# Reviewer # 1

General comment

This study attempts to retrieve from space (ocean color satellite data) information on particle size distribution and carbon-based phytoplankton size classes in open ocean waters. This significant piece of work is actually the extension of previous studies (Kostadinov et al. 2007-2022) which includes validation results. The manuscript is well organized, written and illustrated.

Thank you.

Unfortunately, these validation results are not convincing, most probably as several assumptions made in the methodology are not valid. The authors should carefully revise the assumptions made notably to model the particle size distributions and discuss the impact on the resulting satellite-derived products. Detailed comments are provided hereafter to clarify the methodology and discuss the validation results.

While we agree that the regression statistics of the PSD validation exhibit low R^2 values, they are statistically significant, and we posit that there can be multiple reasons for that that need to be carefully considered. For example, mismatch in spatial and temporal scales of sampling between satellite vs. in-situ data is a possible reason for poor validation. More reasons are discussed below, and also are covered in more detail in Kostadinov et al. (2009).
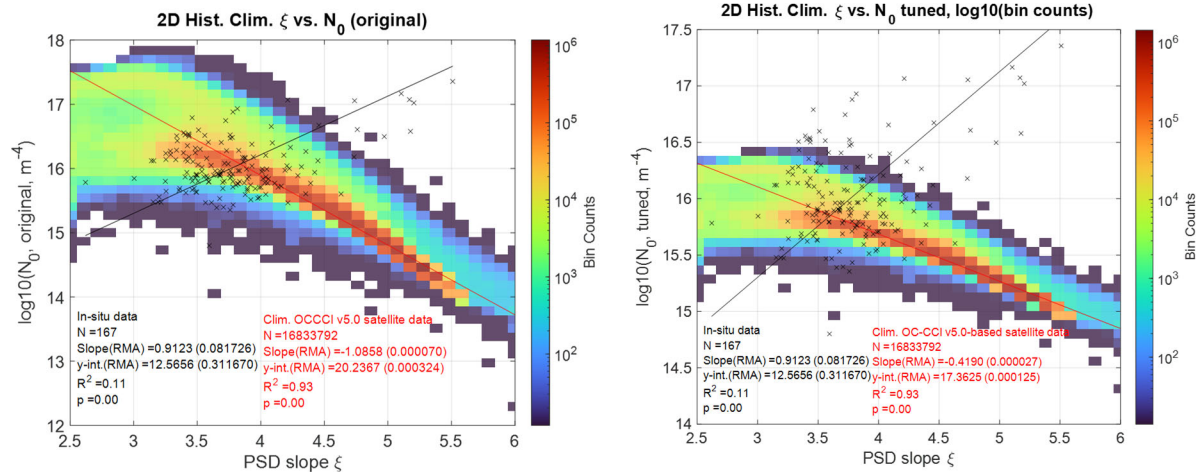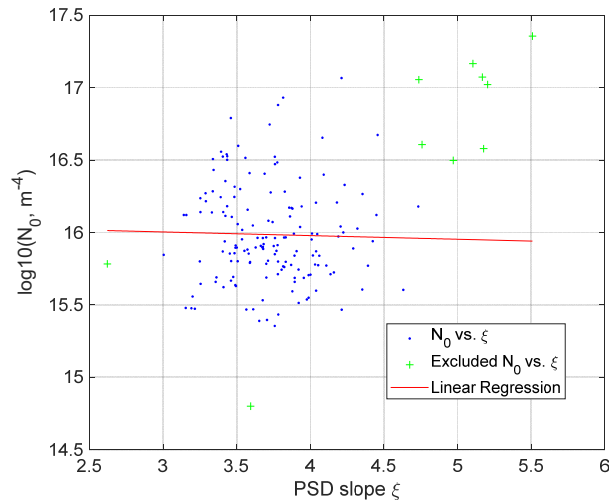
Note that the ξ vs. N_0 relationship in in-situ data (only those that are matched up are shown) is rather weak and driven only by a few outliers. When these are removed, there is no statistically significant linear relationship between the two PSD parameters in the in-situ data (slope 95% confidence interval crosses zero, R^2 << 0.01) (See the regression plot above with outliers excluded; interestingly, most of these outliers come from one area – the California Bight). Thus, while the satellite data, as expected, exhibit strong negative correlation between the PSD slope and N_0, the in-situ data exhibit a weak positive correlation that disappears with removal of a few outliers. See above the bivariate histogram of satellite data (OC-CCI v.5.0 climatology using the new algorithm presented here), with in-situ match-ups superimposed. While one possible reason for that can indeed be that the satellite algorithm uses wrong/incorrect model/parameterizations, we posit that there are multiple additional or alternative reasons for this discrepancy. One such important reason is the large difference of spatio-temporal coverage between the satellite and the in-situ data sets. Geographic and temporal coverage of the in-situ data is rather limited, especially when matched up with satellite data (only 167 PSD match-ups are available after the match-ups were re-done per request of the other reviewer, some more are expected to be added in revised manuscript, see comments to other reviewer). This suggests that the in-situ data is not necessarily able to capture a relationship that the satellite data does. We note that this relationship has a theoretical underpinning because of at least two reasons: a) the power-law tends to apply over large size ranges (e.g. Hatton et al., 2021), for which there are theoretical reasons (e.g. Brown et al, 2004) , and b) what we know about global ocean ecosystems, namely that oligotrophic areas exhibit relative dominance of smaller phytoplankton, as opposed to increased importance of larger phytoplankton in more eutrophic areas. Because of b) above, we expect backscattering in the ocean to become "bluer", i.e. to have a steeper spectral slope, in oligotrophic areas. This is indeed observed in satellite data and is qualitatively interpreted in this way in Loisel et al. (2006). Therefore, we expect, in the ocean, globally and on average, N_0 to decrease with increasing ξ. This is not necessarily going to be captured by in-situ data of limited spatio-temporal coverage that is also fit over a relatively small size range as compared to the full optically significant size range. This latter point brings us to another possible reason why in-situ data (which has its own limitations and uncertainties) may not correspond well to satellite-derived PSDs.

