

A first attempt at testing correlation between MODIS ocean colour data and *in situ* chlorophyll-a measurements within Maltese coastal waters

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ABSTRACT

The study of spatio-temporal trends for key water quality parameters in the Maltese coastal waters is hindered by the lack of systematic observations spanning over the full domain and for sufficiently long time periods. Satellite data offers an alternative source of information, but requires ground truthing against *in situ* measurements. The aim of this study is to attempt the statistical comparison of MODIS ocean colour data, for a near-shore marine area off the north-east coastline of Malta, with *in situ* surface chlorophyll-a measurements, and to extract a twelve-month ocean colour data series for the same marine area. Peaks in surface chlorophyll-a concentration occurred in the January-February period, with lowest values being recorded during the early spring period. Log bias values indicate that the MODIS dataset under-estimates the surface chlorophyll-a values, whilst RMSD and r^2 values suggest that the match-up between satellite and *in situ* values is only partly consistent.

Keywords: Chlorophyll-a concentration · Maltese Islands · Annual dynamics · Ocean colour

1. INTRODUCTION

Despite the Maltese Islands being party to a number of onerous EU Directives whose main mandate is the promotion of a more rigorous water quality monitoring regime, including the Water Framework Directive (WFD) and the Marine Strategy Framework Directive (MSFD), operational monitoring of water quality parameters within the Maltese marine area, including chlorophyll-a, remains thin on the ground. In fact, monitoring of surface chlorophyll-a values within Maltese coastal waters is almost exclusively conducted on a short-term basis (a number of days each year) and mainly to assess the impact of aquaculture operations. In order to address this lacuna, the Malta Environment and Planning Authority (MEPA) issued a tender in 2010 for the environmental monitoring of Maltese waters pursuant to meeting WFD-related obligations.

To date, the only tangible attempt at exploiting remote sensing techniques for characterising the quality of Maltese waters was made by [1], who compared LANDSAT-5 ocean colour, surface temperature and water transparency data with *in situ* data collected on a single day and within a restricted spatial area. The same authors had proposed the extension of their pilot study to other areas of the Maltese marine domain, and had observed that the long-term conduction of such a study would enable the identification of trends and changes, and thus prove indispensable to coastal management in the Maltese Islands. In addition, the Water Framework Directive stipulates that monitoring of surface chlorophyll-a content should be conducted with a six month periodicity.

Ocean colour from satellite has given over the last two decades another dimension to ecosystem studies and marine biology, providing key information on the timing and spatial distribution of phytoplankton blooms, and the magnitude of primary production. Remote observations of ocean colour from space represent therefore a

major tool directly related to the marine biogeochemical distributions and associated processes [2]. Unlike [3], [2] report that ocean colour estimates behave well for the Mediterranean Sea when compared to other marginal seas, but acknowledge that this is likely associated with the location of their validation data set that might not be representative of the whole oligotrophic waters of the basin.

The aims of this study include a preliminary attempt at statistically validating ocean colour data derived from the MODIS platform through a limited number of surface chlorophyll-a field measurements and the extraction of a twelve-month ocean colour time-series for a site within Maltese coastal waters. To date, no publication has addressed the annual variability in surface chlorophyll-a values in Maltese coastal waters.

2. MATERIALS AND METHODS

The marine area of interest, for which ocean colour data were extracted and *in situ* chlorophyll-a measurements were taken, is enclosed within nearshore waters off the north-eastern coast of the island of Malta, as shown in Figure 1.

Within the field sampling protocol, two-litre water samples were collected at a depth of 50cm through the use of a Niskin bottle at six different stations in neritic waters to the north-east of the island of Malta (refer to Figure 1), during April and September 2010. Two or four replicates were collected at each sampling station.

