Author's Response

"Technical Note: Algal Pigment Index 2 in the Atlantic off the Southwest Iberian Peninsula: standard and regional algorithms"

Manuscript Ref.: os-2016-41

Contents

Part A. Point-by-point response to reviewers and relevant changes in the manuscript.

Replies to Comments of Referee V. Suslin and relevant changes in the manuscript.

Questions

Comments from Referees: page 3 line 30: you write " .. when _ is below the threshold _=1". Why _<1 but more or less 1?

Authors' response: The authors agree that this sentence was not easy to read, and have changed it accordingly. It should be: "…when $\eta \leq 1$".

Authors' changes in manuscript: In page 4, line 17, where it was "when η is below the threshold $\eta=1$.", it is now "…when $\eta \leq 1$.".

Comments from Referees: What the satellite data selection criteria you used in this study to analyze the quality of the Algal Pigment Index 2 in Sagres? It is clear that all was done 99 series * 3 (A, B, C) = 297 ground truth measurements, and the main factor is cloudy. What have any other criteria (except cloud) been used?

Authors' response: The selection of satellite images was restricted to images without clouds and contamination, as indicated by not having specific Product Confidence (PCD) flags. The most common flags were PCD1_13 and PCD 19, where: PCD1_13 flag is a composite confidence flag for all the reflectance wavebands, and indicates a failure in the atmospheric correction for at least one of these wavebands and PCD 19 is a flag for uncertain aerosol type and optical thickness, i.e., also linked to the atmospheric correction. High levels of sun glint affected some of the days, and the corresponding flag was taken into account to check if the data were contaminated by a bright pattern of specular reflectance from the sun. An ice haze flag was also checked for some of the MERIS images when there was high radiance in the blue region of the spectrum caused by ice in the atmosphere or by a very high optical thickness. More details are in Cristina et al. 2014 and Cristina et al. 2016.

Authors' changes in manuscript: The authors have now included a section in Page 3, Line 2 about the image selection criteria, quoting "The selection of satellite images was restricted to images without clouds and contamination, as indicated by not having specific Product Confidence (PCD), sun glint and ice flags. More details on the image selection criteria and full description of flags are reported in Cristina et al. 2016 (Cristina, S., Cordeiro, C., Lavender, S., Goela, P.G., Icely, J., Moore, G., Newton, A. Remote Sensing. 2016. Seasonal-Trend decomposition time series based on Loess applied to MERIS products from the SW Iberian Peninsula: Sagres. Remote Sensing, 8(6), 449; doi:10.3390/rs8060449.)"

Comments from Referees: Page 12: Fig. 1(c,f): Are you sure that in these figures N = 297? I think N = 54. Check please!

Authors' response: The authors thank the referee for noting this issue. In fact, there was an important detail requiring explanation in the manuscript. Regarding Fig.1, two different analyses are shown: a validation exercise (in left and middle panel) of MERIS products data against in situ reference data, and the other analysis (right panel) is the assessment of the performance of the regional NN algorithm for the retrieval of TChl*a*.

The different numbers of data points arise from the differences between the two analyses, the greater number of data points is used to evaluate the algorithm on the basis of its best performance (e.g. Cristina et al., 2016, Sá et al., 2015; Kajiyama et al., 2013). The x and y axes of the figures in the left and middle panels (Figs. 1a-d) represent the values of API2 product as retrieved by both MERIS and by the regional algorithm using MERIS reflectances, respectively. In these cases, the total numbers of points compared were 54. In contrast, Figs. 1c and 1f represent the regional algorithm trained using in situ reflectances collected from the in situ deployment of a Satlantic® radiometer. In this case, 4 to 8 reflectance casts were collected with the radiometer for each location corresponding to one in situ TChl*a* measurement. As the objective was the regional algorithm performance assessment, all those points were used for this comparison, showing the best case scenario for the use of the regional algorithm. However, we can still show that comparison results remain consistent with the reported statistical values (Figure A1 in attachment) even when using only one radiometric cast per location (i.e., N=54 as in right panels of Fig. A1) to compare MLP(R_{rs}^{SITU}) with in situ references (TChl*a* (ABS, HPLC)).

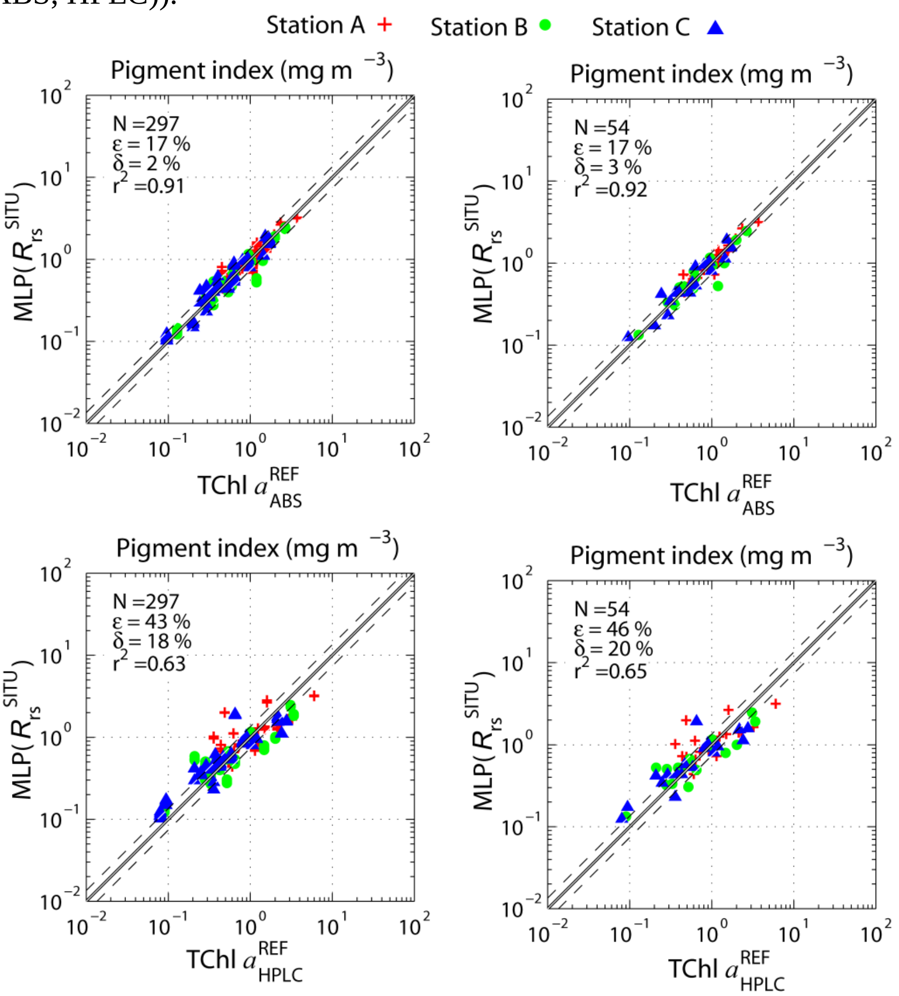

Figure A1 – Comparison of the performance of the regional NN algorithm results using only N=54 points (right panels), or with N=297 points (left panels, as originally Figs. 1c and 1f in the manuscript), both against TChl*a* references (retrieved through a_{ph}(442) and with HPLC).

Authors' changes in manuscript: A more detailed explanation has now been included in the manuscript to explain better the difference between number of data points, in Page 5, line 2, quoting: "The total number of samples used to validate $\mathrm{MER}^{\mathrm{API2}}$ and $\mathrm{MLP}(R_{\mathrm{rs}}^{\mathrm{MER}})$ algorithms results with respect to the in situ reference measurements was N=54. In contrast, the total number of samples for assessing the performance of regional MLP algorithm with in situ reference measurements ($\mathrm{MLP}(R_{\mathrm{rs}}^{\mathrm{SITU}})$, was N=297. This larger number of samples is based on the data from 4-8 radiometric casts for each in situ TChl*a* sample at each location."

Comments from Referees: Page 13: In Fig. 2(b) I believe that you had the opportunity to show all measurements N = 297, not only N = 54!

