

Interactive comment on “CoastColour Round Robin datasets: a database to evaluate the performance of algorithms for the retrieval of water quality parameters in coastal waters” by B. Nechad et al.

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Reviewer#2 The comments are followed by answers, and when applicable, by modifications in the text. Note that extra-modifications are included under section “OTHER COMMENTS”, after sections “GENERAL COMMENTS” and “SPECIFIC COMMENTS”.

GENERAL COMMENTS

In this paper the authors compare the performance of different algorithm’s performance

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in retrieving in water properties in coastal waters. They compare MERIS Level 2 matchups, in situ reflectance measurements and Hydrolight simulations. The database itself is a very important contribution since it puts together several dataset available around the world of reflectance and water constituents (chl, TSM, CDOM). Abstract: the abstract is more of a summary of the material and methods rather than a summary of findings. This paper has a lot of information and results and I think that this manuscript could be improved by summarizing what the main results are. In the results and discussion section I found it hard sometime to see what the take-home message was.

Answer: the paper focuses on CCRR dataset description and analysis, not on the inter-comparison of algorithms performance. Hence, The main results of the paper, as summarized in the conclusion, show particularly the diversity of water types in the CCRR datasets, and document the relationships existing between the biogeochemical, IOPs and AOPs in the different CCRR sites and the consistency (and good quality) of these measurements between the in situ, MERIS and simulated datasets. The message is that these datasets are fully validated and documented here, and made available for the scientific community dealing with remote sensing algorithm validation/calibration. To avoid any false expectations of algorithm intercomparison results, the first paragraph of the abstract has been changed, stating clearly the scope of the paper:

“The use of in situ measurements is essential in the validation and evaluation of the algorithms that provide coastal water quality data products from ocean colour satellite remote sensing. Over the past decade, various types of ocean colour algorithms have been developed to deal with the optical complexity of coastal waters. Yet there is a lack of a comprehensive inter-comparison due to the availability of quality checked in situ databases. The CoastColour Round Robin (CCRR) project funded by the European Space Agency (ESA) was designed to bring together three reference datasets using these to test algorithms and to assess their accuracy for retrieving water quality parameters. This paper provides a detailed description of

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these reference datasets that include the Medium Resolution Imaging Spectrometer (MERIS) Level 2 match-ups, in situ reflectance measurements and a synthetic data generated by radiative transfer model (HydroLight). These datasets are available from doi.pangaea.de/10.1594/PANGAEA.841950”.

SPECIFIC COMMENTS

P188, L12: a flow chart in fig4 is mentioned but it looks like figure 4 is in fact the same as figure 6? I couldn't find any flow chart on figure 4

Answer: Figure 4 has now been correctly inserted, thanks.

Throughout the manuscript: I would suggest to use the abbreviation 'Med.' Instead of 'Md.' for the Mediterranean, it seems more intuitive.

Answer: The purpose was to reduce the long name for the Morocco and Western Mediterranean Sea site. On some figures, even the contracted name (with “Med”) was longer than all the other site names which needed a cosmetic modification, and led to “Morocco-W.Md. Sea”, then to “E.Md. Sea” for consistency.

The authors define TChl as the chlorophyll from the HPLC and Chl as the chlorophyll from fluorometry and spectrophotometry but then from p.190 onwards a new abbreviation called CHL is introduced for chlorophyll from HPLC (?). On p.190, L22 for example: ‘The CHL data were measured by HPLC. . .’. How is the abbreviation CHL different from TChl and Chl? P.194,L16: ‘the median HCL..’, is this HPLC or fluorometric data?

Answer: In the abstract and in the introduction, CHL was defined as chlorophyll-a concentration, and used to designate chlorophyll-a concentrations in sections 2.2(“In situ reflectance dataset”) and 2.3(“Simulated dataset”). In sections 2.1.1(under “Chlorophyll-a and TSM”) and 3.2(“Chlorophyll-a concentration”), specific notation Chl-a was defined and used for chlorophyll-a concentration obtained by fluorometry, and TChl-a by HPLC. When we compare chlorophyll-a concentration to other parameters (TSM, IOPs or RLw) we use the generic name “CHL”, and also when we analyze the

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distributions of TChl-a or Chl-a (when available) throughout the sites like in the section: “Chlorophyll-a concentrations (either Chl-a or TChl-a) exhibit median values less than 1 mg m⁻³ from the E. Md. Sea, GBR region, Morocco-W. Md. Sea, Tasmania and Trinidad and Tobago sites. Some of these sites have been extensively studied, and characterized as ultra to oligotrophic (CHL \leq 1 mg m⁻³), or mesotrophic to eutrophic waters.”