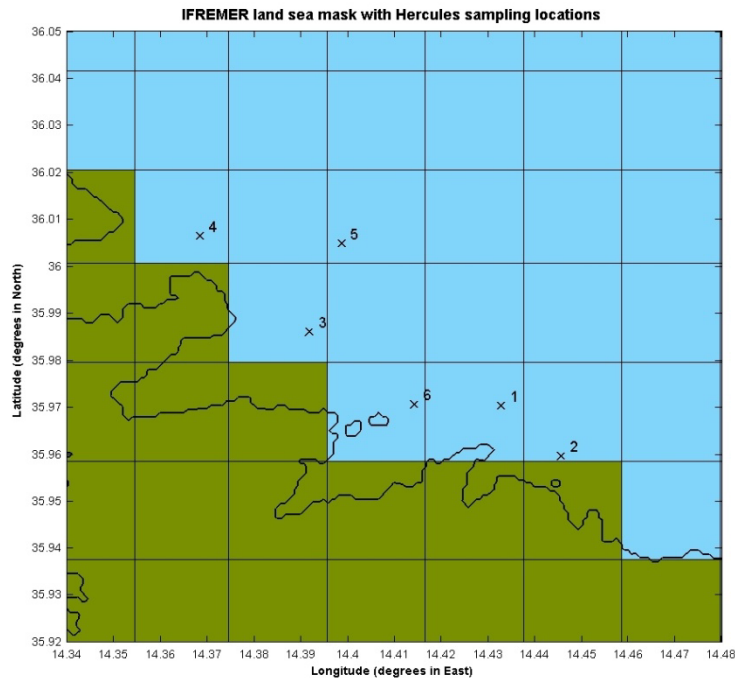


Figure 1 – Geographical location of the six coastal water sampling stations used, adopted, along with a system of replicates, in assessing the *in situ* surface chlorophyll-a values.

Chlorophyll-a content analysis was carried out according to the methodology given in [4]. The water samples were filtered through a 0.45 μ m membrane filter; pigment retained on the filters was extracted in 90% acetone and measured using a spectrophotometer.

Since the ocean colour dataset provided by the JRC (Joint Research Centre) Institute within the MyOcean project (version V0) extended spatially over a big domain, only a small subset of the dataset was extracted (the Maltese Coastal Area was defined as extending from 13.99°E to 14.79°E in longitudes and from 35.656°N to 36.219°N in latitudes). The aim was to extract the ocean colour time series at specific grid cells only. These grid cells correspond to the locations of the *in situ* measurements. The satellite data were defined at the centre of each grid cell, with the ocean colour data extracted through the MODIS platform being averaged around noon (12pm).

The main algorithms used to process ocean colour are the OC4v4 and the newer version OC4v6, which are standard algorithms developed by NASA intended for global applications. On the other hand, we know that the oligotrophic waters of the Mediterranean Sea are ‘optically different’ with respect to a global standard, with the global ocean colour algorithm OC4v4 exhibiting uncertainty levels in the chlorophyll-a estimation which are incompatible with the expected requirements of the ocean colour mission (chlorophyll uncertainty <35%) when applied to the Mediterranean Sea [5]. In fact, regional algorithms (such as BRIC and DORMA in [5]) have been demonstrated to perform better in retrieving chlorophyll-a concentrations in oligotrophic conditions and applying OC4v4 or v6 leads to significant overestimates. Therefore, the Group for Satellite Oceanography (GOS-ISAC) of the Italian National Research Council (CNR) based in Rome has developed a regional formula that corrects for this over-estimation.

Ideally, the comparison of the in-situ data products should have been performed with such Satellite Ocean-Colour reanalysis data being produced by GOS-ISAC, which utilises the regional algorithm specifically developed for the Mediterranean Sea. However, the production of this dataset is still ongoing (at the time of writing), and has not yet been released. Therefore, we had to use the data provided by JRC for this study. In a future study, a re-analysis with the data released by the GOS-ISAC will be performed.

The protocol proposed by [3] and used in [5] for testing possible correlations between MODIS ocean colour and *in situ* chlorophyll-a values was adopted. Such a protocol is based on the computation of the RMS log error and of the bias in log.

