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1 Regional ocean-colour chlorophyll algorithms for the 2 Red Sea

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13 Abstract

The Red Sea is a semi-enclosed tropical marine ecosystem that stretches from the Suez Canal and Gulf of Aqaba in the north, to the Gulf of Aden in the south. Despite its ecological and economic importance, its biological environment is relatively unexplored. Satellite ocean-colour estimates of chlorophyll concentration (an index of phytoplankton biomass) offer an observational platform to monitor the health of the Red Sea. However, little is known about the optical properties of the region. In this paper, we investigate the optical properties of the Red Sea in the context of satellite ocean-colour estimates of chlorophyll concentration. Making use of a new merged ocean-colour product, from the European Space Agency (ESA) Climate Change Initiative, and *in situ* data in the region, we test the performance of a series of ocean-colour chlorophyll algorithms. We find that standard algorithms systematically overestimate chlorophyll when com-

pared with the *in situ* data. To investigate this bias we develop an ocean-colour model for the Red Sea, parameterised to data collected during the Tara Oceans expedition, that estimates remote-sensing reflectance as a function of chlorophyll concentration. We used the Red Sea model to tune the standard chlorophyll algorithms and the systematic overestimation in chlorophyll originally observed was removed. Results suggest the overestimation was likely due to an excess of CDOM absorption per unit chlorophyll in the Red Sea when compared with average global conditions. However, we recognise that additional information is required to test the influence of other potential sources of the overestimation, such as aeolian dust. We present a series of regional chlorophyll algorithms for the Red Sea designed for a suite of ocean-colour sensors and available for further testing.

14 *Key words:* Phytoplankton, Ocean colour, Remote sensing, Chlorophyll, Red
15 Sea, Validation

16 **1. Introduction**

17 The Red Sea is a narrow, semi-enclosed oceanic basin situated between the
18 continents of Africa and Asia. At its southern end, it is connected to the Gulf
19 of Aden and Arabian Sea, through the strait of Bab-el-Mandeb, and at its north-
20 ern end to the Mediterranean Sea through the Suez Canal. Situated between
21 12° N and 28° N, it provides the shortest commercial shipping route between

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22 the Atlantic and Indian Ocean and thus is a major economic asset to the region
23 (Johns and Sofianos, 2012). The Red Sea is also the world's northernmost tropi-
24 cal sea and among the warmest and most saline seas on the planet (Belkin, 2009;
25 Longhurst, 2007; Raitzos et al., 2011). These unique environmental conditions
26 (high temperature and salinity) reflect those predicted in other marine regions
27 several decades from now (Christensen et al., 2007).

28 The Red Sea is categorised as a large marine ecosystem (Belkin, 2009) and
29 sustains coral reefs that provide habitat for a diverse range of marine organ-
30 isms (Baars et al., 1998), including sponges, bi-valves, pelagic larvae, fish, crus-
31 taceans, mollusks and echinoderms. At the base of the marine food-web, phyto-
32 plankton act as an integral component of these coral reef ecosystems transferring
33 energy to higher levels of the marine food-web, sustaining fisheries and provid-
34 ing sustenance to many inhabitants of the region. Despite the economic and
35 ecological importance of the Red Sea, despite extensive knowledge on its phys-
36 ical characteristics (e.g. Sofianos and Johns, 2003; Yao et al., 2014b,a) given its
37 strategic position as a commercial shipping route, and despite extensive studies
38 analysing the bio-optical properties of the Gulf of Eilat (Iluz et al., 2003; Soko-
39 letsky et al., 2003, 2004; Labiosa et al., 2003; Stambler, 2005, 2006) located at
40 the northern tip of the Red Sea, knowledge on large-scale biological dynamics
41 in the region is relatively limited to knowledge on the phytoplankton seasonal
42 cycle, rates of uptake of carbon and nitrogen by phytoplankton and the influence
43 of coral reef ecosystems on Red Sea productivity (Acker et al., 2008; Raitzos
44 et al., 2013; Qurban et al., 2014; Racault et al., 2015).

45 The main source of data used to investigate large-scale biological dynamics
46 in the Red Sea has been synoptic estimates of chlorophyll concentration (denoted
47 here as C and referred to in this paper as the chlorophyll concentration, being the
48 sum of monovinyl chlorophyll-a, divinyl chlorophyll-a, chlorophyllide-a, and
49 chlorophyll-a epimers and allomers (Werdell and Bailey, 2005), a measure of
50 phytoplankton biomass) derived using satellite ocean-colour data (Acker et al.,
51 2008; Raitzos et al., 2013; Brewin et al., 2013a). The temporal and spatial cover-
52 age of ocean-colour data surpass that of any *in situ* biological datasets currently
53 available for the Red Sea. Since the advent of the first ocean-colour sensor,
54 NASA's Coastal Zone Color Scanner, satellite ocean-colour data have been used
55 to understand the optical properties of the Red Sea (e.g. Kirby et al., 1993) and
56 other biogeochemically-relevant variables such as the chlorophyll concentration.
57 More recently, Acker et al. (2008) used ocean-colour data from the SeaWiFS and
58 MODIS-Aqua sensors to investigate variations in chlorophyll concentration in
59 the northern Red Sea, and Raitzos et al. (2013) used data from MODIS-Aqua to
60 describe the seasonal succession of chlorophyll and its relationship to the physi-
61 cal forcing.

