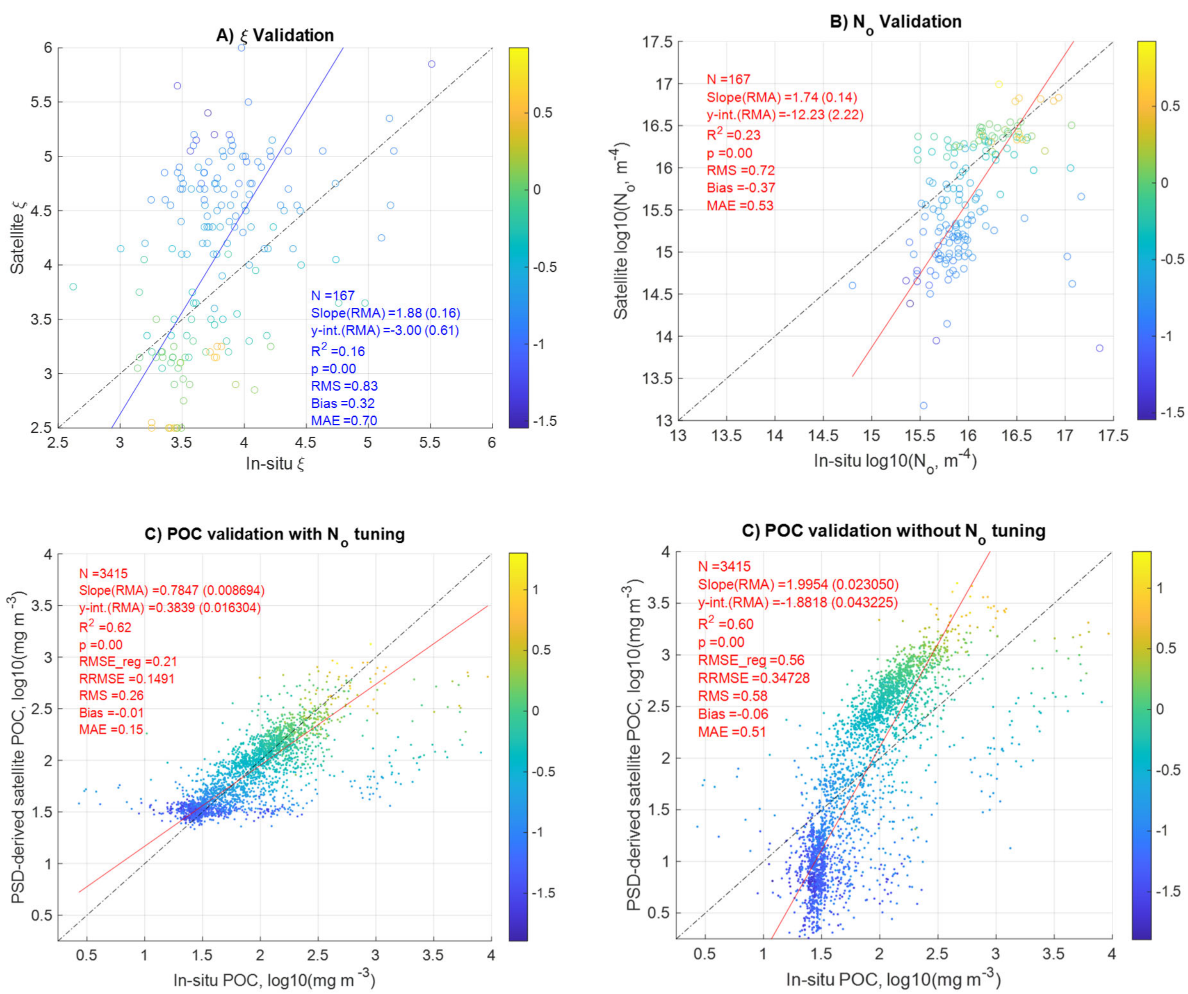
One significant observation is that satellite and in-situ PSD parameters do fall in similar ranges. While the 2.5 to 6 PSD slope range is prescribed in our model, this is particularly impressive for N_0, which is retrieved via the magnitude of modeled and observed bbp, and is not prescribed. This is an indication, that at least to first order or so, the algorithm is able to estimate the abundance of particles correctly. Given the large sources of uncertainty inherent in, for example, not knowing the index of refraction of particles accurately (and this is part of the Monte Carlo assessment of uncertainty), this is an encouraging result.