Authors' response: The authors thank the referee for noting this issue. In fact, there were important details requiring explanation in the manuscript. In Fig. 2b the two techniques for retrieval of reference TChl*a* are compared. As explained by the authors in the previous comment, the number of in situ measurements for TChl*a* retrieval (either through absorption or by HPLC) at surface was only 54. The number of samples was instead set to 297 in Figs 1c and 1f, because at each location sampled for TChl*a* retrieval, 4 to 8 radiometric casts were collected. However the radiometric dataset is not represented in Fig. 2b, only in situ TChl*a* measurements.

Authors' changes in manuscript: As mentioned in the previous comment, now the manuscript will include a more detailed explanation on the difference between the number of data points (Page 5, Line 2).

GENERAL COMMENTS

This research is actual. The regional bio-optical algorithms demand for more reliable results by using satellite ocean color data. This study is a continuation of the work of these authors (eg, IEEE GEOSCIENCE AND REMOTE SENSING LETTERS, Digital Object Identifier 10.1109 / LGRS.2016.2529182) for the development of a regional satellite algorithm in the Atlantic off the southwestern Iberian Peninsula.

Specific comments

Comments from Referees: in "Introduction" issue: To outline a significance of your research to add reference/ references to other regional algorithms (for example, for the Mediterranean Sea) GREGG , W.W. and CASEY , H.W., 2004, Global and regional evaluation of the SeaWiFS chlorophyll data set. Remote Sensing of Environment, 15 December, 93, Iss. 4, pp. 463–479, doi:10.1016/j.rse.2003.12.012.

Authors' response: The authors acknowledge the suggestion, and have now included this reference in the introduction section.

Authors' changes in manuscript: In page 2, Lines 12/13, the following sentence and references were added, quoting: "In such cases, regionalized bio-optical algorithms are required (Bricaud et al., 2002, Gregg and Casey, 2004)."

Comments from Referees: Statistics of in situ measurements by seasons is missed (among N=54/297 for stations A, B and C separatly). In particular, it could be useful in connection with Fig. 2b.

Authors' response: The authors agree with the referee on the utility of the analysis of the seasonality. Notwithstanding, the scope of this brief technical note was to evaluate the performance of a regional algorithm for the retrieval of TChl*a* and also on the product definition itself. The analysis of seasonal components and trends would also imply the consideration of forcing agents (e.g. upwelling), which could be considered as an interesting follow up work, but a bit far from the scope of the present technical note.

Comments from Referees: Warning: "Tchla (Ref, ABS)" cannot be equated with the concentration of chlorophylla in Sagres, we can only speak of in situ aph (442). Do you agree?

Authors' response: In this technical note, the authors are discussing pigment indices derived from different quantities, having taken into account the definition of algal pigment indices (API1 and API2) by the European Space Agency. API1 is equivalent to the concentration of TChl*a* as determined by HPLC, and API2 is a proxy of TChl*a* concentration determined by means of an empirical relationship between $a_{ph}(442)$ and TChl*a*. In page 3, lines 27/28, it is explained that TChl*a* (Ref, ABS) is the in situ API2 equivalent measure estimated through $a_{ph}(442)$, using the following expression: $MER^{API2} = A \times a_{ph}(442)^B$, where A=21.0 and B=1.04 (derived from field measurements in the German Bight and Norwegian waters as in Doerffer and Schiller, 2007). To ensure that the comparisons were the most reliable possible, the choice of the in situ references was made based on these definitions.

Comments from Referees (Technical corrections): Page 3 line 2: "Total chlorophyll *a* (Tchla) .." repeat reference. The first reference to "Tchla" was on page 1 line 16 in Abstract.

Authors' response: Thanks for noticing. The manuscript has been revised acknowledging the Referee's recommendation.

Authors' changes in manuscript: The Referee's request has been addressed in the revised manuscript, where it was "... Total chlorophyll *a* (TChl*a*) …" (page 3 line 2), it has been changed to "…TChl*a* …" now in page 3 line 4.

Comments from Referees (Technical corrections): Page 3 line 8: instead " .. neural nets NN" stay " .. neural nets" or " .. NN". The first reference to "NN" was on page 2 line 14.

Authors' response: Thanks for noticing. The manuscript has been revised acknowledging the Referee's recommendation.

Authors' changes in manuscript: The Referee's request has been addressed in page 3 in line 26 in the revised manuscript, where it was "... is estimated with two neural nets NN", and has now been changed to "…is estimated with two NN".

Comments from Referees (Technical corrections): Page 3 line 8: "BOA"The first reference to "BOA" was on page 2 line 6.

Authors' response: Thanks for noticing. The manuscript has been revised acknowledging the Referee's recommendation.

Authors' changes in manuscript: The Referee's request has been addressed in page 3 in line 26 in the revised manuscript, where it was "…bottom of the atmosphere (BOA)…", and has been changed to "…computes BOA…".

Comments from Referees (Technical corrections): Page 3 line 16: http://ocportugal.org/sites/default/files/api2Sgr.pdf - Page not found

Authors' response: Thanks for noticing. The revised manuscript has the corrected link.

Authors' changes in manuscript: The correction of the link in the revised manuscript was made in page 4 line 4, instead …"http://ocportugal.org/sites/default/files/api2Sgr.pdf"…, and now is going to be "...http://ocportugal.org/sites/default/files/mlpSgrAPI2.pdf".

Comments from Referees (Technical corrections): Page 3 line 7: remove ":" in "2.2.1 MERIS Standard algorithm API2:". The same for "2.2.1 Regional MLP NN algorithm:" on page 3 line 13

Authors' response: Thanks for noticing. The manuscript has been revised acknowledging the Reviewer's recommendation.

Authors' changes in manuscript: The ":" were removed from "2.2.1 MERIS Standard algorithm API2:" and "2.2.1 Regional MLP NN algorithm:". These two sub-sections were changed in the revised manuscript to "2.2.1 MERIS Standard algorithm API2" in page 3 line 25 and "2.2.2 Regional MLP NN algorithm" in page 4 line 1.

Comments from Referees (Technical corrections): Page 4 line 1: "2.1 In situ reference data" move before issue "2.2.1 MERIS Standard algorithm API2".

Authors' response: This section has been moved following the referee's suggestion.

Authors' changes in manuscript: The Section "2.1 In situ reference data" in page 4 line 1 has now been moved to page 3, line 8.

Comments from Referees (Technical corrections): "Page 12: In Figure 1(a), a caption of the X axis can be seen partially."

Authors' response: Thanks for noticing. The Figure 1(a) has been revised and the axis legend can now be seen in full.

Authors' changes in manuscript: Fig. 1 was altered, to meet this requirement. The new figure is included.

Replies to Comments of Reviewer #2 (Anonymous Referee) and relevant changes in the manuscript.

GENERAL COMMENTS

As a technical note, this manuscript provides details the match up analysis between satellite retrieved estimates of chl-a and in situ measurements from different sources for a small region off the Iberian Peninsula. The results would be interesting to a limited readership who are interested in the same region. However I do think the paper has a major flaw; the authors find that the comparison of in situ chl-a parameters from different sources (absorption vs HPLC) yields better results than the comparison of retrieved parameters with either absorption or HPLC in situ results. These results are affected by the comparison of only 54 pairs of data for the retrieved vs in situ compared to 297 for the in situ abs vs HPLC. The potentially better metrics for the comparison of in situ parameters could be totally or in part due to the sample size being approximately 6x that of the retrieved vs in situ comparisons. I presume that the smaller data set is due to cloud cover etc so that you could only retrieve 54 data points that matched to an in situ measurement. If this is the case then the comparison between in situ abs vs HPLC should also only be for these same 54 data sets, so that all comparisons are being made on the same data sets. Overall I think the idea of the paper is suitable as a technical note in OSD, but I would like to see the data and conclusions drawn after the authors re-analysed the data using the same 54 data sets for all comparisons, before I commented on the worth of the final paper.