We note that the in-situ data used in the validation, especially for PSD, has its own limitations and should not unequivocally be considered the "sea-truth" without any reservations. In the case of PSD It is assembled from two different instruments with quite different principles of operation, and the power-law fit is done only in the range of 2 to 20 micrometers diameter, much smaller than the optically significant range. As noted by the reviewer, the power-law fit is not always great, and it can be sensitive to the diameter range used to fit it. The relationship of satellite PSD slope retrieved to the PSD slopes measured in-situ is therefore expected to be noisy, as observed. In fact, other investigations have also not always been able to demonstrate a strong or any relationship between PSD and bbp shape – e.g. Kostadinov et al., 2012; Organelli, 2020, but see also Slade and Boss, 2015. The overall trend/tendency of higher or slower slope is, however, captured, in our validation, which in our view renders the PSD slope validation reasonable, but with improvements desirable in future implementations.

In short, we believe that the relatively poor validation result and the above satellite to in-situ correlation discrepancy does not necessarily mean the satellite algorithm is "wrong". We fully acknowledge that the power-law PSD has its limitations, and more of the assumptions/limitations of the algorithm are ideally going to be relaxed in future work. Global relationships averaged over a month or longer vs. a measurement in single point in time and space are likely to work better.

Regarding the validation with POC and pico-phytoplankton C data, and the tuning procedure, it is of importance that similar tuning procedure was also implemented in an earlier version of the algorithm, Kostadinov et al. (2016). This earlier version used only one particle population and modeled it as homogeneous spheres. The algorithm construction here is substantially improved since it uses two different particle populations and a more realistic representations of phytoplankton cells. However, in much of the open ocean (especially the oligotrophic areas), the backscattering optical signal is still dominated by the NAP represented by homogeneous spheres and spanning a larger size range than phytoplankton. One and the same Monte Carlo range of Mie inputs (e.g. real indices of refraction) may not be realistic globally, from subtropical oligotrophic to coastal, to Southern Ocean vs. Northern Hemisphere high latitudes, due to , for example, non-uniform dust input in the ocean, and proximity to coasts. This likely needed regionalization/improvement is out of scope here, but should be investigated in the future.

Some of the assumptions made are necessitated by the goal to have an operational algorithm able to be applied to current multi-spectral satellite data. It is also a goal to have an algorithm based on first principles as much as possible (as mechanistic as possible). This represents a compromise. The goal to have an operational algorithm limits the degrees of freedom and number of independent variables possible to retrieve. More discussion is provided in response to your specific comments below. We will also add text in the manuscript emphasizing some of the key points of our responses here to make model limitations clearer to the user.

Detailed comments

Line 45, Equation 1:

To my knowledge this very convenient power law size distribution of particles does not apply to phytoplankton particles in oceanic waters. Can you please provide relevant references to support your statement?

Line 53:

Again, probably the main/major issue in this study: phytoplankton cells in oceanic waters DO NOT follow a power-law PSD. If I am wrong please prove it based of already published quality field data.

We respond to the previous two comments together as they address the same issue.