62 A difficulty with biological interpretation of ocean-colour data from the Red
63 Sea has been the lack of *in situ* data required for validation and uncertainty char-
64 acterisation. There have been some validation efforts: for instance, Barbini et al.
65 (2004) showed reasonable agreement between satellite-derived chlorophyll and
66 *in situ* lidar fluorescence-derived chlorophyll in the Red Sea. Using *in vivo* fluo-
67 rometric chlorophyll measurements collected over large spatial scales, Brewin

68 et al. (2013a) demonstrated that the performance of standard MODIS-Aqua
69 chlorophyll products in the Red Sea was comparable to that in other regions of
70 the global ocean. Nonetheless, conclusions drawn on biological variability using
71 ocean-colour data in the Red Sea still remain uncertain, due primarily to lack of
72 suitable *in situ* datasets and limited understanding of the optical properties. A
73 further complication in using ocean-colour data for the Red Sea is difficulties in
74 atmospheric correction, for instance, due to the presence of high concentrations
75 of atmospheric dust aerosols from the surrounding arid continents which can
76 render many satellite ocean-colour pixels unusable for analysis of chlorophyll
77 concentration (Acker et al., 2008).

78 Between September 2009 and March 2012, the Tara Oceans expedition con-
79 ducted a ~91,000 km voyage to capture the global distribution of marine plank-
80 tonic organisms (Boss et al., 2014; Werdell et al., 2014a). A hyperspectral ab-
81 sorption and attenuation meter (WETLabs, Inc. AC-S) together with a flow-
82 through system (Slade et al., 2010; Boss et al., 2014) was used for continuous
83 measurements of absorption and attenuation by marine particles along the entire
84 Tara cruise track (Boss et al., 2014). During January 2010, the Tara cruise con-
85 ducted a meridional transect of the Red Sea (Fig. 1) providing the first compre-
86 hensive dataset of absorption and attenuation by particles at large spatial scales
87 in the Red Sea.

88 Recently, efforts have also been made to improve coverage of ocean-colour
89 data through the merging of data from different ocean-colour platforms (e.g.
90 the GlobColour project; Maritorena et al., 2010). In 2010 the European

91 Space Agency launched the Ocean Colour Climate Change Initiative (OC-CCI;
92 Brewin et al., 2013b) with the goal of creating a long-term, consistent, error-
93 characterised time series of merged ocean-colour products (MODIS-Aqua, Sea-
94 WiFS and MERIS), for use in climate-change studies. One of the advantages of
95 the OC-CCI dataset (version 1, see <http://www.oceancolour.org/>) is that, by using
96 an atmospheric correction algorithm called POLYMER (Steinmetz et al., 2011)
97 on MERIS, which performs retrievals in the presence of sun glint, significant
98 increases in ocean-colour coverage were attained (Steinmetz et al., 2011).

99 In this paper, we make use of *in situ* bio-optical data collected in the Red Sea
100 as part of the Tara Oceans expedition (Boss et al., 2014; Werdell et al., 2014a), to-
101 gether with previous *in situ* datasets (Barbini et al., 2004; Brewin et al., 2013a), to
102 investigate the optical properties of the Red Sea in the context of satellite ocean-
103 colour estimates of chlorophyll concentration. Using satellite (OC-CCI data)
104 and *in situ* match-ups, we evaluate the performance of a suite of chlorophyll
105 algorithms in the Red Sea. Discrepancies between satellite and *in situ* chloro-
106 phyll are investigated by developing an ocean-colour model for the Red Sea,
107 parameterised to data from the Tara Oceans expedition. The model describes re-
108 lationships between inherent optical properties of water constituents (absorption
109 and backscattering) and chlorophyll concentration. The ocean-colour model is
110 used to: i) improve our understanding of the optical properties of the region; and
111 ii) tune empirical satellite chlorophyll algorithms for use in the Red Sea. Uncer-
112 tainties in our approach are discussed and conclusions are cautiously stated given
113 the under-sampled nature of this region and its unique atmospheric properties.

114 **2. Methodology**

115 *2.1. Study site*

116 The Red Sea is an elongated basin with a mean depth of 524 m and a surface
117 area of $\sim 4.5 \times 10^{11} \text{ m}^2$ (Patzert, 1974). A deep trench runs along the centre of
118 the Red Sea from north to south reaching maximum depth of about $\sim 2300 \text{ m}$,
119 with shallower waters generally found at the southern end and deeper waters
120 toward the north (Fig. 1a). The Red Sea splits into two gulfs at the northern
121 end, the Gulf of Aqaba and the Gulf of Suez. The transport through these gulfs
122 is extremely small, meaning the only significant connection between the Red
123 Sea and the open ocean is through the Strait of Bab el Mandeb at the south
124 (Sofianos and Johns, 2003), where the Red Sea interacts with the Gulf of Aden
125 (Fig. 1a) and seasonal water exchange occurs (Yao et al., 2014b). Horizontal
126 circulation in the Red Sea is dominated by eddies (Yao et al., 2014a; Zhan et al.,
127 2014) and overturning is influenced by cyclonic recirculation and by overturning
128 circulation in the northern Red Sea, with sinking occurring along the eastern
129 boundary and upwelling along the western boundary (Yao et al., 2014a). The
130 Red Sea is surrounded by arid land masses with low precipitation, little riverine
131 input (Patzert, 1974) and high evaporation rates (Sofianos and Johns, 2003). The
132 atmospheric properties over the Red Sea (high evaporation rates and large dust
133 storms (Prakash et al., 2015)) challenges remote-sensing of ocean colour (Acker
134 et al., 2008).

