## **Responses to Reviewer #1**

## Dear Reviewer,

Thank you very much for the extremely valuable critical comments on our work. Below we present our detailed point-by-point responses and the description of actions taken in regards to your comments. We believe that we have provided satisfactory explanations to your criticisms, and have made appropriate revisions in our paper.

#### Reviewer's comment:

The article, Parameterization of the spectral light absorption coefficient of phytoplankton in the Baltic Sea: general, monthly and two component variants of approximation formulas by Justina Meler, presents a way of accounting for the variability in phytoplankton absorption coefficients using an additional term ( $\Sigma$ Ci/Tchla) in the parameterization. A good attempt, as against the traditional method that takes into account only pigment concentrations. The dataset clearly presents the complexities and challenges, coastal systems have to offer in ocean color remote sensing, wherein regional parameterizations are highly essential. The article is therefore of relevance to the scientific community. However, in its current form it is lengthy (needs to be concise) and contains too many figures. It is therefore requested to perform major revisions (listed below), thoroughly check the text and get it checked from a native speaker.

## Author's response:

Thank you for pointing out the positive aspects of our manuscript.

In order to make the work more concise, the new version of the manuscript text has been reorganized, some fragments has been shortened, and the number of drawings has been reduced. The new version of the text has also been corrected by a native speaker.

## Author's changes in the manuscript:

The order of presentation of our own results has been changed. In section 3.2 one and twocomponent parameterizations are presented, while section 3.3 refers to errors of estimation. In the shortened section 3.4 we briefly refer to selected examples of parameterization known from the literature. Mathematical details regarding obtaining two-parameter parameterization have been moved to Appendix 2. The revised version of manuscript contains 9 reorganized figures in the main text, and one in the Appendix 2 (overall, the reorganized drawings contain 7 fewer individual panels than the original version).

## Reviewer's comment:

Major issues: 1) In the introduction, relevant background knowledge on how the ratio  $(\Sigma Ci/Tchla)$  would account for the variability in phytoplankton absorption is missing. Its implications in inferring ecosystem dynamics etc. in different situations. What do high and low values of the ratio imply?

## Author's response:

Generally, the composition of all accessory pigments may be different for various photosynthesizing marine species, it may reflect adaption of organism to different light conditions (processes of photo- and chromatic adaptations), as well as acclimation at the plant community level. The ratio ( $\Sigma$ Ci/Tchla) used by us for practical purposes allows, in the first approximation, to assess the differentiation between phytoplankton populations characterized by the same concentrations of the basic photosynthetic pigment - chlorophyll *a*.

#### Author's changes in the manuscript:

The information provided in the Introduction section has been supplemented.

#### Reviewer's comment:

2) Parameterizations are developed and tested on the same dataset. How about testing on an independent dataset on an independent dataset (especially when the authors have a huge dataset)? Test the parameterizations on a dataset (from the reported sampling sites, may be set aside data from a year) that was not included in developing the coefficients presented in tables A1, A2 and A3; refer to Mascarenhas et al. 2018 (http://www.mdpi.com/2072-4292/10/6/977/pdf)

## Author's response:

Our main goal was to use all available information to determine new forms of parameterization tailored to the data collected on the Baltic, and we did not intend to carry out a strict validation. We realize that an independent data set would be needed for such an objective. We have tried to emphasize these issues in the improved manuscript. However, in order to satisfy the reviewer's curiosity, we conducted a supplementary calculation exercise. We divided our data dataset into a "training" and "validation" subsets. The "training" set consisted of 2/3 of data selected from each month. The remaining 1/3 of the data created a "validation" set. Using the "training" dataset we found alternative versions of one- and two-component parameterizations. We found that differences between A and E coefficients of one component parameterization were not more than 8% and 4% respectively (see additional Figure R1.a and b). Also relatively small were the differences between coefficients of two-component parameterizations (not shown). We found that these alternative versions of parameterizations have generally small systematic errors (either positive or negative, from -17% to +16.5%) (see Figure R1.c), and in terms of standard error factor x (characterizing the statistical error acc. to logarithmic statistics) they are only slightly less accurate in some portions of the spectrum (see Figure R1.d).

## Author's changes in the manuscript:

The sentence stating that our intention was to briefly compare examples of parameterization known from the literature, and not to validate our own results has been added to the last paragraph of section 3.4 of the revised manuscript.

#### Reviewer's comment:

3) A different approach (than the monthly parameterizations) would be considering different ranges of Tchla concentration and corresponding values of the ratio ( $\Sigma$ Ci/Tchla). This will provide an understanding of the effect of concentration ranges (low-medium-high) on parameterization parameters.