Authors' response: The authors thank the referee for noting this issue. In fact, there was an important detail requiring explanation in the manuscript. Regarding Fig.1, two different analyses are shown: a validation exercise (in left and middle panel) of MERIS products data against in situ reference data, and the other analysis (right panel) is the assessment of the performance of the regional NN algorithm for the retrieval of TChl*a*. The different numbers of data points arise from the differences between the two analyses, the greater number of data points is used to evaluate the algorithm on the basis of its best performance (e.g. Cristina et al., 2016, Sá et al., 2015; Kajiyama et al., 2013). The x and y axes of the figures in the left and middle panels (Figs. 1a-d) represent the values of API2 product as retrieved by both MERIS and by the regional algorithm using MERIS reflectances, respectively. In these cases, the total number of points compared were 54. In contrast, Figs. 1c and 1f represent the regional algorithm trained using in situ reflectances collected from the in situ deployment of a Satlantic® radiometer. In this case, 4 to 8 reflectance casts were collected with the radiometer for each location corresponding to one in situ TChl*a* measurement. As the objective was the regional algorithm performance assessment, all those points were used for this comparison, showing the best case scenario for the use of the regional algorithm. However, we can still show that comparison results remain consistent with the reported statistical values (Figure A1 in attachment) even when using only one radiometric cast per location (i.e., N=54 as in right panels of Fig. A1) to compare MLP(R_{rs}^{SITU}) with in situ references (TChl*a* (ABS, HPLC)).

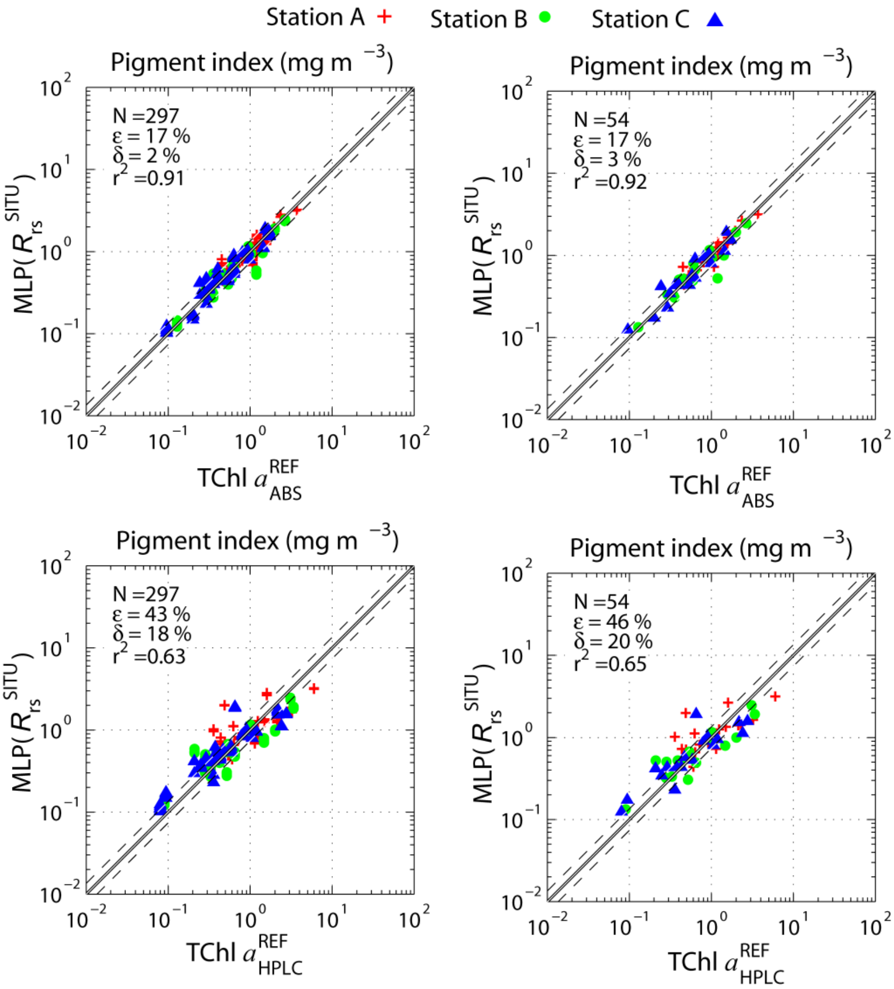

Figure A1 – Comparison of the performance of the regional NN algorithm results using only N=54 points (right panels), or with N=297 points (left panels, as originally Figs. 1c and 1f in the manuscript), both against TChl*a* references (retrieved through $a_{ph}(442)$ and with HPLC).

Authors' changes in manuscript: A more detailed explanation has now been included in the manuscript to explain better the difference between number of data points, in Page 5, line 2, quoting: "The total number of samples used to validate MER^{API2} and MLP(R_{rs}^{MER}) algorithms results with respect to the in situ reference measurements was N=54. In contrast, the total number of samples for assessing the performance of regional MLP algorithm with in situ reference measurements (MLP(R_{rs}^{SITU}), was N=297. This larger number of samples is based on the data from 4-8 radiometric casts for each in situ TChl*a* sample at each location."

Specific comments

Comments from Referees: A general comment is that there was a lot of acronyms and I think it would be useful to have a table which defined all the acronyms.

Authors' response: The Referee's suggestion to create a table with all the acronyms was appreciated and included in the revised manuscript (Table 3).

Authors' changes in manuscript: Page 12 includes Table 3 with the list of the acronyms used in the manuscript.

Comments from Referees: Pg 2, line 21: "of the Southwestern Iberian…" should be "off the Southwestern Iberian..."

Authors' response: Thank you for noticing. The sentence has been modified in the revised manuscript.

Authors' changes in manuscript: In page 2, line 21, where it was "of the Southwestern Iberian…", has been changed to "…off the Southwestern Iberian…".

Comments from Referees: Pg 3, line 8: delete neural nets and bottom-of-the-atmosphere as they have both already been defined.

Authors' response: Thanks for noticing. The manuscript has been revised acknowledging the Reviewer's recommendation.

Authors' changes in manuscript: The Referee's request has been addressed in page 3 in line 26 in the revised manuscript, where it was "…bottom of the atmosphere (BOA)…", has been changed to "…computes BOA…".

Comments from Referees: Pg 3, line 16: could not access web address provided – "page not found" message

Authors' response: Thanks for noticing. The revised manuscript has the corrected link.

Authors' changes in manuscript: The correction of the link in the revised manuscript was made in page 4 line 4, where…"http://ocportugal.org/sites/default/files/api2Sgr.pdf"… has been changed to "...http://ocportugal.org/sites/default/files/mlpSgrAPI2.pdf".

Comments from Referees: Pg3, line 21: "applicability should be application"

Authors' response: Although other terminology could be applied, like the Referee's suggestion, the authors decided to maintain the same terminology, to assure the consistency with previously published studies (Cristina et al., 2016, Sá et al., 2015; Kajiyama et al., 2013) on similar topics.

Comments from Referees: Pg 3, line 23: "applicability should be application"

Authors' response: Although other terminology could be applied, like the Referee's suggestion, the authors decided to maintain the same terminology, to assure the consistency with previously published studies (Cristina et al., 2016, Sá et al., 2015; Kajiyama et al., 2013) on similar topics.

Comments from Referees: Pg 3, line 25: “PCA should be in brackets – (PCA)”

Authors’ response: Thanks for noticing. The manuscript has been revised acknowledging the Referee recommendation.

Authors’ changes in manuscript: Where it was “…Principal Component Analysis PCA ...” in the page 3, line 25, it has been changed in page 4 line 13 of the revised manuscript “…Principal Component Analysis (PCA)...”.

Comments from Referees: Pg 3, line 29: remove “novelty index” or “ÅN´ ” as this term has already been defined

Authors’ response: Thanks for noticing this. The manuscript has been revised acknowledging the Referee’s recommendation.

Authors’ changes in manuscript: Where it was “…is its novelty index η ...” in the page 3, line 29, has been changed in page 4 line 17 of the revised manuscript “…is its η ...”.

Comments from Referees: Pg 3, line 30: replace “when _ is below the threshold _=1.” With “when _ < 1.”

Authors’ response: The authors agree that this sentence was not easy to read, and have changed the statement to: “…when $\eta \leq 1$”.

Authors’ changes in manuscript: In page 4, line 17, where it was “when η is below the threshold $\eta=1$.”, it is now “…when $\eta \leq 1$.”.