135 The seasonal cycles of phytoplankton, as estimated from remote-sensing of
136 ocean colour, indicate higher concentrations during the winter months, attributed

137 to vertical mixing in the north and horizontal advection of nutrient-rich water
138 in the south, and minimum concentrations during the summer, associated with
139 strong seasonal stratification (Raitsos et al., 2013). However, during summer
140 months higher concentrations of phytoplankton can occur in some regions. The
141 Red Sea is surrounded by productive coral reefs (Fig. 1a) which contrast in phy-
142 toplankton seasonality to open ocean waters (peaking during summer months;
143 Racault et al., 2015) and are thought to contribute to the horizontal transfer of
144 nutrients and phytoplankton by eddies to open waters (Acker et al., 2008; Raitsos
145 et al., 2013). For further details on phytoplankton seasonal cycles, spatial struc-
146 tures, trophic regimes and inter-annual variations, inferred using ocean-colour
147 data, the reader is referred to the recent works of Raitsos et al. (2013, 2015) and
148 Racault et al. (2015).

149 2.2. *In situ* data

150 Three sources of *in situ* data were used in this study (Fig. 1):

- 151 • *In situ* hyperspectral absorption and attenuation data collected on a flow-
152 through system (Boss et al., 2014; Werdell et al., 2014a) during the Tara
153 Oceans expedition in the Red Sea in January 2010 (hereafter denoted
154 Tara).
- 155 • *In vivo* fluorometric data on chlorophyll concentration collected from three
156 research cruises during 2008, 2010 and 2011 (Brewin et al., 2013a), as part
157 of the Research Cruises expedition programme of the Red Sea Research
158 Center (RSRC) of King Abdullah University of Science and Technology
159 (KAUST).

- 160 • *In vivo* Lidar fluorescence data on chlorophyll concentration in the Red Sea
161 (Barbini et al., 2004) collected as part of the Mediterranean Sea, Indian and
162 Pacific Oceans Transect (MIPOT) oceanographic campaign between Italy
163 and New Zealand in November 2001.

164 All three sources of *in situ* data have been used previously for comparison with
165 satellite ocean-colour observations (Barbini et al., 2004; Brewin et al., 2013a;
166 Werdell et al., 2014a), though their inter-consistency is subject to caution, as
167 discussed in Section 5.1.1. These datasets are explained in more detail in the
168 following sections.

169 2.2.1. *Tara data*

170 During January 2010, hyperspectral particulate absorption ($a_p(\lambda)$, where λ
171 is the wavelength) and particulate attenuation ($c_p(\lambda)$) data were collected in the
172 Red Sea on the R/V Tara Oceans expedition using a WET Labs AC-S hyper-
173 spectral spectrophotometer and Sea-Bird Electronics SBE45 MicroTSG unit
174 (Boss et al., 2014; Werdell et al., 2014a; Picheral et al., 2014). Water from the
175 ship's flow-through system (~ 2 m depth) was passed through a Vortex debub-
176 bler and then through a WET Labs AC-S. The flow-through system sent the
177 water either directly to the AC-S instrument or through a $0.2\mu\text{m}$ cartridge fil-
178 ter preceding the AC-S instrument. Spectral $a_p(\lambda)$ and $c_p(\lambda)$ in the wavelength
179 interval 400-740 nm were then calculated by subtracting the filtered measure-
180 ments from the unfiltered measurements, providing calibration-independent es-
181 timates of $a_p(\lambda)$ and $c_p(\lambda)$ accounting for instrumental drifts and residual cali-
182 bration errors. These data were downloaded from the NASA SeaBASS website

183 (<http://seabass.gsfc.nasa.gov/> : Werdell et al., 2003) and processed following the
184 methods described in Slade et al. (2010). The system has been evaluated previ-
185 ously in a wide variety of oceanic waters (Dall’Olmo et al., 2009, 2011, 2012;
186 Slade et al., 2010; Westberry et al., 2010; Boss et al., 2014) and used to evalu-
187 ate satellite ocean-colour products (Brewin et al., 2012a; Werdell et al., 2014a).
188 Boss et al. (2014) and Werdell et al. (2014a) provide a more detailed description
189 of the processing methods used during Tara.

190 In total, 9169 spectra (one-minute binned averages) of $a_p(\lambda)$ and $c_p(\lambda)$ were
191 extracted from the Tara dataset spanning the Red Sea (Fig. 1). The hyperspectral
192 data were available at ~ 4 nm intervals between 404 and 736 nm. Data on $a_p(\lambda)$
193 and $c_p(\lambda)$ were extracted at the following wavelengths representative of recent
194 ocean-colour sensors (e.g. SeaWiFS, MODIS, MERIS and VIIRS): 410, 412,
195 443, 486, 488, 490, 510, 530, 547, 551, 555, 560, 620, 665 and 670nm. Where
196 data at the exact wavelengths were not available, spectral interpolation was used.
197 Data for $a_p(\lambda)$ were also extracted at 650, 676 and 715nm, for estimation of the
198 chlorophyll concentration. To derive chlorophyll concentration (C) we used the
199 method of Boss et al. (2014) and Werdell et al. (2014a), whereby the phyto-
200 plankton absorption coefficient at 676 nm ($a_{ph}(676)$) is first estimated using the
201 line height method of Davis et al. (1997) as modified by Boss et al. (2007), such
202 that