While the reviewer is correct that the PSD of a specific species is not likely to follow a power-law and will be expected to instead peak in the characteristic size of that species, here we are aiming to model the global ocean ecosystem as a whole, over large spatio-temporal scales and on average, as well as for all species present. Individual cases, especially during mono-specific strong blooms, are likely to deviate from the power law (e.g. Reynolds et al., 2010 for coastal waters), but ecosystems as a whole, especially on average and globally, are more likely to follow the power law more closely (e.g. Hatton et al., 2021).

There has been a lot of theoretical work on the power-law, particularly as applied to size of organisms and ecosystems, and the power-law has theoretical foundations/underpinnings (e.g. Brown et al., 2004; Hatton et al., 2021 and refs. therein). There's also been investigations demonstrating the power-law does not apply well, especially in coastal ecosystems (e.g. Reynolds et al., 2010; Runyan et al., 2020; Reynolds et al., 2021 and refs. therein). It is a lot harder to find information and data on living phytoplankton only, and their specific PSDs, because it has been historically difficult to separate living phytoplankton and measure, say, their PSD or carbon (e.g. Graff et al. 2012, 2015). This makes validation of one of our main products – phytoplankton C, difficult. This is mentioned in the paper.

A recent study (Haentjens et al., 2022) investigated in-situ measurements of phytoplankton-specific PSDs. They do fit their data to a power-law, but more importantly, their figures illustrate that to first order, the phytoplankton-specific PSD shape is consistent with a power-law. For example, see their Fig. 3, Fig. 5, and Supplement Fig. S8. They do state that the drop off for the smallest size bin is real due to lack of *Prochlorococcus*, but could also be an instrument/methodology artifact. We acknowledge that a drop-off in the size distribution will be expected at the limits of the size range of autotrophs, hence the power-law is not expected to apply equally well over the same size range everywhere and always in the global ocean. Again, our algorithm aims to capture first order effects and be applicable globally; regionalization may be needed to address this further, e.g. build an algorithm with different modeled size limits for phytoplankton in different regions.

Hatton et al. (2021) offer an assessment of the PSD of marine life over a huge range of sizes (body mass), demonstrating that a specific power law applies, in the context of the Sheldon (1972) hypothesis that equal biomass tends to occur in each logarithmically-spaced size bin. This also follows from our Eq. 1, for a specific PSD slope ($\xi = 4$), and when the upper and lower limits of the size bins follow a geometric progression. We note that the assessment of Hatton et al (2021) offers a strong support for the power law (their Fig. 1), and also separately analyzes autotrophs from other marine organisms with overlapping size ranges. Note from their Fig. 2a that to first order, approximately equal autotroph biomass occurs in logarithmically spaced size bins, consistent with a

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power-law for phytoplankton alone and consistent with Sheldon's hypothesis (for the ocean as a whole). We emphasize here "to first order" – over larger size ranges and on average for global oceanic ecosystems. We acknowledge that individual cases in space time may not closely conform to a power-law, hence giving one possible explanation (out of several) for the relatively poor validation.

Quinones et al. (2003) investigate the size spectra of planktonic biomass and find that the power-law is followed at all stations, and biovolume-wise the Sheldon hypothesis is followed in terms of slope. We also note that Fig. 2 of Lombard et al. (2019) demonstrates that to first order the power law applies to large size ranges of planktonic organisms, sampled with different instruments. We acknowledge that phytoplankton share their size domain with other organisms (bacteria on the low end and zooplankton at the high end). So, it may be reasonable to accept that the contribution of phytoplankton to the size classes would fall off at the two ends of their range – but see the Hatton et al. (2021) discussion above.

While we acknowledge the limitations of the power-law (e.g. Reynolds et al., 2021 and refs therein; Bernard et al., 2007; Reynolds et al., 2010; Organelli et al., 2020 – see slope for small particle sizes), in spite of support for it from the literature as shown above (see also, for example, Buonassissi and Dierssen 2010), we would also like to present here a strong motivation for using the power-law PSD, as well for using the same PSD slope for both phytoplankton and NAP (which assumption is also questioned by the reviewer later on). A primary goal of this work is to build a model that is based on first principles as much as possible, and of course to stay as close to reality as possible. Some of the assumptions are hard to verify due to lack of global data sets of the variables involved. Importantly, a second major goal of the manuscript is to develop an operational algorithm that is possible to apply to current mainstream, multispectral global ocean color data, e.g. the OC-CCI data set. That puts a limit to the degrees of freedom available for retrievals, especially since only certain wavelength ranges work well with the satellite bbp retrievals we use (the choice of wavelengths is important – see for example Organelli et al. 2020). Ideally, of course, it would be good to model phytoplankton, NAP, and perhaps a third particle population to represent mineral contributions, fully independently and with more complex PSDs as needed, however, these parameters would not be possible to retrieve realistically from multispectral data.