Some of the figure seem to be in low quality. (Fig. 7, 15). Also I think every figure should be self-explanatory. So for example I would add in the caption of Figure 7 what the green line is and what the red and blue ‘+’ represent.

Answer: The figures have been (re)produced in eps format, and are of good quality. The figures are already heavily loaded (with site names, x and y label, statistics), adding extra information would make the figure less readable. The meaning of the red and blue plus, and of the green line are explained in the caption of the first figure with the box and whisker plots (Figure 6). For all the captions of all subsequent figures where the box and whisker plots appear, the caption states that the graphical conventions of Figure 6 apply. For Figure 7.c, there was no explanation of what the red line represents (now this has been added): “Figure 7: The distribution of a) TChl-a and b) Chl-a concentrations (in mg m⁻³) as given in the in situ dataset at all measurement depths, and c) Chl-a versus TChl-a. The number of measurements taken at each test site is reported on the right axis of the graph. The graphical convention in a) and b) is identical to Error! Reference source not found.. In c) the solid line represents the 1:1 ratio, the dashed lines $\pm 30\%$, and the red line the linear regression fitting the log-transformed TChl-a and Chl-a measurements.”

p.196,L5: ‘ The ranges of Kd(443) and Kpar measurement (Fig. 6c and d)..’. I am assuming the authors meant Figure 9?

Answer: Yes. It is corrected now, thanks.

p.196, L13: “The noticeable shift between Kd (or Kpar) in Acadia and Cape Verde may

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be partly explained by the different Chl a ranges: around 0.2 mgm⁻³ in Cape Verde and 2 mgm⁻³ in Acadia (Fig. 7a).”- I couldn't see the chlorophyll data for Cape Verde on Figure 7a

Answer: Indeed. There is no CHL from Cape Verde. This has been changed to comparison between the total backscattering from Cape Verde and from Acadia. “The noticeable shift between the ranges of bb measured in the Acadia and Cape Verde sites may partly explain the shift between (Kd (or Kpar) in Acadia and Cape Verde (Figure 9.a).”

p196,L25: shouldn't 'their models..' be singular? The author talk of Hydrolight, correct? Same line: ‘. . .adopted the distributions documented in..’. Assume the author talk about the distribution of chlorophyll? If so I would change it to ‘distributions of chlorophyll document in..’ as to avoid any confusion

Answer: It is about the way TSM and CHL (and also CDOM) were modelled: randomly generated to be part of the inputs to HydroLight, with a log-normal distributions for CHL and for TSM, and with a constrain on their covariations. These are different models for TSM and CHL.

p.197, L5. I would reference Figure 10 a here. Throughout the text I would suggest the authors check to make sure that they cite the figures they are talking about. There is a lot of figure and sometime it is hard to follow which figure they are discussing.

Answer: Yes. Reference to Figure 10 was added here. Thanks! References to all figures were checked.

p.198,L25:’The different periods of sampling relative to the algal blooms events in each site (Fig. 3).’ I am not sure how the author concluded this from Fig. 3 since the period of algal bloom or each of the sites is not presented on this figure?

Answer: The figure (Fig.3) shows that the sampling is not uniform or regularly made throughout the seasons for all the sites. The information on algal bloom periods is

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actually not given in that figure. The sentence was changed to: “The different periods of sampling throughout the seasons for each site (Figure 3) may partly explain this general discrepancy between the aphy*(44X) data, which can be highly impacted during algal bloom events.”

OTHER COMMENTS

-> List of acronyms:

- ERI acronym is fixed (Earth Research Institute (ERI))

-> Abstract: specify the in situ measurements and simulations are multi- or hyper-spectral.

- Added in the abstract: “The datasets mainly consisted of 6 484 multispectral or hyper-spectral marine reflectance associated with various geometrical (sensor viewing and solar angles) and sky conditions and water constituents”

-> Introduction: add definition of Rrs and RLw, as both are used in the text.

- Added in the introduction: “Three types of data were prepared for the CCRR: a) match-ups: where in situ WQ is available simultaneously with a cloud-free Medium Resolution Imaging Spectrometer (MERIS) product; b) in situ reflectances: where an in situ water-leaving reflectance measurement (denoted by RLw which is derived from the remote-sensing reflectance, Rrs following $RLw = \pi Rrs$)”

-> Section 2.1.1 Rectification of data size (carefully checked, now consistent with numbers in Tables 3.a and 3.b).

“Metadata including depth, temperature and salinity, exceeded 20 000 for each parameter, whereas the number of bio-geochemical, IOPs and AOPs were much lower: 11 208 chlorophyll-a concentration measurements, 538 TSM measurements, 957 reflectance spectra (the other AOP data do not reach 200 data each), and less than 700 IOP data (for each parameter) except for turbidity (N=2 187).”