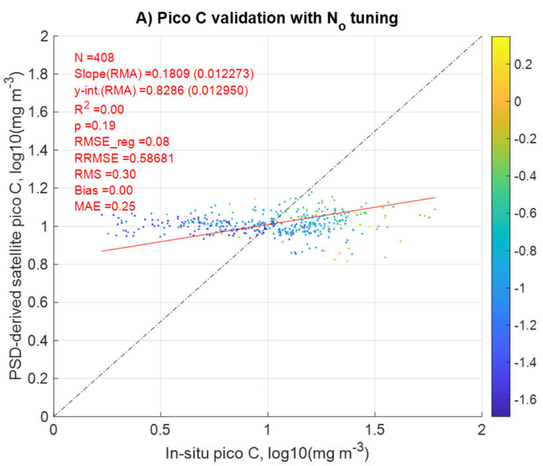
Contrary to the in-situ data, the satellite data exhibit strong negative ξ to N_0 correlation. One possible interpretation of this is that physical reality in the global ocean indeed does not show this relationship in and the satellite observation is incorrect, an artifact of the modeling. However, we posit that this is not too likely, because a) satellite bbp exhibits steeper spectral slopes in oligotrophic waters (e.g. Loisel et al., 2006), and from first principles this is due to smaller particles dominance, and b) from ecological principles we know that oligotrophic waters are characterized by smaller organisms, e.g. dominance of cyanobacteria in the subtropical gyres. Therefore globally over the entire ocean and on average we would expect a clear negative correlation between x and N_0. This is indeed observed in the satellite data, as shown above. We note that the algorithm does not preclude retrievals that could show the opposite relationship – e.g. a place with very high abundance of very small particles vs. a place with very low abundance of relatively larger particles. It's just that the global ocean does not exhibit this relationship.

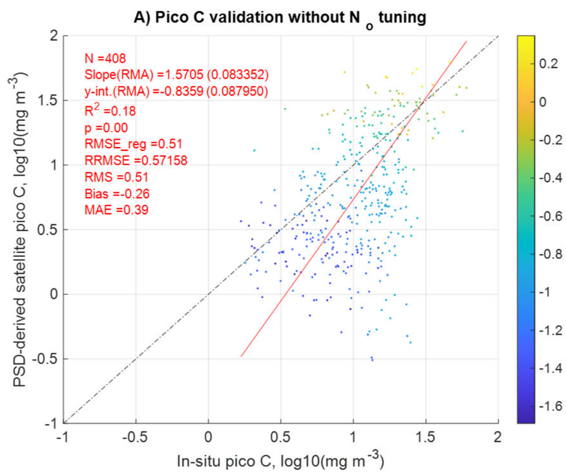
Next, we note the limited and likely biased spatio-temporal coverage of the in-situ data and posit that one possible reason for the lack of the correlation in in-situ data is indeed this limited coverage. Indeed, the lead author recollects a conference presentation from a while ago demonstrating the opposite x to N_0 correlation in in-situ data from the Gulf of Maine, similarly to the in-situ data presented here (with the outliers). The satellite data of course has uncertainties and assumptions, and we also note that the in-situ data comes from multiple instruments and is fitted over a relatively narrow size range. Therefore, discrepancies between in-situ PSD data at a single point and satellite data are expected.

5. The use of the same satellite matchup for multiple validation seems not acceptable to me as it is not an independent evaluation. You could/should average the in-situ data prior to matching up.

We have averaged the in-situ data (ξ, log10(N_0), POC and pico-phyto C) for these duplicates and updated the validation plots to be used in the revised manuscript (see below). The overall scientific results and conclusions from these validation statistics have not changed. For the PSD N=177 before, whereas after duplicate removal N = 167; for POC: N = 4,238 vs N = 3,415, and for pico phyto C: N = 412 vs. N = 408 before and after, respectively. This illustrates that the most substantial reduction in number of match-ups was with POC, and for the other two variables it's minimal. We will add language to the methods to reflect this new duplicate removal.







Minor comments.

1. Figures numbers are not consistent with order of their citation.

Thank you for noting that, wherever possible (without disrupting logical flow for text and order of figures), this will be fixed in the revision.

2. Line 1445: remove ‘using’.

Thank you for catching this (line 145), fixed.

