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ORIGINAL RESEARCH ARTICLE

Comparison of in situ and satellite ocean color determinations of particulate organic carbon concentration in the global ocean☆

Marek Świrgoń [a,b], Malgorzata Stramska [a,b,*]

[a] *Department of Earth Sciences, University of Szczecin, Szczecin, Poland*
[b] *Institute of Oceanology, Polish Academy of Sciences, Sopot, Poland*

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Summary Ocean color satellite missions have provided more than 16-years of consistent, synoptic observations of global ocean ecosystems. Surface chlorophyll concentrations (Chl) derived from satellites have been traditionally used as a metric for phytoplankton biomass. In recent years interpretation of ocean-color satellite data has progressed beyond the estimation of Chl. One of the newer ocean color products is particulate organic carbon (POC) concentration. In this paper we carry out comparisons of simultaneous satellite and in situ POC determinations. Our results indicate that the performance of the standard NASA POC algorithm (Stramski et al., 2008) is comparable to the standard empirical band ratio algorithms for Chl.

1. Introduction

The bio-optical relationships linking optical properties of the ocean to chlorophyll-*a* concentrations (Chl) have been the focal point of numerous studies in the last three decades (Bricaud et al., 1995; Mobley, 1994; Morel, 1988). One of the most often investigated relationships has been that linking the surface Chl to the remote-sensing reflectance. This was motivated by the goal of developing reliable satellite remote sensing methods for monitoring the phytoplankton biomass and primary productivity from space (see Siegel et al., 2013 and the references therein). Empirical relationships for estimating Chl from remote sensing reflectance have been used

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* Corresponding author at: Institute of Oceanology, Polish Academy of Sciences, Powstańców Warszawy 55, Sopot 81-712, Poland. Tel.: +48 58 73 11 600; fax: +48 58 55 12 130.
E-mail address: mstramska@wp.pl (M. Stramska).
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for routine processing of global satellite imagery of ocean color since the beginning of the SeaWiFS mission in 1997 (O'Reilly et al., 1998, 2000).

In the past several years, interpretation of ocean-color satellite data has progressed beyond the estimation of Chl to include new products. For example, it is now possible to determine the dominant phytoplankton functional groups present in oceanic surface waters (e.g., Alvain et al., 2005; Brewin et al., 2011) and to retrieve information about particle size distribution (Kostadinov et al., 2010; Loisel et al., 2006). In addition, information about important components and processes of the oceanic carbon cycle such as the primary productivity (Antoine et al., 1996; Behrenfeld and Falkowski, 1997; Woźniak et al., 2007), the particulate organic carbon concentration (Duforet-Gaurier et al., 2010; Gardner et al., 2006; Stramska and Stramski, 2005; Stramski et al., 2008), and the colored dissolved and detrital organic matter absorption (Maritorena et al., 2002; Siegel et al., 2002) can be derived from satellite data. Before these new data products are broadly used in oceanographic studies, it is extremely important to validate the performance of the various ocean color algorithms with observations. The main objective of this paper is to evaluate the performance of the standard NASA POC algorithm (Stramski et al., 2008).

2. Data sets and methods

For POC product match-up analysis we have used coincident in situ data and satellite data from SeaWiFS and MODIS Aqua. We searched 16 years of satellite data from 1997 to 2012 for matchups with in situ data. In situ POC data have been obtained from public databases of the U.S. Joint Global Ocean Flux Study (U.S. JGOFS, http://usjgofs.whoi.edu/jg/dir/jgofs/) and the SeaWiFS Bio-optical Archive and Storage System (SeaBASS), the publicly shared archive maintained by the NASA Ocean Biology Processing Group (OBPG) (http://oceancolor.gsfc.nasa.gov). We have selected only these in situ data sets for which POC determinations were made using JGOFS protocols (Knap et al., 1996) and filters were acidified for removal of inorganic carbon prior to combustion. We have assumed that POC values of 10 mg m^{-3} and less were invalid in situ POC determinations if found outside the hyperoligotrophic waters of the South Pacific Subtropical Gyre (Stramski et al., 2008). We have found 2418 surface in situ POC concentration data fulfilling these requirements. For comparisons with in situ data we have downloaded SeaWiFS and MODIS – Aqua Level 2 POC data product from the NASA's Ocean Color Web (reprocessing versions R2010.0 and R2013.1, respectively). The POC data product provided by NASA is based on Stramski et al. (2008) algorithm. The full details of the approach used by NASA in standard processing of satellite ocean color data are given at http://oceancolor.gsfc.nasa.gov/. Spatial resolution of satellite data was about 1.1 km at nadir for the Merged Local Area Coverage (MLAC) SeaWiFS data and 1 km for the Local Area Coverage (LAC) MODIS Aqua data. We also used Global Area Coverage (GAC) SeaWiFS data with effective resolution of about 4.5 km.