## Author's response:

Following the Reviewer's comment we have performed additional calculation exercise. The results are summarized in two additional Figures: R2 and R3. We have divided our dataset into separate groups according to different *Tchla* concentrations (33rd and 67th percentiles of *Tchla* distribution were used as limit values for these sets). However the obtained results reviled that changes in concentration ranges does not help to explain the differences in the classic one-component parameterizations matched for data from different months (see equations given in Figure R3).

#### Author's changes in the manuscript:

No changes were made to the manuscript in connection with this particular comment.

## Reviewer's comment:

*4)* In the introduction, in addition to studies in the Baltic and the Black Sea, consider also those of other ocean basins. For e.g. refer to the following

- Mascarenhas et al. 2018 Parameterization of Spectral Particulate and Phytoplankton Absorption Coefficients in Sognefjord and Trondheimsfjord

- Nima et al. 2016 Absorption properties of high-latitude Norwegian coastal water

- Stramska et al 2003 Bio-optical relationships and ocean color algorithms for the north polar region of the Atlantic.

- Matsuoka et al 2007 Bio-optical characteristics of the western arctic ocean: Implications for ocean color algorithms

## Author's response:

Thank you for indicating these literature items. They were all quoted in the manuscript. Some of them have been included in the examples demonstrating the diversity of coefficients reported in the literature.

#### Author's changes in the manuscript:

The indicated items are cited in the Introduction section. Selected items were used in section 3.4 (see Figures 4d and e, 5c and d, 9).

#### Reviewer's comment:

5) Figures could be combined representing the two different parameterization scenarios e.g. Fig 6 and Figures 11 c,d. Less relevant ones could be provided as supplementary material.

Author's response: Agreed.

## Author's changes in the manuscript:

The suggested drawings have been merged according to the reviewer's suggestion (see new Figure 6). All figures have been rearranged, 7 panels from multi-panel figures have been removed, one six-panel figure has been moved to Appendix 2.

<u>Reviewer's comment</u>:*6)* Provide equations of trends in fig 6 and 11c,d.

<u>Author's response</u>: Agreed.

<u>Author's changes in the manuscript</u>: The equations have been added to the new Figure 6.

#### Reviewer's comment:

7) Figure captions need to be clearly distinguished from the normal text. Maintain appropriate spacing between the two.

#### Author's response:

We would like to apologize for this editing mistake, which appeared at the stage of creating an electronic document submitted to the editorial office of the journal.

<u>Author's changes in the manuscript</u>: The new version of the manuscript has been checked in this respect.

<u>Reviewer's comment:</u>*8)* List out the objectives precisely in points instead of a paragraph.

<u>Author's response</u>: Agreed.

<u>Author's changes in the manuscript</u>: The last paragraph of the Introduction section has been modified.

# Reviewer's comment:

9) All along the article there is a constant effort to explain what this study has to offer in comparison to previously published works (using similar dataset). List out the features and make them clear to the reader in one instance, e.g. at the end of the introduction after listing your objectives or before. Avoid such statements in the methods or the results section.

Author's response: Agreed.

Author's changes in the manuscript:

Explanations which facts have already been documented in the previous work of our team have been grouped in the third paragraph of the Introduction section.

<u>Reviewer's comment:</u> 10) Pay attention to the formation of paragraphs (of a consistent size) throughout the article.

<u>Author's response</u>: Agreed.

Author's changes in the manuscript:

The sizes/lengths of the paragraphs have been modified (among others in section 2. Materials and methods).

Reviewer's comment:

Minor issues:- Watch over differences between British vs American English styles. Check for consistency throughout the article.

<u>Author's changes in the manuscript</u>: The language style has been checked (British English)

# Reviewer's comment:

- Title

Parameterization of the spectral light absorption coefficient of phytoplankton in the Baltic Sea: general, monthly and two component variants of approximation formulas Instead,

**Parameterization of phytoplankton spectral absorption coefficients in the Baltic Sea**: general, monthly and two component variants of approximation formulas

Author's response: Agreed.

Author's changes in the manuscript:

The title has been corrected according to the Reviewer's suggestion. In the entire manuscript a shorter form was used: "phytoplankton absorption" (in this matter, the recommendation of the Reviewer #2 was also taken into account).

Reviewer's comment:

- Page 1 Line 8: approximate formulas, empirical equations instead Line 12: varied between x and y; be precise no '> '

Line 18-20: sentence not clear, needs to be reframed. Line 22: to fully describe **the process of** photosynthesis Line 26: pigments *it* they contain.