Comments from Referees: Pg 4, line 3: replace “an hyperspectral” with “a hyperspectral”

Authors’ response: Thanks for noticing this. The revised manuscript has replaced the word.

Authors’ changes in manuscript: Where it was “…an hyperspectral...” in the page 4, line 3, has been changed to “…a hyperspectral ...”in page 3 line 10 of the revised manuscript.

Comments from Referees: Pg 4, line 3: delete “located below the surface” as it is implied by the preceding “subsurface”.

Authors’ response: Thanks for noticing this. The sentence was deleted following the Referee recommendation.

Authors' changes in manuscript: The sentence from the page 4 line 3 "…a subsurface radiance sensor $L_u(\lambda)$ located below the surface...", has been changed to "… a subsurface radiance sensor $L_u(\lambda)$..." in page 3 line 8.

Comments from Referees: Pg 4, line 10: replace "in GF/F" with "on GF/F"

Authors' response: Thanks for noticing this. The word was changed following the Referee recommendation.

Authors' changes in manuscript: The word from the page 4 line 10 "…in GF/F...", has been changed to "…on GF/F..." in page 3 line 18.

Comments from Referees: Pg 4, line 14: the sodium hypochlorite bleaching does not remove the detrital contribution; it removes the pigment contribution. The phytoplankton contribution is determined as the difference between the total particulate and detrital absorption which are recorded before and after the hypochlorite bleaching, respectively.

Authors' response: The authors agree that the sentence was not clear, and the manuscript will be changed accordingly.

Authors' changes in manuscript: In page 4, line 13/14, where the text "The phytoplankton absorption was determined from the total particle absorption, through the measurements before and after sodium hypochlorite bleaching of the filters to remove the contribution of detrital absorption" has been changed to "The phytoplankton absorption was determined as the difference between the total particulate and detrital absorption which were measured before and after sodium hypochlorite bleaching (Ferrari and Tassan, 1999; Goela et al., 2013), respectively.

Comments from Referees: Pg 7, line 4: "An additional explanation could be that TChlABSREF was determined using $a_{ph}(442)$, which is likely better related to Rrs than TChlHPLCREF (both $a_{ph}(442)$ and Rrs directly represent optical properties)." $a_{ph}(442)$, might be better related to Rrs, but TChlHPLC is a direct measurement of the chl-a concentration whereas the $a_{ph}(442)$ is an indirect measurement of the absorption due to phytoplankton. It is estimated as the difference between the total particulate and detrital absorption, both of which are measured, but would carry errors associated with the technique (extraction efficiency of the pigments, the dominance of a detrital signal etc) which would affect the accuracy of the estimation of $a_{ph}(442)$.

Authors' response: The authors agree that this statement should be included in the manuscript.

Authors' changes in manuscript: This statement was added to the argument, in Page 7, line 10, quoting: "Some caveats would however apply to this argument, because $\mathrm{TChl}a_{\mathrm{HPLC}}^{\mathrm{REF}}$ is a direct measurement of the TChl*a* concentration whereas $\mathrm{TChl}a_{\mathrm{ABS}}^{\mathrm{REF}}$ is an indirect measurement which has errors associated with the laboratorial determination of aph(442)".

Comments from Referees (Figures and captions): A general comment is that if the reader prints this publication, the font size used on the figures is quite small and can make reading difficult, especially both parts of Figure 2.

Authors' response: Thank you for noticing. The font size in the figure was expanded.

Authors' changes in manuscript: The figures in attachment have a larger font size.

Comments from Referees (Figures and captions): Figure 3: should have a description of each panel in the legend rather than referring to a section in the text. It is difficult to read both the section and the plot at the same time on a computer.

Authors' response: Thanks for the comment. The authors agree, and now a more detailed legend is presented.

Authors' changes in manuscript: The legend of Figure 3 was changed to: "Comparison between Sagres regional Multilayer Perceptron (MLP) algorithm map with MERIS pigment index product map Algal Pigment Index 2 for the 25th August 2010, showing a) the product map of the regional MLP, b) standard API2 MERIS product map, c) difference between $\mathrm{MER}^{\mathrm{API2}}$ and MLP($R_{\mathrm{rs}}^{\mathrm{MER}}$), d) region of applicability of MLP($R_{\mathrm{rs}}^{\mathrm{MER}}$), f) results of the application of the regional MLP to the Portuguese coast in the three regions of interest (shown in e). Please see Sect. 3.2 for a more detailed description of the panels."

Part B. MARKED MANUSCRIPT

Technical Note: Algal Pigment Index 2 in the Atlantic off the Southwest Iberian Peninsula: standard and regional algorithms

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Abstract. In this study, Algal Pigment Index 2 (API2) is investigated in Sagres, an area located in the Atlantic off the southwestern Iberian Peninsula. Standard results provided by MEdium Resolution Image Spectrometer (MERIS) ocean color sensor were compared with alternative data products, determined through a regional inversion scheme, using both MERIS and in situ remote sensing reflectances (R_{rs}) as input data. The reference quantity for performance assessment is in situ total chlorophyll *a* (TChl*a*) concentration estimated through phytoplankton absorption coefficient (i.e., equivalent to API2). Additional comparison of data products has also been addressed to TChl*a* concentration determined by High Performance Liquid Chromatography. The MERIS matchup analysis revealed a systematic underestimation of TChl*a*, which was confirmed with an independent comparison of product maps analysis. The study demonstrates the importance of regional algorithms for the study area that could complement upcoming standard results of the present Sentinel-3/OLCI space mission.

Keywords: absorption, MERIS Algal Pigment Index 2, Multi-Layer Perceptron (MLP) neural nets, ocean color, remote sensing.

1 Introduction

The MERIS space sensor, operated by the European Space Agency (ESA) on-board of the Envisat platform from 2002 to 2012, has been continuously supported by investigations for the assessment and improvement of data products. Commissioned studies include the validation of radiometric data such as the R_{rs} (Cristina et al., 2014; Kajiyama et al., 2014), as well the analyses of derived product maps (Kajiyama et al., 2014; D'Alimonte et al., 2014, Cristina et al., 2016). These MERIS validation activities have established an important basis to address Earth Observation (EO) capabilities through the Ocean Land Color Instrument (OLCI) sensor launched on the Sentinel-3 satellite in February 2016. OLCI data products are

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the main component of the Copernicus European program to monitor the marine environment, and the retrieval of Chlorophyll *a* (Chl*a*) is a core task of the Sentinel-3 space mission. Chl*a* is needed to estimate the phytoplankton biomass in the ocean and to contribute to a variety of inter-related investigations and applications, including climate data records, environmental legislation, and a number of economic activities such as fisheries and aquaculture. After the removal of the atmospheric contribution to the signal recorded at the top of the atmosphere, Chl*a* can be estimated from the bottom-of-atmosphere (BOA) R_{rs} values using the standard approach with polynomial algorithms based on band-ratios of the input radiometric quantities. The corresponding MERIS data product is denoted Algal Pigment Index 1 (API1) (Morel and Antoine, 2011). The use of band-ratio is based on the assumption that seawater optical properties are driven by Chl*a*. A tendency to overestimation has however been documented in optically complex marine conditions (D'Alimonte et al., 2014). This can occur when optically active constituents such as Colored Dissolved Organic Matter (CDOM) and detrital particulate matter exceed their typical levels. The Chl*a* retrieval accuracy declines in these optically complex conditions because the band-ratio approach attributes variations of the R_{rs} spectral slope to changes of Chl*a*. In such cases, regionalized bio-optical algorithms are required (Bricaud et al., 2002, Gregg and Casey, 2004). Alternative ocean color inversion schemes adopted to improve the Chl*a* retrieval from space include artificial Neural Nets (NN) using R_{rs} at selected wavelengths as input. In the case of MERIS standard deliverables, this corresponds to the API2 data product (Doerffer and Schiller, 2007).

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Although NNs can in principle model any relationship between apparent and inherent optical properties, their performance is in practice mostly determined by the dataset used for their training. Specific analyses are then needed to compare the standard MERIS API2 results with independent estimates. This main requirement is addressed in the present work by: 1) developing and assessing the performance of an independent regional Multilayer Perceptron (MLP) scheme to retrieve results equivalent to MERIS API2 values; and 2) comparing MERIS standard and regional API2 product maps.