The RMS is an estimate of the error of the MODIS data set. It represents the value within which 67% of the data set fall [3]. The decision to logarithmically transform chlorophyll-a data before statistical evaluation is based on the following considerations:

- (i) the natural distribution of chlorophyll-a, which is log normal [6]
- (ii) some of the *in situ* chlorophyll-a values were very low and log transformation avoids ascribing too much weight to such extreme cases
- (iii) the data set was not normally distributed

Other statistical parameters include:

- bias in log, calculated as:
$$\frac{\sum(\log S - \log I)}{n}$$
- relative difference, which is another estimate of bias, and which is calculated as:
$$\frac{\sum[(S - I)/I]}{n}$$
- average absolute relative difference, which is calculated as:
$$\frac{\sum[|(S - I)/I|]}{n}$$
- coefficient of determination (r^2) on log-transformed data.

where S = ocean colour value and I = *in situ* chlorophyll-a value.

Together, these statistical measures provide information on the performance and uncertainty of the MODIS ocean colour data set in the Maltese coastal domain.

Prior to conducting such an analysis, ocean colour data which were coincident (occurring within the same time, +/- 1 day) and collocated (occurring within a single grid cell) were identified. Restricting the comparative analyses to just ocean colour and *in situ* chlorophyll-a data collected on the same day would have resulted in a highly restricted number of match-up pairs.

3. RESULTS AND DISCUSSION

Table 1 gives the results of the statistical validation exercise conducted, along with descriptive statistics for *in situ* chlorophyll-a and for ocean colour data. Figure 2 gives the annual variation in MODIS ocean colour values for the six sampling stations of interest.

Table 1 – RMG log error, mean *in situ* chlorophyll-a value, bias and coefficient of determination values for *in situ* surface chlorophyll-a ocean colour comparisons.

	Number of match-up pairs used for comparison	<i>In situ</i> chlorophyll-a values range (mg/m ³)	Mean <i>in situ</i> chlorophyll-a value (SD) (mg/m ³)	Ocean colour data values range (mg/m ³)	Mean ocean colour value (SD) (mg/m ³)	RMSD	Bias in log	Relative bias	Average absolute relative difference	r ²
April 2010 dataset	18	0.118 - 0.511	0.226 (0.097)	0.100 - 0.363	0.163 (0.070)	0.25	-0.14	-19.7%	44.4%	0.168
September 2010 dataset	10	0.130 - 0.500	0.369 (0.172)	0.139 - 0.589	0.238 (0.131)	0.69	-0.41	-23.4%	36.3%	0.116