# Author's changes in the manuscript:

Because the term 'approximation formulas' is used in title of the work, in the first sentence of the abstract, we decided to give both forms, i.e.: 'approximate formulas (empirical equations)". Other suggestions have been taken into account.

# Reviewer's comment:

- Page 2

Line 1: ...with which their populations absorb sunlight (**References???**) Line 3: of all these relationships Line 15: They proposed ....power function (provide the equation) Line 20: empirical data, instead of empirical material Line 20: 'case 1' instead of "case 1" (single quote marks, also elsewhere in the manuscript) Line 21: contents in enclosed parenthesis (chlorophyll a concentration ranging from 0.02 to 25mg m-3) Line 27: concentration ranging from Line 33: A more recent paper, Mascarenhas et al. 2018

# Author's changes in the manuscript:

(line1) - we have changed the place in the Introduction section, where the following literature items are mentioned for the first time: Morel and Bricaud 1981 and 1986; (line 3) - corrected; (line 15) - for brevity, we have provided the information that the appropriate mathematical formulas are given later in the text (see equation 3.a in Section 3.2); (line 21 and 27) - information on chlorophyll *a* ranges of was removed for brevity; (line 33) - the suggested position was added to the list of other examples.

# Reviewer's comment:

- Page 3 Line 16: 9 years or 10 Lines 22-31: instead of the paragraph, list the objectives as Line 28: if possible??? This should be clear by now!

Author's changes in the manuscript:

(line 16) - the whole paragraph has been modified; (lines 22-31, line 28) - the paragraph has been modified according to these suggestions.

Reviewer's comment: - Page 4 Figure 1 caption: ....., enlarged view of the enclosed area.

<u>Author's changes in the manuscript:</u> Figure 1 caption has been modified.

Reviewer's comment:

- Page 5 Lines 3 to 6: Authors attempt to emphasize differences in comparison to previously published works. This could be done at the end of section in brief. Not here and there or in the beginning of the section. Line 13: pore size of GF/F Line 15: kept <del>deep</del> frozen

Author's changes in the manuscript:

(lines3 to 6) - as stated earlier all these information are now given in the third paragraph of the Introduction. (line 13) - information has been added; (line 15) - corrected.

<u>Reviewer's comment:</u> - Page 6 Structure the paragraphs appropriately

<u>Author's changes in the manuscript</u>: The sizes/lengths of the paragraphs have been modified.

Reviewer's comment:

- Page 7 statistical formulas could be avoided, will help keep the length reasonable.

<u>Author's changes in the manuscript</u>: Detailed mathematical formulas were transferred to the footnote under Table 3.

<u>Reviewer's comment:</u> - Page 8 Line 4: at selected wavelengths

<u>Author's changes in the manuscript:</u> Corrected.

<u>Reviewer's comment:</u> - Page 9 Line 5: ....and their ratio to Tchla

<u>Author's changes in the manuscript:</u> Corrected.

Reviewer's comment: - Page 14

#### Figure 5 a,c: provide detailed legends for every spectra

<u>Author's changes in the manuscript</u>: The new version of Figure 5 has been supplemented as suggested.

<u>Reviewer's comment</u>: - Page 15 Figure 6: (see the caption legend to in panel (b))

<u>Author's changes in the manuscript</u>: The caption to the new version of Figure 6 has been corrected as suggested.

<u>Reviewer's comment:</u> - Page 19 Line 1: Example of a Two component parameterization Line 2: (see also Figure 3)

<u>Author's changes in the manuscript</u>: Corrected.

Line 5: As a step towards improving....

<u>Reviewer's comment:</u> - Page 24 Line 5: check the percentages

Author's changes in the manuscript:

In the original manuscript, the ranges including data from all light wavelengths were given, while only selected wavelength were shown in tables. These particular fragment has been removed from the revised version of the manuscript.

<u>Reviewer's comment:</u> - Page 25 Line 2: now we shall.....with those of cite them here directly

<u>Author's changes in the manuscript</u>: Not applicable. The fragment has been modified.

<u>Reviewer's comment:</u> - Page 29 Line 3: Importantly, when matched.....

<u>Author's changes in the manuscript</u>: We have corrected the sentence fragment to avoid misunderstanding.

<u>Reviewer's comment:</u> - Page 30 Line 1: seawater optical components

<u>Author's changes in the manuscript</u>: The last five sentences of section 4 have been removed as suggested by the Reviewer # 2.



Figure R1. (a) and (b): Comparison of coefficients A and E of the one-component parameterization: for original variant matched to all data, and for the alternative variant matched to the data set limited to 2/3 of available data; (c) and (d) comparison of the main characteristics of the estimation error logarithmic statistics (mean logarithmic estimation error and standard error factor) calculated for original variants of one- and two-component parameterizations (all data used for training/all data used for error calculation) and for alternative variants validated against 1/3 of data.