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-> Section 2.1.1 TSM data have been removed from the CSIC data:

- In the CSIC dataset, TSM measurements are not correlated to Chl-a in the Morocco-W. Md. Sea site, at the Guadalquivir estuary flow and offshore, because of light limitation for phytoplankton (due to high TSM concentrations frequently observed at this site). However, the quasi-constant values measured between 30 and 45 mg/l, are probably due to the measuring protocol with no sufficient rinsing of filters. Isabel Caballero de Frutos (CSIC) was about to redo new measurements in this region during year 2015. No results yet. In the meanwhile, the TSM and PIM data from CSIC were removed from the paper. Figures 8 and 10 were updated accordingly and the text too.

- The paragraph on CSIC data was updated as: “The CSIC dataset contains 736 Chl-a and 667 POM measurements collected in the Gulf of Cadiz (southwest Iberian Peninsula) within the Morocco-W. Md. Sea site. The measurements were taken in the nearshore area (<30 km) of the Guadalquivir estuary from 2005 to 2007, and offshore during 2008 with slightly lesser measurements during the periods June-August (19% of the data). Chlorophyll analysis was conducted by filtering samples of 500 ml through Whatman GF/F glass fiber filters (0.7 μm pore size), extracting in 90% acetone, and measuring chlorophyll-a by standard fluorometric methods using a Turner Designs Model-10 following JGOFS protocols (IOC/UNESCO, 1994). TSM concentrations were measured gravimetrically on pre-weighted Whatman GF/F (0.7 μm pore size) after rinsing with distilled water, following JGOFS protocols (IOC/UNESCO 1994). Organic matter lost on ignition was determined by reweighting the filters after 3 hours in the oven at 500°C, giving the concentrations of PIM and POM (by subtraction). TSM and PIM measurements were contaminated by salt (filters not correctly rinsed) and showed low variability of TSM and PIM, with 90% of TSM measurements comprised between 31.1 and 48.3 g m⁻³. Therefore, only Chl-a and POM measurements were retained from the initial CSIC dataset.”

-> Section 2.1.1: CSIRO dataset: remove an outlier in aphy

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- The aphy outlier was removed, Table 3.b updated (62 measurements at the GBR site, and 681 from all sites)

- Figure 13 was replotted for GBR region: 62 aphy spectra instead of 63

- All figures in Figure 15 were updated

-> Section 2.1.1: add reference to Ifremer dataset.

“The Ifremer dataset consisted of 975 Chl-a measurements collected at 30 different locations within the Armorican Shelf (north-west of France), from 2005 to 2009. Data were available from the French phytoplankton surveillance network (REseau PHYtoplankton, REPHY, Gohin 2011).”

-> Section 2.1.1: minor corrections, NOMAD dataset (Chl, IOPs and AOPs).

- Now the texts read: “The NASA SeaWiFS Bio-optical Archive and Storage System (SeaBass, (Werdell et al., 2003)), the source of the NOMAD dataset, includes both the HPLC and fluorometric methods.”

“The spectral backscattering coefficient provided in NOMAD dataset was obtained using HOBI Labs HydroScat-2 and HydroScat-6 sensors, WET Labs ECObb and ECOVSF sensors, and Wyatt Technology Corporation DAWN photometers. The details on bb data processing are given in Werdell (2005).

“From the NOMAD database, Lw and Es measurements were extracted for the match-up locations between 2005 and 2010, and converted to RLw spectra. Various instruments were used for the measurements of the remote-sensing reflectance, Rrs, in the NOMAD dataset (Werdell and Bailey, 2005), including in-water profiling or above-water measurements. All in- and above-water data from various instruments and data providers were consistently processed to Rrs, with the methods described in Werdell and Bailey (2005).”

-> Section 2.1.1: complete description of USCB measurements (Southern California

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site).

- The methods and instruments of ERI/USCB data were updated in Table 6 (for RLw measurements), and in the text for RLw, backscattering and absorption measurements (see the two paragraphs below):

“The USCB RLw measurements in the Southern California region were obtained using above-water radiometric measurements of one Dual FieldSpec spectrometer (ASD) instrument and under-water measurements of a Biospherical Instruments (San Diego, California) profiling reflectance radiometer (PRR-600), as described by Toole et al.,(2001). Sea-surface radiance, L_s , at viewing zenith angle of 45° , sky radiance (that would be reflected into L_s), L_{sky} and spectralon upwelling radiance, L_{spec} were measured by the ASD. The above water reflectance was estimated following Toole et al. (2000): the above-water irradiance was calculated from spectralon measurements according to $E_d = \pi L_{spec}/spec$ where $spec$ is the reflectance of the plaque, the water-leaving reflectance was calculated as $RLw = \pi (L_s - L_{sky})/E_d - residual(750)$, where $residual(750)$ corrects for any residual reflected sky radiance, assuming zero water-leaving radiance at 750 nm. Underwater downwelling irradiance, E_d , and upwelling radiance, L_u were measured along vertical profiles using the Biospherical PRR-600, then interpolated to above water radiance and irradiance respectively, leading to a new estimate of RLw spectra which were merged with ASD reflectances (see Toole et al. (2000) for details).”