In light of the above discussion, we note that our algorithm ultimately retrieves one slope and N_0 value, from the total particulate backscattering. The algorithm's assumptions are then used to assign these to phytoplankton vs. NAP PSDs. We agree that these are restrictive and not fully tested assumptions. However, adding two power-law PSDs with different slopes results in a non-power law PSD and requires retrieval of more parameters, making the inversion more complex, where not only degrees of freedom but also uniqueness of solutions may become an issue and needs further investigation. Two power-law PSDs with the same slope and different N0 add to a power-law PSDs, making the problem tractable.

We are also not convinced that using a different distribution from a power law for phytoplankton is going to make a big difference at low oceanic chlorophyll concentrations.

In fact, submicron particles are important for the shape of bbp, and their treatment may turn out o be more important that the exact shape of phytoplankton PSD. For example, our modeled signal is dominated by bbp due to NAP in oligotrophic areas (see also Bellacicco et al., 2018). This covers a

large surface area of the oceans. This of course requires quantitative verification, and testing different PSD parameterizations is planned as a priority next step. The proper form of phytoplankton PSD is a difficult concern to respond to – because it is not clear what distribution phytoplankton do have in the open ocean, data on this are limited – however, see our Haentjens et al. (2022) discussion above.

We would also like to note that the phyto C: POC = 1:3 everywhere in the ocean assumptions is more of a concern and more restrictive to us than the power-law PSD form. We believe that it's a priority to address that assumptions as best as feasible in later iterations.

We will add language to the manuscript's discussion to summarize all of the above considerations.

Line 64:

"a single population of particles (approximated by homogeneous spheres)"

This is another strong assumption which definitely does not apply to phytoplankton cells in in marine waters. Please discuss it and say what is the impact in your methodology.

We note that this sentence pertains to the earlier KSM09 (Kostadinov et al., 2009) algorithm. One of the major purposes of the effort of this manuscript is exactly to relax this assumption to the extent feasible within this effort. I.e., we are no longer assuming a single population of particles like KSM09 does – here we model two separate particle populations, phytoplankton and NAP, the optical properties of which are modeled differently and separately. Importantly, phytoplankton are *not* modeled as homogeneous spheres, rather as coated spheres, to better approximate their internal structure and hence backscattering.

Line 85:

Where do minerogenic particles come from in open ocean waters?

Minerogenic particles are delivered globally via dust deposition as part of the atmospheric dust cycle. In fact, aeolian iron sources can be important biologically both in the ocean and on land - see for example, Nogueira et al. (2021), Gao et al. (2001), Mahowald et al. (2005) and Wagener et al. (2008).

We thank you for this question, it illustrates another area of possible improvement that can prove to be important – at the moment minerogenic contributions to the particle assemblage are considered a source of random uncertainly via the choice of Mie inputs and the Monte Carlo simulations, and in future iterations they could be quantified in a spatially and/or temporally explicit manner, which should improve algorithm performance and reduce uncertainty.

Line 93 'an initial effort of validation':

Such an effort to at least first validate the assumptions made in your recent and present studies and notably validate the PSD algorithm should have been made already, before going forward applying non-validated algorithms to satellite data and interpret the results obtained

We note that this is the initial paper describing the novel PSD algorithm, and it does come with a validation, including the PSD parameters and derived variables. The assets (published scientific code and data) are part of this paper. We state that it is an initial validation, because it's the first for this algorithm, and because more is planned. Further validation (including with more data and more variables) is planned, and validation results are and will be taken into account for further algorithm development. Prior iterations of the algorithm and publications (e.g. Kostadinov et al., 2009, 2010, 2016, 2017) do contain validation and/or inter-comparisons.

Line 98 'backscattering are modeled using Mie theory (Mie, 1908) for homogeneous spherical particles and the Aden-Kerker (Aden and Kerker, 1951) method for coated spheres.':

Is Mie theory well adapted to your study?

What not considering also the more realistic case of non-spherical particles?

Mie theory is applied to NAP, which are modeled as homogeneous spheres. Phytoplankton are modeled as coated spheres. The reviewer is of course right that not all particles closely conform to these spherical models, and random shoes should be considered. Considering random shapes complicates the optical solutions greatly, and it's non-trivial to find solutions that work for the needed size ranges for optical oceanography (e.g. Clavano et al., 2007). The EAP framework using coated spheres has the advantage in that it provides a realistic model for a phytoplankton cells – backscattering is significantly affected by use of coated vs. homogeneous spheres, as we show here and as is shown, for example, in Organelli et al. (2018). We agree that random-shaped particles should be considered for both NAP and phytoplankton and spherical vs. random shaped will affect backscattering (e.g. Clavano et al., 2007), but given the limitations above and the need to specify more parameters such as shapes, we consider this to be out of scope for this work, and something to be considered for future tests and iterations.