$$a_{ph}(676) = a_p(676) - [39/65a_p(650) + 26/65a_p(715)]. \quad (1)$$

203 The chlorophyll concentrations (C) were then estimated from $a_{ph}(676)$ following

204 Werdell et al. (2014a), according to

$$C = \left[\frac{a_{ph}(676)}{0.0152} \right]^{0.9055} . \quad (2)$$

205 The coefficients for Eq. 2 were computed from 52 corresponding High Per-
206 formance Liquid Chromatography (HPLC) samples of chlorophyll and $a_{ph}(676)$
207 (computed using Eq. 1, samples taken within 1h) collected along the entire Tara
208 Oceans expedition (see Fig. 1 of Werdell et al., 2014a). The method of using
209 the line-height of the absorption peak at red wavelengths to estimate chlorophyll
210 concentration has been found to perform with high accuracy when compared
211 with discrete *in situ* HPLC chlorophyll data in a wide range of natural optical
212 environments and diverse phytoplankton cultures (Dall’Olmo et al., 2009, 2012;
213 Westberry et al., 2010; Roesler and Barnard, 2014). Furthermore, the line height
214 determination is also: effective in removing the contributions of absorption by
215 colored dissolved organic matter (CDOM) and non-algal particles; relatively in-
216 dependent of the effects of biofouling; and unlike the *in vivo* fluorometric method
217 for estimating chlorophyll, the absorption line height is insensitive to incident ir-
218 radiance and non-photochemical quenching (Roesler and Barnard, 2014).

219 Following Werdell et al. (2014a), the particulate backscattering coeffi-
220 cient (b_{bp}) was estimated from the a_p and c_p data by using the scattering-to-
221 backscattering ratio as a function of chlorophyll, according to the method of
222 Twardowski et al. (2001), such that

$$b_{bp}(\lambda) = (0.0096C^{-0.253})[c_p(\lambda) - a_p(\lambda)]. \quad (3)$$

223 Whereas b_{bp} modelled from a_p and c_p is less ideal than direct measurement of
224 b_{bp} , the scattering-to-backscattering ratio has been shown to vary consistently
225 according to trophic conditions for a variety of open-ocean waters (Twardowski
226 et al., 2001; Whitmire et al., 2007; Dall’Olmo et al., 2012).

227 2.2.2. RSRC data

228 During 2008, 2010 and 2011, oceanographic data were collected from three
229 research cruises as part of the Research Cruises expedition programme of the
230 RSRC of KAUST (Fig. 1). Continuous *in vivo* fluorescence vertical profiles
231 were collected at each station using a WET Labs ECO-FLNTUs (FLNTURTD-
232 964) fluorometer attached to a CTD. A total of 401 *in situ* samples from the three
233 RSRC cruises were used in the analysis, consisting of average chlorophyll con-
234 centrations within the first optical depth. Brewin et al. (2013a) provide a detailed
235 description of the processing methods used during the three RSRC cruises (see
236 Section 2.1 of Brewin et al. (2013a)) and additional details are also provided as
237 Supplementary material. Of the 401 *in situ* samples, 33 were from 2008, 107
238 from 2010 and 261 from the 2011 cruise.

239 2.2.3. MIPOT data

240 As part of the MIPOT oceanographic campaign, conducted between Italy
241 and New Zealand, measurements of surface chlorophyll concentration were de-
242 rived using a lidar fluorosensor aboard the RV *Italica* (Barbini et al., 1999,
243 2001a,b, 2003, 2004). Between 18th to the 22nd November the RV *Italica* passed
244 through the centre of the Red Sea (Fig. 1), resulting in 505 measurements of
245 *in situ* chlorophyll concentration. This data were downloaded from the NASA

246 SeaBASS website <http://seabass.gsfc.nasa.gov/> (Werdell et al., 2003).

247 2.3. Satellite data

248 2.3.1. OC-CCI data

249 The OC-CCI project is one of 14 ESA funded CCI projects and focuses
250 specifically on creating a consistent, error-characterised time-series of ocean-
251 colour products, for use in climate-change studies (Brewin et al., 2013b).
252 From 2014, Version 1 of the OC-CCI dataset is available for community use
253 (<http://www.oceancolour.org/>). The dataset consists of a time-series of merged
254 and bias-corrected MERIS, MODIS-Aqua and SeaWiFS data at 4km-by-4km
255 resolution. Briefly, top-of-atmosphere reflectance data for SeaWiFS, MODIS-
256 Aqua and MERIS, at visible wavebands, were processed using atmospheric-
257 correction models, SeaDAS (Fu et al., 1998) for SeaWiFS and MODIS-Aqua
258 (SeaDAS version 7.0 using standard SeaDAS flags) and POLYMER (Steinmetz
259 et al., 2011) for MERIS. Remote-sensing reflectance (R_{rs}) data from MODIS-
260 Aqua and MERIS are then band-shifted to match the wavelengths of SeaWiFS
261 using an in-water bio-optical model (e.g. see Mélin and Zibordi, 2007). MODIS-
262 Aqua and MERIS are then bias-corrected to SeaWiFS at each wavelength, using
263 a pixel-by-pixel bias-correction model developed using daily match-up data be-
264 tween the respective sensors during over-lapping time periods, and finally the
265 data are merged into a single product. For further information on OC-CCI
266 processing, extensive documentation can be found on the following website
267 <http://www.esa-oceancolour-cci.org/>.