The region under study is the Atlantic off the Southwestern Iberian Peninsula, where in situ reference data were collected at three stations off the Sagres region at 2, 10 and 18 km from the coast (henceforth stations A, B and C, respectively). The study is conducted based on both matchup analyses and product map inter-comparisons, with timely presentation of the results acknowledging, not only the planned MERIS data reprocessing, but also the need for a benchmark for the analysis of the upcoming OLCI API2 deliverables. An added value of this study is to confirm that qualitative evaluations based on product maps comparison can complement matchup data at the early mission stages of OLCI, when the statistical significance of matchup analysis is limited.

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2 Data and Methods

Field campaigns were performed from 2008 to 2012 at the three study sites, with simultaneous collection of water samples and radiometric measurements. MERIS Level 2 Full Resolution (FR, 290 m x 260 m) and Reduced Resolution (RR, 1.20 km x 1.04 km) satellite images were extracted for matchup analysis and product map comparison, respectively, and analyzed with the Basic ERS & ENVISAT (A) ATSR and MERIS Toolbox (BEAM version 4.9). The MEGS 8.1 processor (MERIS third reprocessing) was used to derive level 2 data, in agreement with previously reported extraction procedures (Cristina et al., 2014, 2015). The selection of satellite images was restricted to images without clouds and contamination, as indicated by not having specific Product Confidence (PCD), sun glint and ice flags. More details on the image selection criteria and full description of flags are reported in Cristina et al. (2016). TChl*a* concentration (monovinyl Chl*a* + divinyl Chl*a* + chlorophyllide *a* + phaeopigments) was determined by High Performance Liquid Chromatography (HPLC), according to Wright and Jeffrey (1997), herein referred as $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{HPLC}}$. The protocols adopted for TChl*a* extraction, identification and quantification procedures are reported in Goela et al. (2014, 2015).

2.1 In situ reference data

In situ radiometric measurements were acquired with the tethered attenuation coefficient chain sensor (TACCS, Satlantic®), supporting a hyperspectral surface irradiance sensor $E_s(\lambda)$ and a subsurface radiance sensor $L_u(\lambda)$, as well as a tethered attenuation chain equipped with four irradiance sensors at nominal depths of 2, 4, 8 and 16 m. Normalized water leaving reflectance (ρ_N) was computed with Eq. (1):

$$\rho_N(\lambda) = \pi \frac{L_W(\lambda)}{E_S(\lambda)}, \qquad (1)$$

where L_w is the water leaving radiance determined by propagating L_u from below to above the sea surface and corrected for self-shading following (Gordon and King, 1992). $\rho_N(\lambda)$ corresponds to the remote sensing reflectance R_{rs} upon scaling with π.

For the determination of in situ absorption of phytoplankton pigments at 442 nm ($a_{ph}(442)$), seawater filtrates (0.5 L) were collected on GF/F filters (pore size 0.7 µm), which were then analyzed with the transmittance-reflectance technique as in (Tassan and Ferrari, 2002), using a dual beam-spectrophotometer (GBC® CINTRA 40), equipped with an integrating sphere. The phytoplankton absorption was determined as the difference between the total particulate and detrital absorption, which were measured before and after sodium hypochlorite bleaching (Ferrari and Tassan, 1999; Goela et al., 2013), respectively. The API2 in situ equivalent algal pigment index $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{ABS}}$, was then estimated by converting $a_{ph}(442)$ into API2, using the same regression coefficients presented in Sect. 2.2.2.

2.2 Chlorophyll *a* retrieval algorithms

2.2.1 MERIS standard algorithm API2:

This standard product is estimated with two NNs. The first NN computes BOA R_{rs} values by removing the atmospheric radiometric contribution. The second NN utilizes the BOA R_{rs} to derive the absorption of phytoplankton pigments at 442 nm ($a_{ph}(442)$). The final API2 product is then computed as $\mathrm{MER}^{\mathrm{API2}} = \mathrm{A} \times a_{ph}(442)^{\mathrm{B}}$, with power-law regression coefficients A=21.0 and B=1.04 derived from field measurements in the German Bight and Norwegian waters (Doerffer and Schiller, 2007).

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2.2.2 Regional MLP NN algorithm

The regional MLP for retrieving the data product equivalent to API2 has been trained with the in situ data collected at the Sagres site (instructions for independent implementation by users are provided as supplemental material http://ocportugal.org/sites/default/files/mlpSgrAPI2.pdf). This MLP is here applied to two different sets of input data for assessment of performance and for comparison of results. The first set consists of the in situ R_{rs} values (R_{rs}^{SITU}), and the second set includes standard MERIS BOA R_{rs} data (R_{rs}^{MER}). Corresponding data products are denoted MLP(R_{rs}^{SITU}) and MLP(R_{rs}^{MER}), respectively. In both cases, R_{rs} at 490, 510 and 560 nm were selected as input channels, in agreement with the reference study (Cristina et al., 2014).

A novelty detection scheme (D'Alimonte et al., 2014; Bishop, 1994) was used to verify the algorithm applicability range by evaluating the representativeness of the input data in the training dataset (D'Alimonte et al., 2003; Mélin et al., 2011; Sá et al., 2015). The adopted applicability range is based on a novelty index (η) presented in published works (D'Alimonte et al., 2013; Sá et al., 2015). A revision is however applied for the scope of this work. This updated version considers all dimensions of the Principal Component Analysis (PCA) of selected input data, rather than only the first three components considered in the past (see the supplemental material for details). This updated definition is more effective for cases where the variability of training and application data tends to occur at different wavelengths (details not presented here). Key features are: 1) η is bounded between 0 and ∞; 2) the more the R_{rs} spectrum is similar to the in situ MLP training measurements, the lower is its η; and 3) an R_{rs} spectrum is considered within the MLP applicability range when η≤1.

3 Results

The main tasks of this study are: 1) to evaluate the performance of regional MLP algorithm and the MER^{API2} results with respect to the in situ $\mathrm{TChl}a_{\mathrm{ABS}}^{\mathrm{REF}}$ reference measurements; 2) to verify the applicability of the regional MLP(R_{rs}^{MER}) and to compare product maps with MER algal pigment indices; and 3) to extend the analysis by also considering $\mathrm{TChl}a_{\mathrm{HPLC}}^{\mathrm{REF}}$ for data product assessment.

The statistical figures used to evaluate the estimated (y) in relation to the reference in situ TChl$a$ (x), were absolute (ε) and signed (δ) percent differences, defined as:

$$\varepsilon = \frac{1}{N}\sum_{i=1}^{N}\frac{|y_i - x_i|}{x_i}\times 100;\ \delta = \frac{1}{N}\sum_{i=1}^{N}\frac{y_i - x_i}{x_i}\times 100\ , \qquad (2)$$

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Moved up [1]: 2.1 In situ reference data¶
In situ radiometric measurements were acquired with the tethered attenuation coefficient chain sensor (TACCS, Satlantic®), supporting an hyperspectral surface irradiance sensor $E_s(\lambda)$ and a subsurface radiance sensor $L_u(\lambda)$ located below the surface, as well as a tethered attenuation chain equipped with four irradiance sensors at nominal depths of 2, 4, 8 and 16 m. Normalized water leaving reflectance was computed with Eq. (1)
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where L_w is the water leaving radiance determined by propagating L_u from below to above the sea surface and corrected for self-shading following (Gordon and King, 1992). $\rho_N(\lambda)$ corresponds to the remote sensing reflectance R_{rs} upon scaling with π.¶
For the determination of in situ a_{ph}, seawater filtrates (0.5 L) were collected in GF/F filters (pore size 0.7 µm), which were then analyzed with the transmittance-reflectance technique as in (Tassan and Ferrari, 2002), using a dual beam-spectrophotometer (GBC® CINTRA 40), equipped with an integrating sphere. The phytoplankton absorption was determined from the total particle absorption, through the measurements before and after sodium hypochlorite bleaching of the filters to remove the contribution of detrital absorption (Ferrari and Tassan, 1999; Goela et al., 2013). The API2 in situ equivalent algal pigment index $\mathrm{TChl}a_{\mathrm{ABS}}^{\mathrm{REF}}$, was then estimated, converting $a_{ph}(442)$ into API2, using the same regression coefficients presented in Sect. 2.2.1.¶

where N is the total number of samples and i is the sample index. For product maps comparison, the absolute (ε^*) and signed (δ^*) unbiased differences were instead determined as:

$$\varepsilon^* = \frac{1}{N}\sum_{i=1}^{N}\frac{|y_i - x_i|}{y_i + x_i} \times 200;\ \delta^* = \frac{1}{N}\sum_{i=1}^{N}\frac{y_i - x_i}{y_i + x_i} \times 200\ , \quad (3)$$

where x_i and y_i are the MLP(R_{rs}^{MER}) and MER^{API2} values, respectively, taking the mean of the two values as a reference. In addition, the coefficient of determination r^2 between the evaluated quantities is also reported. The total number of samples used to validate MER^{API2} and MLP(R_{rs}^{MER}) algorithms results with respect to the in situ reference measurements was N=54. In contrast, the total number of samples for assessing the performance of regional MLP algorithm with in situ reference measurements (MLP(R_{rs}^{SITU}), was N=297. This larger number of samples is based on the data from 4-8 radiometric casts for each in situ TChl*a* sample at each location.