**Figure R2.** (*extended variant of Figure 3 from the revised manuscript*). (a): Box plot presenting the range of variation of chlorophyll *a* concentration (*Tchla*) for all the data analysed, for each sampling month, and for three selected ranges of *Tchla*; (b): as (a) but showing the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments to the chlorophyll *a* concentration ( $\Sigma C_i$ ); (c): as (a) but showing the ratio of the sum of accessory pigments accessory pigments accessory pigments accessory pigments ( $\Sigma C_i$ ) and  $\Sigma C_i$  accessory pigments ( $\Sigma C_i$ ) accessory pigments ( $\Sigma C_i$ ) and  $\Sigma C_i$  and  $\Sigma C_i$  and  $\Sigma C_i$  and  $\Sigma C_i$  accessory pigments ( $\Sigma C_i$ ) accessory pigments ( $\Sigma C_i$ ) and  $\Sigma C_i$  and  $\Sigma C_i$  accessory pigments ( $\Sigma C_i$ ) accessory pigments ( $\Sigma C_i$ ) accessory pigments ( $\Sigma C_i$ ) accessory pigments ( $\Sigma C_i$  and  $\Sigma C_i$  and  $\Sigma C_i$  accessory pigments ( $\Sigma C_i$ ) accessory pigments ( $\Sigma C_i$ ) accessory pigments ( $\Sigma C_i$ ) accessory pigments ( $\Sigma C_i$ )



**Figure R3.** (alternative to Figure 6a and b from the revised manuscript) (a): Relationship between coefficient  $a_{ph}^*(440)$  and the chlorophyll a concentration *Tchla* and its functional approximations determined in this study for all the data analysed, for selected sampling months, and for limited ranges of *Tchla* (see the legend to panel b; equations are given below the panel); (b): as (a) but for  $a_{ph}^*(675)$ . The grey dots on each panel represent individual data points from our database.



**Figure R4.** (a): Box plot presenting the range of variation of the ratio of the photoprotective carotenoids to chlorophyll *a* concentration (*PPC/Tchla*) for all the data analysed, and for each sampling month; (b) and (c) relations between the ratio  $a_{ph}(\lambda)_{cal/a_{ph}}(\lambda)_m$  and the pigment concentration ratio *PPC/Tchla*, and their functional approximations (the equations are given in the panels).

**Table R1.** Arithmetic statistics of estimation absolute errors\* of coefficient  $a_{ph}(\lambda)$  in selected spectral bands when the different variants of the parameterization derived in this study were applied to the entire dataset (n= 1002). The calculated values are given for three scenarios: when the general variant of the one-component parameterization was used; when variants specific to individual months were chosen (the first alternative value is given in parentheses); and when the two-component parameterization was used (the second alternative value is given in parentheses).

λ [nm]	absolute systematic error	absolute statistical error
	$\langle \varepsilon_a \rangle [m^{-1}]$	$\sigma_{\varepsilon_a}[m^{-1}]$
350	-0.044 (-0.037; -0.044)	0.22 (0.21; 0.22)
400	-0.025 (-0.023; -0.027)	0.17 (0.16; 0.18)
440	-0.019 (-0.017; -0.022)	0.15 (0.14; 0.15)
500	-0.009 (-0.008; -0.010)	0.09 (0.08; 0.07)
550	-0.005 (-0.005; -0.005)	0.05 (0 04; 0.05)
600	-0.005 (-0.005; -0.005)	0.03 (0.03; 0.03)
675	-0.007 (-0.007; -0.009)	0.06 (0.06; 0.06)
690	-0.005 (-0.004; -0.005)	0.04 (0.04; 0.04)
700	-0.003 (-0.003; -0.003)	0.02 (0.02; 0.02)

#### \*) Arithmetic statistics of the absolute error:

- <u>mean of the absolute error</u> (representing the systematic error according to arithmetic statistics):  $\langle \varepsilon' \rangle = N^{-1} \sum_{i=1}^{N} \varepsilon'_i$ , where  $\varepsilon' = P_i - O_i$ ,  $O_i$  - observed/measured values,  $P_i$  - predicted/estimated values - <u>the standard deviation of the absolute error</u> (representing the statistical error according to arithmetic statistics):

$$\sigma_{\varepsilon'} = \sqrt{\frac{1}{N} \left( \sum_{i=1}^{N} (\varepsilon'_i - \langle \varepsilon' \rangle)^2 \right)}$$