For bb and a-measurements:

“Backscattering coefficients provided by USCB were estimated from profiled measurements of the total volume scattering function β at 140° , using a HobiLabs HydroScat-6, collected at the Southern California site. These measurements were corrected for light attenuation along the photon path to the instrument detector (σ -correction of Maffione and Dana, 1997) using concurrent absorption spectra (Kostadinov et al. 2007) for measurements up to 2005, and concurrent beam attenuation and absorption modelled

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from the diffuse attenuation coefficient for downwelling irradiance and the irradiance reflectance (see Antoine et al. (2011) for details). A total of 269 backscattering spectra initially measured at 442, 470, 510, 589 and 671 nm were interpolated at 412, 470, 510 and 589 nm assuming a λ^{-1} spectral dependency of the backscattering coefficient. USCB absorption spectra up to 2005 were obtained using vertical profiles of WET Labs ac-9 measurements, after application of pure water calibration, and standard temperature, salinity and scattering corrections (WET Labs ac-9 Protocol, 2003). Surface absorption values were derived from the upper 15 m absorption spectra, after filtering incomplete, negative or extreme values; spectra were linearly interpolated at 412, 443, 490, 510, 530, 555, 620 and 665 nm (Kostadinov et al., 2007). Measurements of aphy, ag and ad spectra were obtained using a Shimadzu UV2401-PC spectrophotometer. CDOM samples were filtered on 0-2 μ m Poretics membranes, while GF/F filters were used to retain total particulate matter for ap measurement, corrected for pathlength effects following Guillocheau (2003). Pigment extraction was performed in 100% methanol."

-> Acknowledgements

- CSIR Data Providers are now duly acknowledged: "Stewart Bernard, Hayley Evers-King, Mark Mattews and Lisl Robertson for processing the CSIR dataset over the Benguela region, with the support of the Department of Agriculture, Forestry and Fisheries, DAFF."

- CSIRO: "The CSIRO measurements were funded by the CSIRO Wealth from Oceans Flagship and the Australian Integrated Marine Observing System (IMOS)."

- REPHY Data Providers duly acknowledged: "Francis Gohin, Catherine Belin and Alain Lefèbvre for the Ifremer (REPHY phytoplankton network) dataset."

-> New references

- New reference was added (for instruments/methods of Ifremer): "Gohin, F.: An-

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nual cycles of chlorophyll-a, non-algal suspended particulate matter, and turbidity observed from space and in-situ in coastal waters, *Ocean Science*, 7, 705-732, 2011. doi:10.5194/os-7-705-2011"

- New references were added (for instruments/methods of the USCB)

"Guillocheau, N.: β -Correction Experiment Report, ICES, University of California, Santa Barbara, CA, 2003.

Kostadinov, T. S., Siegel, D. A., Maritorena, S., and Guillocheau, N.: Ocean color observations and modeling for an optically complex site: Santa Barbara Channel, California, USA, *Journal of Geophysical Research*, 112, C07011, 1-15, 2007. doi: 10.1029/2006JC003526

Maffione, R. A., and Dana, D. R.: Instruments and methods for measuring the backward-scattering coefficient of ocean waters, *Applied Optics*, 36, 24, 6057-6067, 1997.

Toole, D. A., Siegel, D. A., Wenzies, D. W, Neumann, M. J., and Smith, R. C.: Remote-sensing reflectance determinations in the coastal ocean environment: impact of instrumental characteristics and environmental variability. *Applied Optics*, 39, 3, 456-469, 2000.

Toole, D. A. and Siegel, D. A.: Modes and mechanisms of ocean color variability in the Santa Barbara Channel. *Journal of Geophysical Research*, 106, C11, 26,985-27,000, 2001. WET Labs ac-9 Protocol, revision H (2003), WET Labs, Inc. Philomath, OR, 42 pp."

-> One reference completed:

"Arar, E. J., and Collins, G. B.: Method 445.0 - In vitro determination of chlorophyll a and pheophytin a in marine and freshwater algae by fluorescence. National Exposure Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, Ohio, 1992."

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