3.1 Matchup data analysis

The top panels of Fig. 1 present the matchup comparisons of MER^{API2}, MLP(R_{rs}^{MER}) and MLP(R_{rs}^{SITU}) with respect to the in situ reference $\mathrm{TChl}a_{\mathrm{ABS}}^{\mathrm{REF}}$ (Figs. 1a, 1b and 1c, respectively). While MER^{API2} underestimated TChl*a* (δ = -34%) especially at higher concentrations, the regional products slightly overestimated TChla (δ =11% for MLP(R_{rs}^{MER}) and 2% for MLP(R_{rs}^{SITU}). The best agreement between data sets was obtained with MLP(R_{rs}^{SITU}), while MER^{API2} showed larger uncertainties. Table 1 presents the matchup analysis where the underestimation of MER^{API2} in relation to TChl*a* is relatively constant (35%, 32% and 34%, in stations A, B and C, respectively) in all stations, but the correlation coefficient improves towards offshore (0.22, 0.60, 0.67 in stations A, B and C, respectively).

In general, the matchup analysis with $\mathrm{TChl}a_{\mathrm{HPLC}}^{\mathrm{REF}}$ revealed higher uncertainties for MER^{API2}, MLP(R_{rs}^{MER}) and MLP(R_{rs}^{SITU}), as detailed in Fig. 1 (lower panel). Note that also in this case MLP(R_{rs}^{SITU}) presented the best results, with the highest coefficient of determination and the lowest bias. Similarly to what documented for $\mathrm{TChl}a_{\mathrm{ABS}}^{\mathrm{REF}}$, the bias for $\mathrm{TChl}a_{\mathrm{HPLC}}^{\mathrm{REF}}$ displayed only small differences between the sampling stations. The coefficient of determination instead increased from station A to station C. The underestimation of MER^{API2} in relation to $\mathrm{TChl}a_{\mathrm{HPLC}}^{\mathrm{REF}}$ was also observed, but with a lower bias (Fig. 1d). This fact is schematized in Fig. 2, where MER^{API2} was considered as the baseline. A complementary comparison with MER^{API1} is also presented for completeness. Results indicated an overestimation by the API1 algorithm in relation to both estimations of TChl*a* (details not shown). The tendency of $\mathrm{TChl}a_{\mathrm{ABS}}^{\mathrm{REF}}$ to produce higher values than $\mathrm{TChl}a_{\mathrm{HPLC}}^{\mathrm{REF}}$ was also confirmed.

3.2 Comparison of product maps

The comparison of MERIS API2 standard product and the MLP regional results is presented on Fig. 3. The maps for regional MLP (Fig. 3a) and MER^{API2} (Fig. 3b) are shown in the top panel, and the difference between MER^{API2} and MLP(R_{rs}^{MER}) is shown in Fig. 3c. Overestimations of more than 35% in relation to the regional MLP are colored in pink, and underestimations below 35 % are colored in yellow, while differences between -35% and 35% are in green. Results indicate an underestimation by MER^{API2} of more than 35% in a significant part of the applicability range, especially near the coast.

The MLP(R_{rs}^{MER}) region of applicability is shown in Fig. 3d, and the results from the application of Sagres regional MLP to the Atlantic off the Portuguese coast is presented in Fig. 3e and Fig. 3f. Besides the Sagres area (#3, in blue), two other regions of interest (ROIs) were chosen for comparison of product maps: Figueira da Foz (#1, in red) and Lisbon region (#2, in green, Fig. 3e). Note that ROI #1 and #2 have been selected for their contrasting features: the first influenced by Mondego river plume and the second by the Tagus estuary. The comparison between the MER^{API2} and regional MLP products is presented as a scatter plot (Fig. 3f), following the same color coding of the three ROIs. The underestimation tendency of MER^{API2} in relation to in situ TChl*a* was confirmed through this analysis. The results also indicated more pronounced differences in Mondego and Tagus ROIs, where values of TChl*a* were higher.

The statistical figures of the product map comparison between MER^{API2} and regional MLP are summarized in Table 2. The applicability of the Sagres MLP was verified with the novelty detection scheme. The number of total and valid (i.e., η <1) data points are denoted as N_{tot} and N_{val}, respectively. The Sagres ROI presents the highest number of valid data points, while Tagus region had the highest percentage of novel data points.

4 Discussion

This study analyzed the standard MERIS API2 product by considering the TChl*a* retrieval in the coastal waters of Portugal. Data product comparisons have been performed by developing and applying a regional MLP trained with Sagres in situ data and accounting for its applicability range. The work highlighted a tendency of MER^{API2} to underestimate TChl*a*, both derived through $a_{ph}(442)$ and determined by HPLC. This result is consistent with other studies addressing low productivity waters (Tilstone et al., 2012). This underestimation tendency is more pronounced at higher concentrations but not observed in the results of the regional MLP. Possible explanations can be uncertainties in BOA R_{rs} values, as well as in specific properties of the NN inversion scheme used to compute the standard API2 values. It is noted that the MERIS NN scheme for API2 retrieval is scoped for global applications in both Case 1 and optically complex waters. This general applicability might limit the algorithm performance in the presence of specific bio-optical relationships at the regional scale. An example could be the upwelling along the cost of Portugal (Loureiro et al., 2005; Goela et al., 2015).

As a contribution to the forthcoming OLCI mission, the present work also provides indications to enhance standard OLCI API2 results by including additional training samples in the synthetic dataset used for the development of the MERIS NN scheme. The overestimation of $\mathrm{TChl}a_{\mathrm{ABS}}^{\mathrm{REF}}$ in relation to $\mathrm{TChl}a_{\mathrm{HPLC}}^{\mathrm{REF}}$ has been identified in this study as one of the reasons for the systematic difference observed in the comparison of MER^{API2} with both in situ referred targets (Fig. 2b).

The regional MLP using in situ R_{rs} as input produced highly accurate results (bias of 2%), when relating R_{rs}^{SITU} to reference measurements of $\mathrm{TChl}a_{\mathrm{ABS}}^{\mathrm{REF}}$. When MERIS R_{rs} is used, the bias is slightly higher, probably due to the uncertainties of the atmospheric correction (Cristina et al., 2014). It is also reported that a cross-validation analysis performed by splitting the in situ data in different subsets to develop and assess the regional MLP documented an increase from 2 to 9% of the bias (details not presented). As observed for the standard NN inversion schemes, the performance of the regional MLP could be enhanced through a better representation of the optical properties of the study region: the collection of additional field measurements is hence recommended. Another aspect that has been considered is the reduction in bias when the training dataset was $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{ABS}}$ estimated with a_{ph} at 440 nm (7% of bias). This indicates that the specific selection of the wavelength of the maximum phytoplankton absorption could allow for a better TChl*a* parameterization and hence also lead to a more accurate regional MLP.