268 We chose to use OC-CCI products primarily due to improved coverage in the

269 Red Sea region when compared with individual sensors (see Fig. 2 of Racault
270 et al., 2015) and other merged products (e.g. GlobColour, see Section 8 of
271 Sathyendranath and Krasemann, 2014). Daily level 3 sinusoidal projected R_{rs}
272 data at 412, 443, 490, 510, 555 and 670nm, were downloaded from the OC-CCI
273 website covering the period September 1997 to July 2012. For regional verifi-
274 cation of the OC-CCI products, daily level 3 binned R_{rs} data for SeaWiFS pro-
275 cessed with SeaDAS, MODIS processed with SeaDAS, MERIS processed with
276 SeaDAS and MERIS processed with POLYMER were also used for the January
277 2010 period, which corresponds to the time of Tara Expedition passing through
278 the Red Sea.

279 2.3.2. *In situ satellite match-up data*

280 Daily $R_{rs}(\lambda)$ data from OC-CCI were matched in time (daily temporal
281 matchup) and space (latitude and longitude, closest 4 km pixel) with *in situ*
282 chlorophyll data. For all *in situ* datasets, but particularly the underway cruises
283 (Tara and MIPOT), when one or more *in situ* samples were matched to the same
284 satellite pixel, the *in situ* chlorophyll concentrations were averaged (using \log_{10}
285 transformation) and considered as a single match-up. A total of 410 OC-CCI
286 match-ups were obtained, 185 for Tara, 142 for RSRC and 83 for MIPOT. The
287 geographical distribution of these match-ups is shown in Fig. 1. For Tara, an ad-
288 ditional 84 SeaWiFS match-ups were available, 152 for MODIS, 96 for MERIS
289 processed with SeaDAS and 154 for MERIS processed with POLYMER.

290 2.4. *Satellite chlorophyll algorithms*

291 2.4.1. *OC4*

292 Satellite chlorophyll (C) algorithms incorporated into the comparison are
293 described in the following section. The standard NASA OC4 (v6) band-ratio
294 chlorophyll algorithm (O'Reilly et al., 2000) is a polynomial algorithm which
295 relates the ratio of remote-sensing reflectances at three pairs of wavebands with
296 chlorophyll concentration (C), using the following algorithm:

$$X = \log_{10}\{\max[R_{rs}(443), R_{rs}(489), R_{rs}(510)]/R_{rs}(555)\}. \quad (4)$$

297 The chlorophyll (C) is estimated according to:

$$C = 10^{(q_0+q_1X+q_2X^2+q_3X^3+q_4X^4)}, \quad (5)$$

298 where $q_0 = 0.3272$, $q_1 = -2.9940$, $q_2 = 2.7218$, $q_3 = -1.2259$ and $q_4 = -0.5683$
299 (NASA, 2010).

300 2.4.2. *OCI*

301 The band-difference algorithm of Hu et al. (2012) was also explored. This
302 algorithm has been found to perform well at low chlorophyll concentrations
303 ($<0.25 \text{ mg m}^{-3}$ Hu et al., 2012), which are typical of the Red Sea (Brewin et al.,
304 2013a). The approach uses a Colour Index (denoted here as ξ), based on a band-
305 difference between remote-sensing reflectance in the green part of the visible
306 spectrum and a base-line formed linearly between the blue and red wavebands,

307 such that:

$$\xi \approx R_{rs}(555) - 0.5[R_{rs}(443) + R_{rs}(670)]. \quad (6)$$

308 Chlorophyll is then related to ξ using the following equation:

$$C = 10^{A+B\xi}, \quad (7)$$

309 where $A = -0.4909$ and $B = 191.659$. Since Eq. 7 was designed specifically
310 for waters with low chlorophyll ($\leq 0.25 \text{ mg m}^{-3}$), at higher chlorophyll concentra-
311 tions ($> 0.3 \text{ mg m}^{-3}$) OC4 is used (Eq. 5), whereas for chlorophyll concentrations
312 between 0.25 and 0.3 mg m^{-3} , a combination of Eq. 7 and Eq. 5 is used to fa-
313 cilitate a smooth transition between algorithms. The OCI algorithm is expressed
314 as

$$C = \begin{cases} 10^{A+B\xi} & \text{if } [10^{A+B\xi}] \leq 0.25 \text{ mg m}^{-3} \\ \alpha[10^{(q_0+q_1X+q_2X^2+q_3X^3+q_4X^4)}] + (1-\alpha)[10^{A+B\xi}] & \text{if } 0.25 < [10^{A+B\xi}] \leq 0.3 \text{ mg m}^{-3} \\ 10^{(q_0+q_1X+q_2X^2+q_3X^3+q_4X^4)} & \text{if } [10^{A+B\xi}] > 0.3 \text{ mg m}^{-3}, \end{cases} \quad (8)$$

315 where α serves to provide a linear transition from Eq. 7 to Eq. 5 as chlorophyll
316 increases from 0.25 to 0.3 mg m^{-3} . This parameter is computed as $\alpha = (10^{A+B\xi} -$
317 $0.25)/(0.3 - 0.25)$.

318 2.4.3. GSM

319 The semi-analytical Garver-Siegel-Maritorena (GSM) model, initially devel-
320 oped by Garver and Siegel (1997) and later updated by Maritorena et al. (2002),
321 was also used in this study. The GSM model retrieves simultaneous estimates
322 of chlorophyll, absorption by combined detrital and dissolved matter at 443 nm
323 ($a_{dg}(443)$) and particle backscattering at 443 nm ($b_{bp}(443)$) from $R_{rs}(\lambda)$, assum-
324 ing an underlying bio-optical model and using non-linear optimisation. This
325 method was designed to estimate chlorophyll independent of influence from
326 $a_{dg}(443)$ and $b_{bp}(443)$, and output chlorophyll is constrained to lie within the
327 range that was used to parameterise the model ($0.01 < C < 64 \text{ mg m}^{-3}$).