Satellite POC data have been stored for each pixel containing a coincident in situ data point. Only data pairs with a time difference between in situ measurement and satellite overpass less than 2 h and with a low spatial variability in a 3 × 3 pixel square were used in the analysis. The center pixel in satellite image was the nearest to the in situ measurement. The comparison was carried out if at least 6 of 9 satellite pixels were valid and the average difference between the central pixel and all the other valid pixels was less then 25%. In some cases not one but two overpasses during the same day could have been matched with one in situ measurement. In that case, if both match-ups satisfied the criteria described above, we have used the one that had the smaller time difference between the satellite and the in situ measurement. These match-up criteria differ somewhat from those used in Bailey and Werdell (2006).

After the compilation of the data using these criteria, the joint satellite and in situ data set included 260 match-ups of POC concentrations. The geographical positions of these data are indicated in Fig. 1.

The differences between in situ and satellite-derived POC have been quantified by standard methods (Ostasiewicz et al., 2006):

- the absolute average error (AAE)

$$\mathrm{AAE} = \frac{1}{N}\sum_{i=1}^{N}|O_i - P_i|,$$

- the root mean square error (RMSE)

$$\mathrm{RMSE} = \left[\frac{1}{N-1}\sum_{i=1}^{N}(P_i - O_i)^2\right]^{1/2},$$

- the bias (B)

$$B = \frac{1}{N}\sum_{i=1}^{N}P_i - \sum_{i=1}^{N}O_i = \bar{P} - \bar{O},$$

- the mean normalized bias (P_{BIAS})

$$P_{\mathrm{BIAS}} = 100\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N}O_i},$$

- the mean absolute percentage error

$$\mathrm{MPE} = 100\frac{1}{N}\sum_{i=1}^{N}\left|\frac{P_i - O_i}{O_i}\right|,$$

where N is the total number of measurements, O_i is the in situ observation value and P_i is the predicted value (satellite POC determination).

When comparing the in situ and satellite derived POC concentrations one has to remember that both kinds of POC estimates are subject to errors. In-water POC determinations are subject to several potential sources of errors and there is a continued need for further improvement in the methodology. This issue has been discussed in-depth in Gardner et al. (2003) The causes for the overestimation of POC include potential adsorption of dissolved organic carbon