The strong relationship between R_{rs} and the phytoplankton coefficient of absorbance at 442 nm suggests the presence of Case 1 waters. The better agreement with $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{ABS}}$ rather than with $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{HPLC}}$ can be explained by considering that the training of the neural net was performed with $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{ABS}}$. An additional explanation could be that $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{ABS}}$ was determined using $a_{\mathrm{ph}}(442)$, which is likely better related to R_{rs} than $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{HPLC}}$ (both $a_{\mathrm{ph}}(442)$ and R_{rs} directly represent optical properties). Some caveats would however apply to this argument, once $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{HPLC}}$ is a direct measurement of the TChl*a* concentration whereas $\mathrm{TChl}a^{\mathrm{REF}}_{\mathrm{ABS}}$ is an indirect measurement which has errors associated with the laboratorial determination of $a_{\mathrm{ph}}(442)$.

It is then noted that regional relationship between a_{ph} at 442 nm and TChl*a* retrieved by HPLC is close to that used in $\mathrm{MER}^{\mathrm{API2}}$ ($\mathrm{TChl}a_{\mathrm{MERIS}} = 21\ a_{\mathrm{ph}}(442)^{1.04}$, $\mathrm{TChl}a_{\mathrm{SAGRES}} = 27\ a_{\mathrm{ph}}(442)^{1.13}$). However, the local relationship between TChl*a* and $a_{\mathrm{ph}}(442)$ corresponds to a coefficient of determination $r^2 = 0.8$. Hence, about 20% of variability of TChl*a* is not related to $a_{\mathrm{ph}}(442)$.

The ROIs data analysis indicates lower MERIS API2 values with respect to equivalent results derived with the regional MLP, especially when the TChl*a* concentration increases. This finding is in a good agreement with the matchup results, thereby, highlighting the benefit of independent comparison of product maps to qualitatively evaluate data products at an early stage of an ocean color space missions (e.g., OLCI).

5 Conclusions

The scope of this technical note was to analyze MERIS standard API2 product in the Southwestern coast of Portugal. A regional MLP algorithm to retrieve TChl*a*, estimated through phytoplankton absorption coefficient was implemented and applied for this purpose. This regional algorithm produced good agreement with in situ data, hence indicating a high accuracy of regional MLP products. The applicability of the regional MLP in the study area was verified by a novelty detection scheme. On these bases, the study reports an underestimation tendency of $\mathrm{MER}^{\mathrm{API2}}$, which is consistent with other European basins within low ranges of this constituent. The results of the regional MLP were closer to the in situ reference for API2 – TChl*a* estimated with $a_{\mathrm{ph}}(442)$ – than to TChl*a* determined by HPLC. This work also indicates that the use of a regional relationship between phytoplankton absorption and pigment concentration is expected to improve the accuracy of global ocean color remote sensing products.

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This study has highlighted the usefulness of maintaining in situ measurement programs for validation purposes of ongoing ocean color missions. Moreover, it has also demonstrated the importance of developing regional algorithms that not only complement standard approaches, but that can also be applied for the qualitative data assessments of new ocean color missions in its early stage of the product map delivery (e.g., Sentinel-3).

Data availability

The majority of the in situ data used in this work can be accessed through the ESA MERIS MAtchup In-situ Database (http://mermaid.acri.fr/home/home.php) and the MERIS satellite data can be accessed through the Optical Data processor of ESA (http://www.odesa-info.eu/process_basic/basic.php).

Acknowledgements

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Table 1. Comparison between standard (MER^{API2}), regional bio-optical algorithms (MLP(R_{rs}^{MER}) and MLP(R_{rs}^{SITU})) and TChla^{REF}

	N				ε(%)				δ(%)				r^2			
	A	B	C	**All**	A	B	C	**All**	A	B	C	**All**	A	B	C	**All**
MER^{API2} *vs* TChla_{ABS}^{REF}	18	17	19	54	45	35	38	39	-35	-32	-34	-34	0.22	0.60	0.67	0.49
MER^{API2} *vs* TChla_{HPLC}^{REF}	18	17	19	54	48	39	42	43	-21	-24	-26	-24	0.18	0.54	0.66	0.38
MLP (R_{rs}^{MER}) *vs* TChla_{ABS}^{REF}	18	17	19	54	23	32	30	29	8	8	16	11	0.69	0.51	0.85	0.67
MLP (R_{rs}^{MER}) *vs* TChla_{HPLC}^{REF}	18	17	19	54	66	45	49	54	39	16	30	29	0.38	0.49	0.49	0.43
MLP (R_{rs}^{SITU}) *vs* TChla_{ABS}^{REF}	93	91	113	297	16	17	19	17	3	-4	7	2	0.88	0.91	0.91	0.91
MLP (R_{rs}^{SITU}) *vs* TChla_{HPLC}^{REF}	93	91	113	297	56	35	39	43	27	7	20	18	0.48	0.86	0.61	0.63

Table 2. Comparison between regional MLP(R_{rs}^{MER}) and the standard MER^{API2} (The ROIs location is presented in Fig. 3e).

ROI	N_{tot}	N_{val}	**ε*(%)**	**δ*(%)**	r^2
#1	2122	2075	43	-43	0.70
#2	3383	1739	32	-30	0.71
#3	2946	2224	20	-15	0.76
Total	8451	6038	32	-29	0.76

Table 3. List of notations.

API1	Algal Pigment Index 1
API2	Algal Pigment Index 2
BEAM	Basic ERS & ENVISAT (A) ATSR and MERIS Toolbox
BOA	Bottom-of-atmosphere
CDOM	Colored Dissolved Organic Matter
Chl*a*	Chlorophyll *a*
EO	Earth Observation
$E_S(\lambda)$	Surface downwelling incident irradiance
HPLC	High Performance Liquid Chromatography
$L_u(\lambda)$	Subsurface upwelling radiance
$L_w(\lambda)$	Water leaving radiance
$\mathrm{MER}^{\mathrm{API2}}$	MERIS Algal Pigment Index 2 standard product
MERIS	MEdium Resolution Image Spectrometer
MLP	Multilayer Perceptron
$\mathrm{MLP}(R_{rs}^{\mathrm{MER}})$	Regional TChl*a* products computed using inversion schemes based on the MLP NN using standard MERIS BOA R_{rs}
$\mathrm{MLP}(R_{rs}^{\mathrm{SITU}})$	Regional TChl*a* products computed using inversion schemes based on the MLP NN using in situ R_{rs}
NN	Neural Nets
N_{tot}	Number of total (i.e., η <1) data points
N_{val}	Number of valid (i.e., η <1) data points
OLCI	Ocean Land Colour Instrument
PCA	Principal Component Analysis
r^2	Coefficient of determination
ROIs	Regions of interest
R_{rs}	Remote sensing reflectances
R_{rs}^{MER}	Standard MERIS BOA R_{rs}
R_{rs}^{SITU}	In situ R_{rs}
TChl*a*	Total Chlorophyll *a*
$\mathrm{TChl}a_{\mathrm{ABS}}^{\mathrm{REF}}$	API2 in situ equivalent algal pigment index
$\mathrm{TChl}a_{\mathrm{HPLC}}^{\mathrm{REF}}$	TChl*a* concentration (monovinyl Chl*a* + divinyl Chl*a* + chlorophyllide *a* + phaeopigments) determined by HPLC
δ	Signed percent differences
δ^*	Signed unbiased differences
ε	Absolute percent differences
ε^*	Absolute unbiased differences
η	Novelty index
ρ_N	Normalized water leaving reflectance