Line 138 'The two key assumptions are: 1) Phytoplankton and NAP have a power-law PSD (Eq. 1) with the same slope ξ'

Once again, I do not agree for phytoplankton. Moreover why the same slope?

We address this concern in our comment above for lines 45 and 53, where we discuss the applicability of the power-law PSD to phytoplankton.

Tables 1 and 2:

Please justify the choice of the minimum, mean and maximum values considered here as inputs. Are your computations realistic??

For many of these inputs, the main references are Robertson-Lain et al. (2018) and Bernard et al. (2009), and refs. therein, as well as Kostadinov et al. (2009) and refs. therein. We discuss additional references below. For the Dmin of phytoplankton – this is dictated by the size of the smallest autotrophs, *Prochlorococcus*, which tend to have diameter of about 0.5 µm or slightly larger (e.g. Morel et al., 1993). For the largest autotrophs it would depend on ecosystem and is harder to pick, hence

we use a distribution, but as a guidance, individual cells larger than ~ 50 μm in diameter are rare/not expected to be found in the open ocean (e.g. Charles Stock, pers. comm to Kostadinov et al., 2016 author team). Our algorithm is meant for global open ocean applications, not to a particular ecosystem, thus the mean Dmax is meant to be close to that value.

For the Dmin and Dmax of NAP – see Duforet-Gaurier et al. (2018), their Table 1. For NAP, since it's important to capture optically active range of particles, this was investigated with the bbp cumulative plots – our Fig. S4. For this reason, we use Dmin = 0.01 mm for NAP, unlike Duforet-Gaurier et al. (2018). If sub-micron-sized NAP is not included, the steeper end of bbp shapes observed in satellite data cannot be reproduced by the model. Note that Stramski and Kiefer (1991) use an even lower limit of 0.002 μm.

For the indices of refraction – apart from Robertson-Lain et al. (2018) and Bernard et al. (2009), see also Morel and Bricaud 1986, Babin et al. (2003), Wozniak and Stramski (2004), and Duforet-Gaurier et al. (2018).

We will add more references to the table to clarify sources.

Line 218:

Define LISST

The acronym will be defined in the revised manuscript, thank you!

Figure 8 'PSD validation results':

Thank you for showing these validation results which are not satisfactory, as could be expected considering that several assumptions made are (most probably) not valid.

While there is somehow an agreement (or at least a trend) between the satellite and situ No (number of particles), there is no correlation for the slope, therefore no validation of the satellite-derived PSD, assuming the PSD is a power-law.

We note that the PSD slope validation regression is statistically significant, albeit with a low R^2 value. As for N0, we note that the algorithm is able to pick up the concentration of particles, to first order, according to this validation. We find this to be impressive and consider it a success, given that the algorithm makes no a-priori prescriptions about particle concentrations – they are solved for from the magnitude and shape of satellite bbp. The algorithm also allows for a wide variation of real indices of refraction, which results in large uncertainties in N0. We further comment on the PSD validation result in response to your general comment at the beginning of this review, also commenting on why in-situ data may not capture the global satellite patterns.

These poor validation results must be discussed so as its implication on the whole methodology. What would be the results if another (more realistic) function was used to model the PSD?

We will add relevant discussion about the PSD parameterization and as stated elsewhere in our responses.

Figure 10:

These validation results are more convincing. Please specify in the figure legend what you mean by 'empirical tuning'.

Thank you, we will edit the figure legend to include explicit description of the empirical tuning for N_0.

Figure 11.

As in Figure 8, poor validation results.

For this validation, as with the PSD data, the in-situ data set quality, method of derivation, and limitations, as well as spatio-temporal coverage have to be considered. We note, for example, that these are not direct phytoplankton carbon measurements. Albeit poor (and not significant in the case of the tuned version), these results are extremely important to report, as, unlike the rest of the phytoplankton C (and Chl) validations and verifications we present, these results are not improved by the tuning, making it ambiguous whether the tuning should be applied. We believe that the continued need for tuning is a primary issue to resolve foe future improvements, and by presenting all these results together, we aim to prompt the community to work in these directions too. Addressing the tuning further may require not only considering different PSD shapes as you suggest, but also, importantly, considering the distributions of the Mie inputs and that they may need regionalization. The latter, we suspect, is more important.

See also relevant parts of the PSD validation responses we offer above.

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