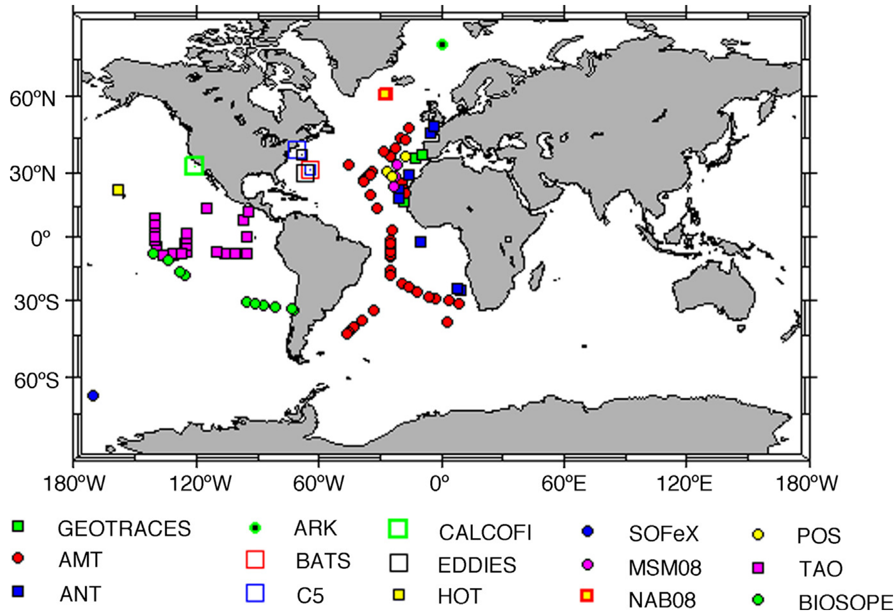

Figure 1 Map showing geographical locations of in situ POC measurements used in this study. Data from the following experiments were used in our comparisons: The Atlantic Meridional Transect (AMT), the ANT-XXIII/1 cruise (ANT), the arkxix2 cruise (ARK), the International Study of Marine Biogeochemical Cycles of Trace Elements (GEOTRACES), the Bermuda Atlantic Time-series Study (BATS), the Eddies Dynamics, Mixing, Export, and Species Composition project (EDDIES), the North Atlantic Bloom Experiment (NAB08), POS, the C5 line cruise (C5), the California Cooperative Oceanic Fisheries Investigations (CALCOFI), the Hawaii Ocean Time-series (HOT), the Tropical Atmosphere Ocean project cruises (TAO), the Biogeochemistry and Optics South Pacific Experiment (BIOSOPE), the Southern Ocean Iron Experiment (SOFeX on Melville), the Maria S. Merian cruise (msm08).

(DOC) onto filters during filtration and contamination of samples during handling. Underestimation of POC can result, for example, from an undersampling of the infrequent large particles, settling of particles below the bottle spigots (Gardner, 1977) or incomplete retention of particles on filters. Therefore the true accuracy of in situ POC determinations remains unspecified. For brevity, in this paper, we refer to in-water POC estimates as \`measured' and to the differences between satellite-derived and in-water POC estimates as \`errors'. Regression analyses included in this paper represent Model II major axis reduced regression (Legendre and Legendre, 1998) as this type of regression model is suitable when the two variables in the regression equation contain errors.

3. Results and discussion

In Figs. 2 and 3 we present the results of comparison between the in situ and the satellite measurements, which passed the comparison criteria described above. Table 1 summarizes the error statistics for data sets presented in Figs. 2 and 3.

Table 1 Summary of the error statistics i.e., the absolute average error (AAE), bias mean normalized bias (P_{BIAS}), mean absolute percentage error (MPE), R^2 coefficient and root mean square error (RMSE) for the POC concentrations [mg m^{-3}] compared in Fig. 2.

	N	AAE	Bias	P_{BIAS} [%]	MPE [%]	R^2	RMSE
All data included							
North Atlantic	109	34.86	−18.59	−19.92	41.75	0.85	64.93
South Atlantic	28	73.68	−72.96	−57.78	52.24	0.41	104.66
North Pacific	74	20.68	7.44	14.63	40.73	0.49	30.84
South Pacific	49	25.50	−11.96	−11.97	20.70	0.83	44.78
AMT data excluded (see explanation in the text)							
North Atlantic	88	23.14	−4.02	−5.83	41.75	0.84	40.15
South Atlantic	3	8.24	−1.57	−2.76	417.04	0.29	11.54
North Pacific	74	20.68	7.44	14.63	40.73	0.49	30.84
South Pacific	49	25.50	−11.96	−11.97	20.70	0.83	44.78
ANT and BIOSCOPE data excluded							
North Atlantic	99	36.13	−22.62	−23.38	42.22	0.85	67.49
South Atlantic	28	73.68	−72.96	−57.78	52.24	0.41	104.66
North Pacific	74	20.68	7.44	14.63	40.73	0.49	30.84
South Pacific	27	9.61	−0.12	−0.24	18.38	0.16	12.12