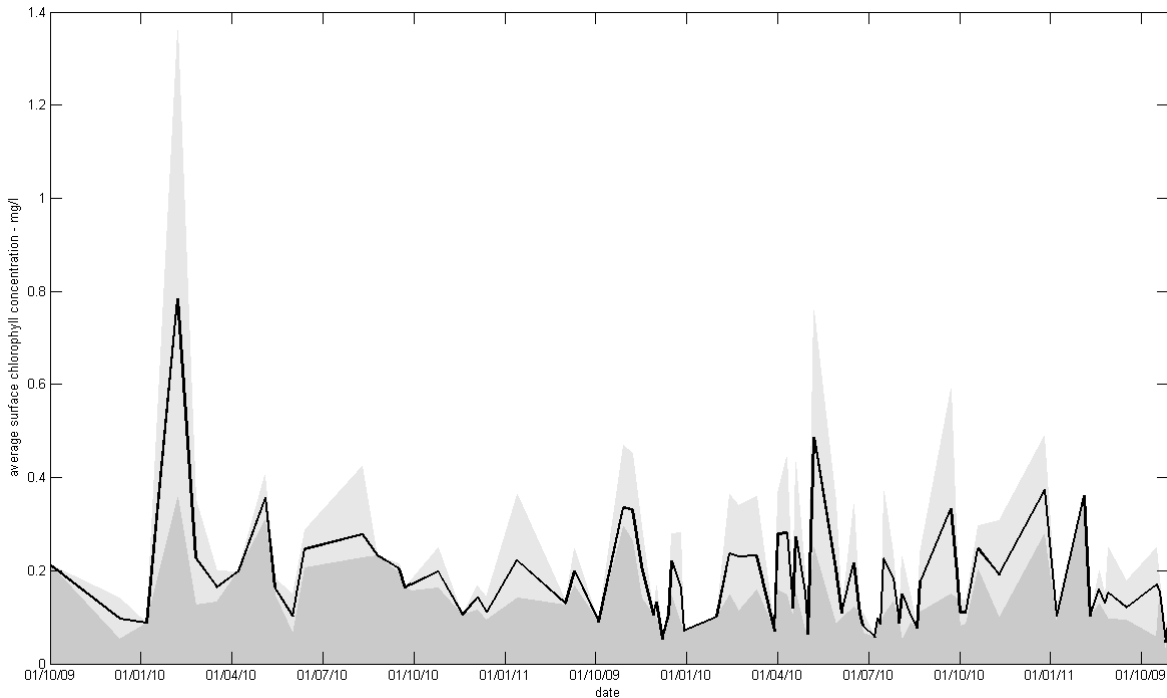


Figure 2 – Minimum, maximum (both shaded) and average (continuous black line) variation in ocean colour values for the marine area of interest during the December 2009-December 2010 period.

With the exception of a small number of outlying values, all *in situ* chlorophyll-a values recorded during the months of April and September fell within a narrow range, such that the standard deviation values for the two *in situ* sampling periods (0.097 and 0.171 mg/m³, respectively) were relatively low, compared to the mean chlorophyll-a values for the same months (0.226 and 0.369 mg/m³, respectively). For the April data set, in fact, just one *in-situ* surface chlorophyll-a value (0.363mg/m³) fell outside the 1 sigma value of 0.097, with the same value being omitted from the correlation analysis and from the related scatter plot. The highest *in situ* chlorophyll-a value obtained (over both sampled months) was 0.511mg/m³, such that all surface chlorophyll-a values obtained are consistent with those of an oligotrophic, optically non-complex, Class/Type I water body [7], of which the Mediterranean Sea is a quintessential example [8]. [9] consider a surface chlorophyll-a concentration of 0.4mg/m³ as the threshold between oligotrophic and mesotrophic conditions. The mean annual ocean colour value for the six grid positions under scrutiny ranged from 0.247mg/m³ to 0.361mg/m³. A high degree of variability was recorded for such values, with standard deviations for the same positions ranging from 0.137 to 0.290, with the highest recorded value (1.360mg/m³) being recorded on the 17th of January 2010. No corresponding, collocated surface chlorophyll-a values exist in literature for comparison.

Two peaks in ocean colour values could be observed, with the most pronounced of these peaks being observed in late January/early February, and a second less well-defined peak being observed in late August/early September. The ocean colour values obtained ranged from 0.040mg/m³ to 1.370mg/m³, with the lowest values generally being recorded during the April-May period. A winter surface chlorophyll-a peak is typical of the Mediterranean Sea, as testified by numerous studies for different regions of the basin (e.g. [10]). [11], in a preliminary survey of phytoplankton from Maltese inshore waters, attribute the high chlorophyll-a values in winter to a dominance by the diatom *Chaetoceros* sp. as a result of optimum ecological conditions during this season. Several studies (e.g. [12] and [13]) document winter diatom blooms (characterized by other species besides *Chaetoceros*, including *Thalassiosira*, *Proboscia*, *Rhizosolenia*, *Leptocylindrus*) in the Mediterranean Sea, labeling these blooms as ‘oases’ in the Mediterranean desert. The anomalously high January/February diatom bloom, in the absence of an ad hoc phytoplankton survey, is also substantiated by a concurrent bloom in some zooplankton taxa, notably Ctenophora (personal observation).