References:

Behrenfeld, M. J., O’Malley, R. T., Siegel, D. A., McClain, C. R., Sarmiento, J. L., Feldman, G. C., Milligan, A. J., Falkowski, P. G., Letelier, R. M., & Boss, E. S. (2006). Climate-driven trends in contemporary ocean productivity. *Nature*, *444*(7120), 752–755. https://doi.org/10.1038/nature05317

Brewin, R. J. W., Dall’Olmo, G., Sathyendranath, S., & Hardman-Mountford, N. J. (2012). Particle backscattering as a function of chlorophyll and phytoplankton size structure in the open-ocean. *Opt. Express*, *20*(16), 17632–17652. https://doi.org/10.1364/OE.20.017632

Kostadinov, T. S., Siegel, D. A., & Maritorena, S. (2009). Retrieval of the particle size distribution from satellite ocean color observations. *Journal of Geophysical Research: Oceans*, *114*(9). https://doi.org/10.1029/2009JC005303

Geider, R. J., MacIntyre, H. L., & Kana, T. M. (1998). A dynamic regulatory model of phytoplanktonic acclimation to light, nutrients, and temperature. *Limnology and Oceanography*, *43*(4), 679–694. https://doi.org/10.4319/lo.1998.43.4.0679

Kostadinov, T. S., Milutinovic, S., Marinov, I., & Cabré, A. (2016). Carbon-based phytoplankton size classes retrieved via ocean color estimates of the particle size distribution. *Ocean Science*, *12*(2). https://doi.org/10.5194/os-12-561-2016

Loisel, H., Nicolas, J. M., Sciandra, A., Stramski, D., & Poteau, A. (2006). Spectral dependency of optical backscattering by marine particles from satellite remote sensing of the global ocean. *Journal of Geophysical Research: Oceans*, *111*(9), 1–14. https://doi.org/10.1029/2005JC003367

Roy, S., Sathyendranath, S., & Platt, T. (2017). Size-partitioned phytoplankton carbon and carbon-to-chlorophyll ratio from ocean colour by an absorption-based bio-optical algorithm. *Remote Sensing of Environment*, *194*, 177–189. https://doi.org/10.1016/j.rse.2017.02.015

Sathyendranath, S., Platt, T., Kovač, Ž., Dingle, J., Jackson, T., Brewin, R. J. W., Franks, P., Marañón, E., Kulk, G., & Bouman, H. A. (2020). Reconciling models of primary production and photoacclimation [Invited]. *Applied Optics*, *59*(10), C100. https://doi.org/10.1364/ao.386252

Stramski, D., Reynolds, R. A., Babin, M., Kaczmarek, S., Lewis, M. R., Röttgers, R., Sciandra, A., Stramska, M., Twardowski, M. S., Franz, B. A., & Claustre, H. (2008). Relationships between the surface concentration of particulate organic carbon and optical properties in the eastern South Pacific and eastern Atlantic Oceans. *Biogeosciences*, *5*(1), 171–201. https://doi.org/10.5194/bg-5-171-2008

Using the rubric of EGU:

We thank you for sharing the rubric responses with us. Our relevant replies to your rubric comments are provided above, or we explicitly respond below where needed.

Scientific significance -3

Scientific quality -3

Presentation quality – 2

1. Does the paper address relevant scientific questions within the scope of OS?

yes

2. Does the paper present novel concepts, ideas, tools, or data?

Yes.

3. Are substantial conclusions reached?

Not really, in my mind, beyond those of model evaluation.

We respectfully disagree that substantial conclusions are not reached. In fact, one important conclusion is that further significant leap in improvement is likely to require a substantial qualitative change in approach – e.g. one or more of – different PSD parameterization, inclusion of absorption (and/or other IOPs) in algorithm development and inversion, and regionalization of optical model inputs, e.g. indices of refraction (to address biases). Another important conclusion is that other existing algorithms/methods exhibit significant disagreements in terms of phyto C, making the need for N_0 tuning ambiguous.

4. Are the scientific methods and assumptions valid and clearly outlined?

Clearly outlined, but validity needs further work.

See our comments on validation above, where we discuss the ξ vs. N_0 relationship, per your suggestion.

5. Are the results sufficient to support the interpretations and conclusions?

No.

See our responses to your previous comments.

6. Is the description of experiments and calculations sufficiently complete and

precise to allow their reproduction by fellow scientists (traceability of results)?

Yes.

7. Do the authors give proper credit to related work and clearly indicate their own

new/original contribution?

Yes.

8. Does the title clearly reflect the contents of the paper?

Yes.

9. Does the abstract provide a concise and complete summary?

Yes.

10. Is the overall presentation well structured and clear?

Yes.

11. Is the language fluent and precise?

Yes.

12. Are mathematical formulae, symbols, abbreviations, and units correctly defined and used?

Yes.

13. Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated?

See above comments.

See above our responses to your suggestions. Thank you for these constructive and helpful suggestions.

14. Are the number and quality of references appropriate?

Yes.

15. Is the amount and quality of supplementary material appropriate?

Yes.