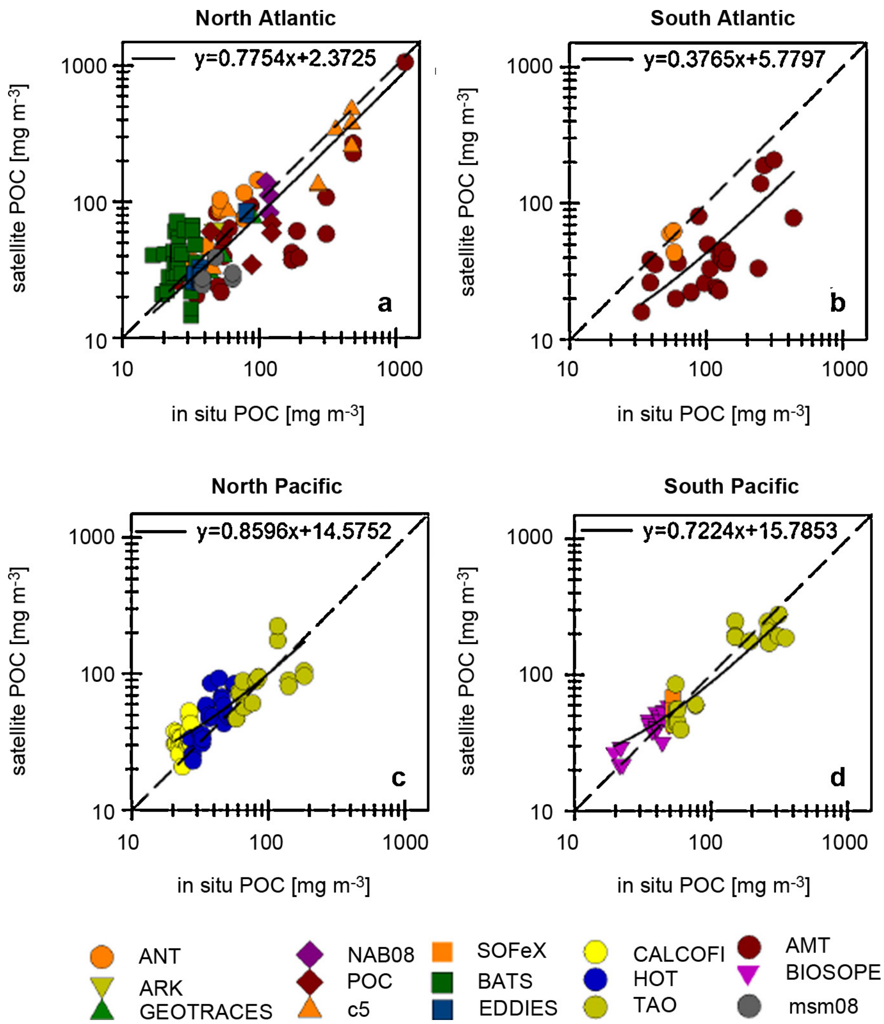

Figure 2 Comparison of in situ and satellite-derived POC estimates on logarithmic scale. Data represent match-ups for the concurrent satellite and field measurements taken during several research projects in various oceanic basins as indicated. The dashed line shows 1:1 relationship, the solid line is the best linear fit to the data. The corresponding error statistics are shown in Table 1. The following experiments are included in Fig. 2: (a) AMT, ANT, ARK, BATS, C5, EDDIES, GEOTRACES, MSM08, NAB08, POS; (b) AMT, ANT; (c) CALCOFI, HOT, TAO and (d) BIOSOPE, SOFeX, TAO.