When contrasting the low RMS difference results obtained during the month of April (0.2514) with those in literature (e.g. [3], [5], [14], [15], [16]), one infers a high degree of fidelity/congruence between ocean colour and in-situ surface chlorophyll-a values recorded. The RMSD values obtained for the month of April also compare well with equivalent values cited within a global comparison study by Clerici et al. (2008). The same authors cite a SeaWiFS global average for RMSD of 0.29, being slightly higher for MODIS (0.31), a difference which they attribute to a smaller statistical basis. The RMSD values obtained during the month of September (0.69) indicate, on the other hand, considerable uncertainty in the satellite estimation of surface chlorophyll-a. Expressed in terms of average absolute relative difference, the differences between satellite and in-situ chlorophyll-a concentrations obtained in April and September 2010 are of the order of 40% and thus are closer to each other than the respective RMS differences of log-transformed concentrations.

The correlation analysis result shows r^2 values of 0.168 and 0.116 for April and September 2010, respectively. These low values are partly explained by the restricted dynamic range of the considered data set; they are also considerably lower than those cited in similar studies in literature which, however, are based on larger data sets. For example, [14] report r^2 values ranging from 0.64 to 0.74 for correlations involving surface chlorophyll-a values measured in the Mediterranean and not exceeding $0.4\text{mg}/\text{m}^3$, whilst [2] report r^2 values ranging from 0.56 to 0.81 for comparisons conducted within different geographical regions. [1] report high r^2 values (ranging from 0.75 to 0.80) for correlations run between LANDSAT ocean colour and *in situ* surface chlorophyll-a values recorded for three semi-enclosed bays along the eastern coastline of Malta.

The negative log bias values obtained indicate that the MODIS ocean colour dataset resorted to under-estimated the surface chlorophyll-a values for the area of interest. The more negative (when compared with other platforms, such as SeaWiFS) bias associated with MODIS is acknowledged by a number of authors – e.g. [17] and [18] – although such values are not yet fully understood. The negative bias values conflict with the findings of [3], [14], [15] and [16], who, for the Mediterranean Basin, report substantial positive bias values for the same basin, but using a different satellite platform (SeaWiFS), which is designed so as to be applied on global rather than on regional scales, or even a different ocean colour algorithm, as in the case of [14]. The latter report negative bias values when running comparisons between OC4v4-derived chlorophyll-a concentrations and *in situ* surface chlorophyll-a values ranging from 0.40 to $10\text{ mg}/\text{m}^3$, and positive bias values when the comparison is conducted with surface chlorophyll-a values within the 0.01-0.40 mg/m^3 range. As for the absolute relative differences, the relative biases for the 2 sampling periods are closer than the log-transformed biases, and are approximately -20%.

One must take into consideration two major caveats facing the current study:

- i) only two comparisons between surface chlorophyll-a and ocean colour values has been conducted so far, with the data set used consisting of just a few datum points, thus underlining the need to widen such a comparison further
- ii) the marine area deployed for the measuring of *in situ* surface chlorophyll-a was located just 2km offshore and can thus be considered as a coastal area. Coastal waters are optically complex due to the input of other substances which mask or modify the signal from phytoplankton and their pigments [19]. [2], in fact, report a higher degree of agreement for open ocean regions than for coastal areas.

In conclusion, bias values indicate that the MODIS data set under-estimates the surface chlorophyll-a values, whilst RMSD and r^2 values suggest that the match-up between satellite and *in situ* values is only partly consistent. More field observations are required to confirm these results. Regional algorithms should also be considered as alternative to improve the agreement between satellite and in-situ retrievals. Obtaining un-biased satellite products would already imply a significant reduction in RMS differences, and is a mandatory first step to properly characterize the local ecosystem.

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