328 2.4.4. OC4-MG

329 The OC4 model is designed for applications in Case-1 waters, in which ab-
330 sorption and scattering by substances other than phytoplankton are assumed to
331 covary with chlorophyll concentration. Morel and Gentili (2009b) developed a
332 correction that can be applied to OC4-type of algorithms, to account for devia-
333 tions in absorption a_g by gelbstoff (coloured dissolved organic matter, CDOM)
334 from the Case-1 assumption. The OC4 algorithm corrected according to Morel
335 and Gentili (2009b) is referred to here as OC4-MG.

336 This approach is based on the assumption that the ratio of reflectance at
337 412 nm to that at 443 nm ($R(412)/R(443)$) is mainly sensitive to CDOM, al-
338 beit influenced to some extent by chlorophyll, and that the ratio of reflectance
339 at 490 nm to that at 555 nm ($R(490)/R(555)$) is essentially dependent on chloro-
340 phyll, although also influenced to some extent by CDOM. The approach uses

341 the bio-optical model of Morel and Maritorena (2001), that implicitly includes
342 a prescribed relationship between CDOM absorption and chlorophyll, and thus
343 produces a unique set of curves relating $R(412)/R(443)$ to $R(490)/R(555)$. De-
344 viations from the prescribed relationship are introduced using a factor ϕ , with
345 $\phi > 1$ indicating an excess and $\phi < 1$ a deficit of a_g per unit chlorophyll.
346 Morel and Gentili (2009b) produced a 2D lookup table relating $R(412)/R(443)$
347 to $R(490)/R(555)$ for specific discrete values of ϕ . Relative anomalies in CDOM
348 (ϕ) with respect to its standard (chlorophyll-related) values can then be computed
349 efficiently using reflectance ratios derived from ocean color, by first converting
350 $R_{rs}(\lambda)$ to $R(\lambda)$ (see Appendix B of Morel and Gentili, 2009b). Once ϕ is obtained,
351 chlorophyll from standard band-ratio algorithms (OC4) can be corrected for the
352 effect of excess or deficit of CDOM (OC4-MG), by using another 2D lookup
353 table (Morel and Gentili, 2009b) and inputting the initial chlorophyll estimate
354 (OC4) and the retrieved ϕ value.

355 2.5. Statistical tests and algorithm ranking

356 To compare the performance of the satellite chlorophyll algorithms with the
357 *in situ* data in the Red Sea, a suite of univariate statistical tests were used follow-
358 ing Brewin et al. (2013b). These included: the Pearson correlation coefficient
359 (r); the root mean square error (Ψ); the average bias between model and mea-
360 surement (δ); the centre-pattern (or unbiased) root mean square error (Δ), noting
361 that $\Delta^2 = \Psi^2 - \delta^2$; the slope (S) and intercept (I) of a Type-2 regression; and the
362 percentage of possible retrievals (η). The equations used for each of these sta-
363 tistical tests are provided in Section 4.1 of Brewin et al. (2013b). All statistical

364 tests were performed in \log_{10} space, considering chlorophyll is approximately
365 log-normally distributed (Campbell, 1995).

366 To rank the performance of the algorithms used in this study we adopted the
367 classification presented in Brewin et al. (2013b). Briefly, for each statistical test
368 (r , Ψ , δ , Δ , S , I and η) the statistic of a model is compared with the average of all
369 models, and a score is assigned based (predominately) on whether the statistic
370 in question is significantly worse (0 points), similar (1 point) or better (2 points)
371 than the average of all models. All points are then summed over each statistical
372 test and the total score for each model is normalised by the average score of
373 all models being tested. A score of one indicates the performance of a model
374 is average with respect to all models, a score greater than one indicates model
375 performance is better than the average, and a score less than one indicates model
376 performance is worse than average.

377 Following Brewin et al. (2013b), the stability of the scoring system and the
378 sensitivity of the scores were tested using the method of bootstrapping (Efron,
379 1979; Efron and Tibshirani, 1993). This involved random re-sampling with re-
380 placement of the *in situ* data (1000 times) to create 1000 new datasets of the same
381 size as the original dataset, but not identical to it (Monte-Carlo approach). The
382 points classification was then re-run for each new dataset and from the resulting
383 distribution of scores, a mean score for each model was computed. Additionally,
384 15.9% and 84.1% confidence intervals (equivalent to one standard deviation for
385 a normal distribution) on the bootstrap distribution were taken and assumed to be
386 the error-bars or confidence limits on the mean score for each model. For further

387 details on the points classification method the reader is referred to Section 4 of
388 Brewin et al. (2013b).

389 **3. Ocean-color model for the Red Sea**

390 In this section we present an ocean-colour model that is tuned to data in
391 the Red Sea. It is based on the classic Case-1 bio-optical assumption (Morel
392 and Prieur, 1977) that ocean-colour reflectance can be related to total chloro-
393 phyll concentration (C) and co-varying material. We consider this assumption
394 a reasonable starting point given that: the focus of the study is on ocean-colour
395 chlorophyll algorithms; the Red Sea is oligo- to meso-trophic in nature (Raitso
396 et al., 2013) with negligible terrestrial or riverine input; and little is known about
397 the optical properties in the region.