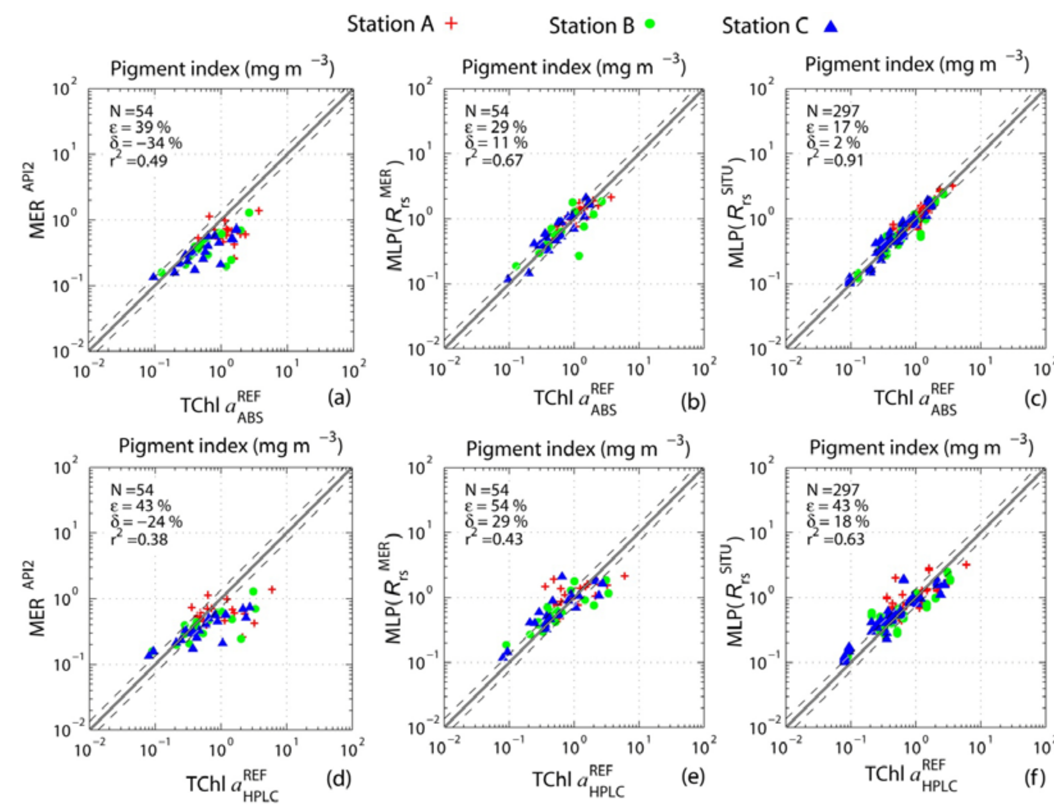
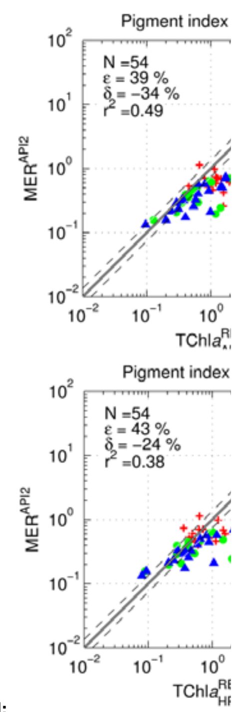


Figure 1: Comparison between MERIS standard Algal Pigment Index 2 and results obtained by applying the Multilayer Perceptron (MLP) regional schemefor the Sagres region. The top row panels present the matchup comparisons with respect to the in situ reference TChla^{REF}_{ABS}, while the lower panels details the matchup comparisons with TChla^{REF}_{HPLC} .



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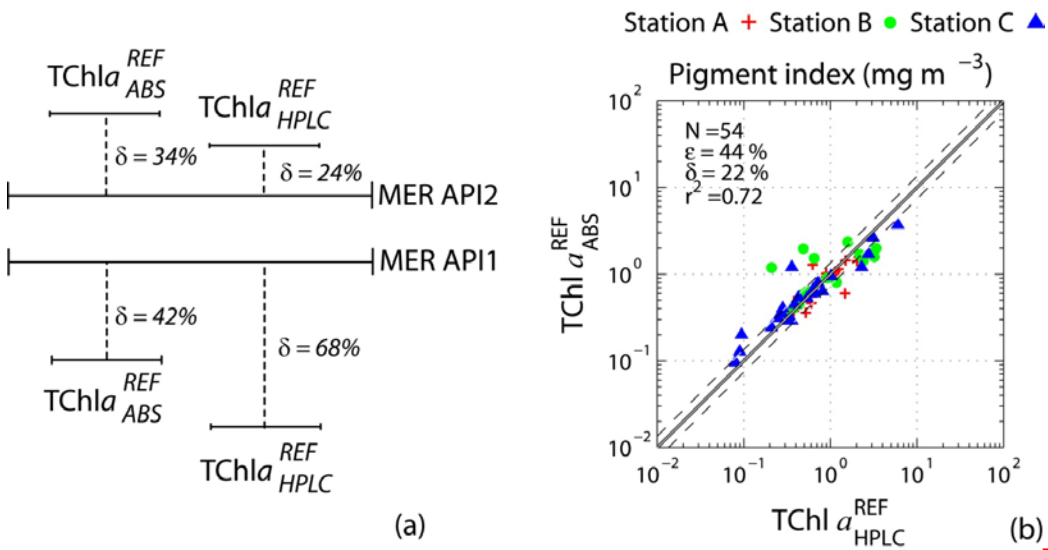
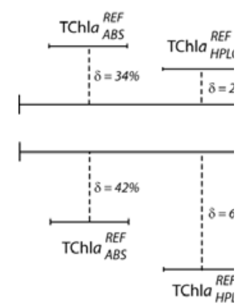


Figure 2: a) Schematic diagram showing, respectively, underestimation and overestimation of MERIS algal pigment indices 1 and 2, relative to TChl*a*, estimated through the absorption coefficient at 442 nm ($\mathbf{TChl}\boldsymbol{a}^{\mathbf{REF}}_{\mathbf{ABS}}$) and measured by HPLC ($\mathbf{TChl}\boldsymbol{a}^{\mathbf{REF}}_{\mathbf{HPLC}}$), and b) scatter plot of the $\mathbf{TChl}\boldsymbol{a}^{\mathbf{REF}}_{\mathbf{ABS}}$ *versus* $\mathbf{TChl}\boldsymbol{a}^{\mathbf{REF}}_{\mathbf{HPLC}}$.



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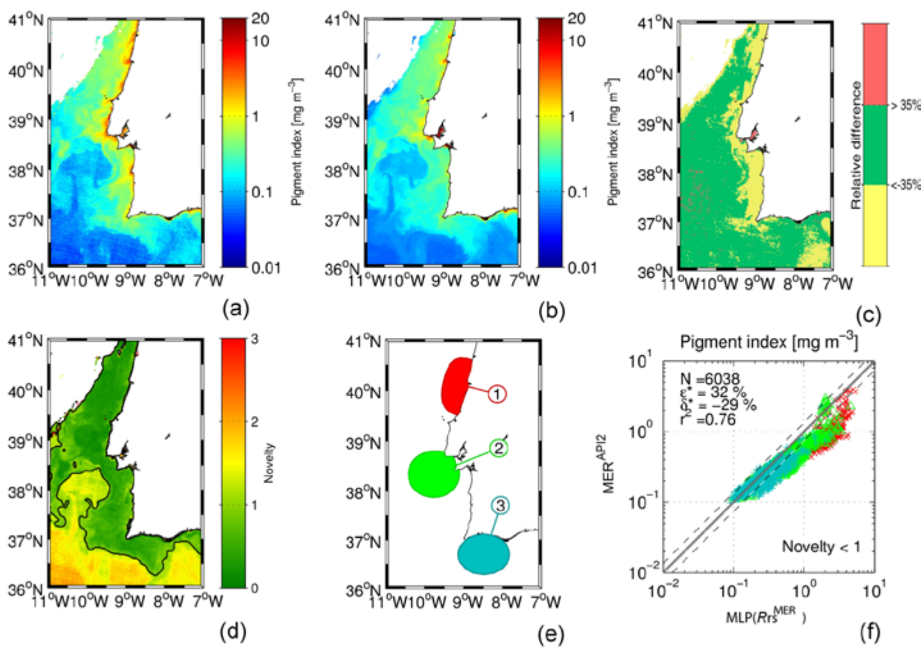

Figure 3: Comparison between Sagres regional Multilayer Perceptron (MLP) algorithm map with MERIS pigment index product map Algal Pigment Index 2 for the 25th August 2010, showing a) the product map of the regional MLP, b) standard API2 MERIS product map, c) difference between MER^{API2} and MLP(R_{rs}^{MER}), d) region of applicability of MLP(R_{rs}^{MER}), f) results of the application of the regional MLP to the Portuguese coast in the three regions of interest (shown in e). Please see Sect. 3.2 for a more detailed description of the panels. (Source: MER_RR_2PRAC20100825_103551_000026292092_00223_44365_0000.N1)

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