Data displayed in Fig. 2 are divided into four regions: the North Atlantic, the South Atlantic, the North Pacific, and the South Pacific. Some ocean regions are not shown, because there were not enough matchups (or no matchups at all) to justify the statistical analysis. Note that a separate evaluation of POC algorithms for the Southern Ocean has been given in Allison et al. (2010). In general, looking at Fig. 1 it is obvious that large areas of the global ocean are not included in our analysis because of lack of in situ POC estimates simultaneous with satellite observations. Regionally, the largest data set from a single experiment comes from BATS (36 data points). However the range of in situ POC concentrations at BATS is rather small, as the site is located in the oligotrophic Sargasso Sea. Analyzing Fig. 2 it would be difficult to notice any clear regional trends. The largest bias and errors (Table 1) have been estimated for the South Atlantic, but this might be due to the fact that almost all of the data included in this data subset are from the AMT cruises (2004, 2005, 2008), when POC samples were collected from a flow-through system. Almost all of the other data shown in Fig. 2 were collected using CTD rosettes. It is possible that using a flow-through system on the cruise could have lead to somewhat different estimates of POC concentration when compared to samples collected with a CTD rosette. Nevertheless we decided to show these data points in Fig. 2 in order to bring to the attention the fact that there might be some unresolved issues with POC samples collected by different methods. The problem is that so far the POC data collection and analysis procedures were not as carefully defined, evaluated, and intercompared as those for chlorophyll concentrations. Table 1 allows one to compare in detail the differences in error statistics if one includes or excludes the ATM data in this statistics. In addition we show how the errors statistics change if data used for the algorithm development (BIOSOPE and ANT cruises) are excluded.

In Fig. 3 the data are redisplayed, but now they are categorized according to satellite sensor and data type. First, all available data are displayed together in Fig. 3a. Second,

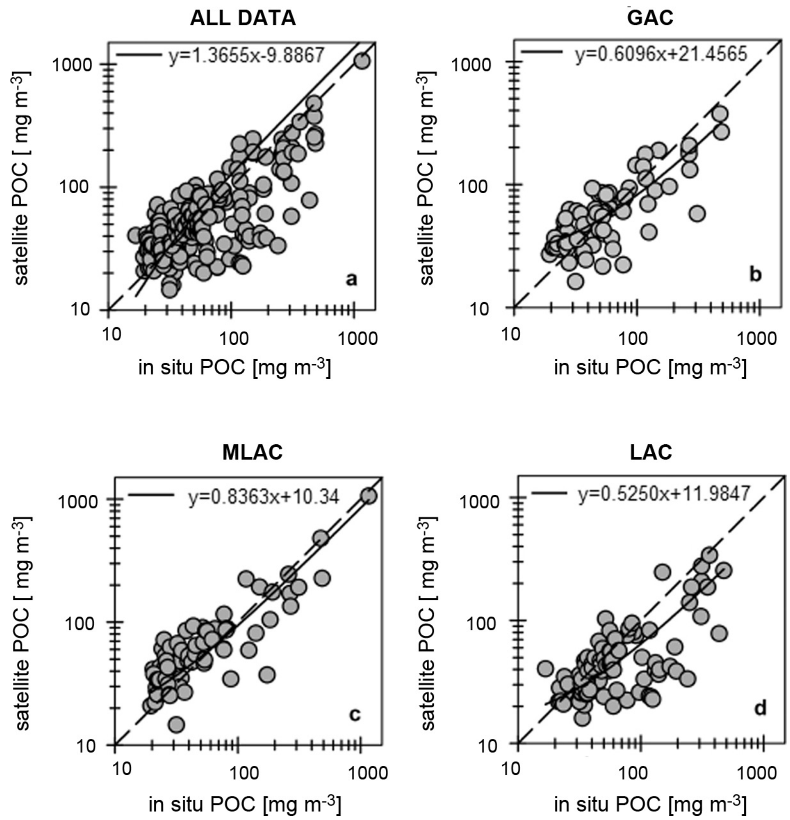

Figure 3 Comparison of in situ POC and satellite-derived POC estimates on logarithmic scale. Data represent match-ups for the concurrent satellite and field measurements taken during several research projects and various satellite data types. The dashed line shows 1:1 relationship, the solid line is the best linear fit to the data. The corresponding error statistics are shown in Table 2. Titles GAC, MLAC, and LAC indicate the SeaWiFS Global Area Coverage data with spatial resolution of about 4.5 km, the SeaWiFS Merged Local Area Coverage data recorded at 1.1 km resolution, and the MODIS-A Local Area Coverage data with 1 km spatial resolution, respectively. In Fig. 3a all of the above data have been plotted together.