398 We begin by assessing the relationship between absorption by particles (in-
399 cluding both phytoplankton and detritus) at 443nm, denoted $a_p(443)$, and chloro-
400 phyll concentration (C) estimated from a_p in the red during Tara, shown in
401 Fig. 2a. Whereas chlorophyll is estimated from a_p between 650-715 nm fol-
402 lowing Eq. 1 and 2, the relationship between $a_{ph}(676)$ and $a_{ph}(443)$ varies due
403 to changes in accessory pigmentation among phytoplankton that influences the
404 blue region of the absorption spectrum with minor influence on the red region
405 (Bricaud et al., 2004), and also because the flattening effect on the absorption
406 spectra, related to the size of the particles, is not the same in the red and in the
407 blue-green parts of the spectrum. As measured during Tara in January 2010,
408 chlorophyll varies between 0.04-1.0 mg m⁻³ (Fig. 2a), confirming the Red Sea
409 is oligo- to meso-trophic. Figure 2a shows two dense groups (or assemblages)

410 of particles: one group (hereafter denoted assemblage 1) is found between 0.06-
 411 0.1 mg m⁻³ of chlorophyll ($a_p(443)$ between 0.009 and 0.013 m⁻¹) and the other
 412 group (hereafter denoted assemblage 2) is found between 0.2-0.6 mg m⁻³ of
 413 chlorophyll ($a_p(443)$ between 0.013 and 0.030 m⁻¹). These assemblages are
 414 also separated geographically, with assemblage 1 found mainly in the northern
 415 oligotrophic waters of the Red Sea and assemblage 2 in the more mesotrophic
 416 southern waters. The optical properties of the two assemblages (with respect to
 417 $a_p(443)$) are significantly different, with the particulate specific absorption co-
 418 efficient at 443 nm ($a_p^*(443) = a_p(443)/C$) of assemblage 1 considerably higher
 419 ($\sim 0.22 \text{ m}^2 (\text{mg C})^{-1}$) than that of assemblage 2 ($\sim 0.05 \text{ m}^2 (\text{mg C})^{-1}$).

420 3.1. Two-component model of chlorophyll

421 Based on the finding that the Red Sea is primarily dominated by two assem-
 422 blages of particles with different optical properties, we develop a two-component
 423 ocean-colour model for the Red Sea. For this model, assemblage 1 is represen-
 424 tative of more oligotrophic conditions and assemblage 2 of mesotrophic condi-
 425 tions. Note that other studies (e.g. Brewin et al., 2011; Devred et al., 2011) have
 426 highlighted the benefits of including a third assemblage representative of more
 427 eutrophic conditions. However, this is not a requirement for the Red Sea consid-
 428 ering chlorophyll rarely exceeds 1 mg m⁻³. We start by relating the chlorophyll
 429 concentration of assemblage 1 (C_1) to the total chlorophyll concentration follow-
 430 ing an equation first presented by Sathyendranath et al. (2001)

$$C_1 = C_1^m [1 - \exp(-S_1 C)], \quad (9)$$

431 where C_1^m represents the asymptotic maximum chlorophyll concentration for as-
432 semblage 1, and S_1 determines the initial increase in C_1 with C . The chlorophyll
433 concentration of assemblage 2 (C_2) can then be computed according to

$$C_2 = C - C_1^m[1 - \exp(-S_1 C)]. \quad (10)$$

434 The parameters of Eq. 9 (C_1^m and S_1) can be computed with knowledge on C_1
435 and C , acquired from either High Performance Liquid Chromatography (HPLC,
436 Brewin et al., 2010, 2011, 2012a,b; Brotas et al., 2013), fluorometric analysis us-
437 ing size-fractionated filtration (Brewin et al., 2014), or from a_{ph} and chlorophyll
438 data, by making assumptions on the relationship between C_1^m and S_1 (Devred
439 et al., 2006, 2011). As there is currently little information in the Red Sea on
440 HPLC or fluorometric analysis using size-fractionated filtration, we chose to use
441 the parameters of Brotas et al. (2013) for pico-phytoplankton within the 1st op-
442 tical depth, such that $C_1^m \sim 0.06$ and $S_1 \sim 17.06$ (see Table 1). We chose to use
443 these parameters for the following reasons: (1) when fitting Eq. 12 (shown be-
444 low) to data in the Red Sea, these parameters resulted in the lowest bias and the
445 highest correlation coefficient between modelled $a_p(443)$ and measured $a_p(443)$
446 when compared with results obtained using other published parameters (e.g.
447 Brewin et al., 2010, 2011, 2012a,b, 2014); (2) with these model parameters, the
448 dominant assemblage transitions from 1 to 2 at around 0.1 mg m^{-3} of chlorophyll
449 (Fig. 2b), consistent with results in Fig. 2a; and (3) these parameters were com-
450 puted using data within the penetration depth of the satellite signal (Brotas et al.,
451 2013). The percentage contribution of each assemblage to total chlorophyll as a

452 function of total chlorophyll is illustrated in Fig. 2b.