the SeaWiFS Global Area Coverage (GAC) data are shown in Fig. 3b. These data were subsampled and recorded onboard the spacecraft and subsequently downloaded twice a day at Wallops and NASA/Goddard and have an effective resolution of about 4.5 km. Next, the SeaWiFS Merged Local Area Coverage (MLAC) data (recorded at full 1.1 km resolution but only in selected parts of the world) are presented in Fig. 3c. Finally, the MODIS-A Local Area Coverage (LAC) data with 1 km nominal resolution are displayed in Fig. 3d. Note that the AMT data are not included in Fig. 3. The error statistics for data shown in Fig. 3 are summarized in Table 2. The categorization of data into 3 subsets (GAC, MLAC, LAC) does not show any evidence that either of the subsets has a much better statistics than the other data subsets. The R^2 coefficient for all data subsets is about 0.8 if AMT data are not included. The lowest mean absolute percentage error (MPE) of about 22% is for the MODIS-A LAC data set, while the lowest percentage of model bias (P_{BIAS}) is for the SeaWiFS GAC data (about 1%).

The results shown in Figs. 2 and 3 indicate that the performance of satellite POC algorithms is acceptable and comparable to the performance of the standard correlational satellite algorithms for chlorophyll (Chl) concentration (Bailey and Werdell, 2006). Similar conclusion has been reached by Duforet-Gaurier et al. (2010), but these authors used more limited data sets (27 data points). Allison et al. (2010) also concluded that the band ratio algorithm is currently the best option for estimating POC from ocean color remote sensing in the Southern Ocean, although they recommended a slightly modified version of the regional algorithm. In spite of these results one has to recognize that the POC database (260 data points) is still modest when compared to global Chl matchup database (~2500 data points in Siegel et al., 2013), and more efforts are needed to carry out global POC measurements to increase this database in the future. In addition, historically much less efforts have been devoted to establishing robust POC in situ data collection protocols, and there have been no round robin or intercomparison experiments between different laboratories. More research efforts should be focused on this issue. In recent years, satellite-derived Chl data improved substantially our understanding of phytoplankton biomass and primary production distributions within the world's oceans. However, of particular interest to ocean biogeochemistry and its role in climate change is not Chl, but carbon. It is therefore important to continue the experimental and conceptual work to improve the reliability of in situ and satellite POC determinations. Another challenging task for the ocean color methods is development of the capability to partition the POC stock into the living and non-living components (Behrenfeld et al.,

Table 2 Summary of the error statistics i.e., the absolute average error (AAE), bias mean normalized bias (P_{BIAS}), mean absolute percentage error (MPE), R^2 coefficient and root mean square error (RMSE) for the POC concentrations [mg m^{-3}] compared in Fig. 3.

	N	AAE	Bias	P_{BIAS} [%]	MPE [%]	R^2	RMSE
All data included							
All data	260	32.87	−15.79	−18.35	38.62	0.76	59.49
GAC	87	30.18	−8.79	−11.35	40.40	0.72	51.51
MLAC	74	31.18	−4.88	−5.25	44.67	0.90	52.95
LAC	99	37.47	−30.09	−34.04	32.04	0.55	70.27
AMT data excluded							
All data	214	22.62	−1.84	−2.65	36.12	0.80	37.91
GAC	75	24.28	−0.63	−0.93	40.12	0.79	36.13
MLAC	71	25.33	2.08	2.93	44.56	0.79	38.81
LAC	68	17.96	−7.28	−10.33	22.89	0.82	39.43
ANT I and BIOSCOPE data excluded							
All data	225	32.48	−16.58	−20.62	40.49	0.76	60.32
GAC	76	30.57	−9.72	−13.14	42.45	0.71	53.11
MLAC	65	28.21	−2.14	−2.64	46.05	0.91	50.92
LAC	84	38.65	−33.95	−39.68	34.41	0.53	72.61

2005). In our final word we would like to stress that even if scientists continue to strive to decrease errors and improve satellite methods, the substantial scientific benefits from use of large scale ocean color satellite observations are unquestionable.

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