453 3.2. Particulate absorption model

454 The particulate absorption ($a_p(\lambda)$) model we adopt follows a similar model
455 presented by Sathyendranath et al. (2001) for phytoplankton absorption. Here,
456 $a_p(\lambda)$ is modelled as a function of chlorophyll (C) according to

$$a_p(\lambda) = a_{p,1}^*(\lambda)C_1 + a_{p,2}^*(\lambda)C_2, \quad (11)$$

457 where $a_{p,1}^*(\lambda)$ and $a_{p,2}^*(\lambda)$ represent the chlorophyll-specific particulate absorption
458 coefficients of assemblages 1 and 2, respectively. Expanding Eq. 11 by inserting
459 Eq. 9 and 10 results in the following expression:

$$a_p(\lambda) = C_1^m [a_{p,1}^*(\lambda) - a_{p,2}^*(\lambda)] [1 - \exp(-S_1 C)] + a_{p,2}^*(\lambda) C. \quad (12)$$

460 By setting C_1^m and S_1 according to Brotas et al. (2013) (Table 1, Fig. 2), Eq. 12
461 was fitted to $a_p(\lambda)$ and C from Tara to derive $a_{p,1}^*(\lambda)$ and $a_{p,2}^*(\lambda)$. The fitting pro-
462 cedure used a standard, non-linear least squares method (Levenberg-Marquardt,
463 IDL Routine MPFITFUN (Moré, 1978; Markwardt, 2008)), and was fitted in
464 \log_{10} space, assuming a log-normal distribution for $a_p(\lambda)$. The retrieved param-
465 eters, provided in Table 1 and plotted in Fig. 3a, were obtained by taking the
466 median and 95% confidence interval on the 1000 bootstraps. This involved: ran-
467 domly re-sampling the data with replacement to create 1000 new datasets of the
468 same sample size as the original dataset but not identical to it or each other; fit-
469 ting Eq. 12 to each dataset to obtain a distribution of parameters; and then taking

470 the median and 95% confidence intervals on the estimated parameter distribu-
 471 tion, the latter to provide an indication of uncertainty on the retrieved parameter.
 472 Assemblage 1 has a higher chlorophyll-specific particulate absorption in the blue
 473 region of the spectrum when compared with assemblage 2 (Fig. 3a). Equation
 474 12 captures the variability in a_p as a function of C with low error (Table 2), and
 475 the proposed relationship between $a_p(443)$ and C is similar to that presented by
 476 Bricaud et al. (1998) using a global dataset, but with no measurements in the Red
 477 Sea (Fig. 3d).

478 3.3. Particulate backscattering model

479 Various models have been presented that relate particulate backscattering
 480 (b_{bp}) to chlorophyll (C) in open-ocean (Case-1) waters (e.g. Morel and Mari-
 481 torena, 2001; Sathyendranath et al., 2001; Twardowski et al., 2001; Huot et al.,
 482 2008). To maintain consistency with the two-component model of particulate
 483 absorption (Eq. 12), we used the approach of Brewin et al. (2012a), such that

$$b_{bp}(\lambda) = C_1^m [b_{bp,1}^*(\lambda) - b_{bp,2}^*(\lambda)] [1 - \exp(-S_1 C)] + b_{bp,2}^*(\lambda) C + b_{bp}^k(\lambda), \quad (13)$$

484 where $b_{bp,1}^*(\lambda)$ and $b_{bp,2}^*(\lambda)$ represent the chlorophyll-specific particulate backscat-
 485 tering coefficients of assemblage 1 and 2 respectively, and $b_{bp}^k(\lambda)$ represents a
 486 constant background. It is worth noting that the two assemblages used in this
 487 study (assemblage 1 and 2) are different from those used in Brewin et al. (2012a).
 488 In the Brewin et al. (2012a) study, where the focus was on developing a model
 489 from oligo- to eu-trophic waters, small cells were grouped as pico-nanoplankton

490 (cells $<20\mu\text{m}$) and larger cells as microplankton (cells $>20\mu\text{m}$). Alternatively in
 491 this study, where the focus is on oligo- to meso-trophic waters, assemblage 1 is
 492 likely more representative of the picoplankton size class and assemblage 2 of the
 493 nanoplankton size class. This difference is reflected in the choice of parameters
 494 for C_1^m and S_1 in Eq. 13.

495 Equation 13 was fitted using $b_{bp}(\lambda)$ and C from Tara to derive $b_{bp,1}^*(\lambda)$,
 496 $b_{bp,2}^*(\lambda)$ and $b_{bp}^k(\lambda)$ using the same fitting procedure as that used in Eq. 12 and
 497 setting C_1^m and S_1 according to Brotas et al. (2013) (Table 1). Following Brewin
 498 et al. (2012a), the spectral dependency of $b_{bp,1}^*(\lambda)$, $b_{bp,2}^*(\lambda)$ and $b_{bp}^k(\lambda)$ were as-
 499 sumed to follow a power function, such that

$$\begin{aligned}
 b_{bp}(\lambda) = & b_{bp,1}^*(\lambda_0)(\lambda/\lambda_0)^{-\gamma_1} \{C_1^m [1 - \exp(-S_1 C)]\} + & (14) \\
 & b_{bp,2}^*(\lambda_0)(\lambda/\lambda_0)^{-\gamma_2} \{C - C_1^m [1 - \exp(-S_1 C)]\} + \\
 & b_{bp}^k(\lambda_0)(\lambda/\lambda_0)^{-\gamma_k},
 \end{aligned}$$

500 where γ_1 , γ_2 and γ_k represent the exponents of the power function describing
 501 the spectral shape of each component of the model, and $\lambda_0 = 443\text{nm}$. Having
 502 obtained a distribution of parameters for $b_{bp,1}^*(\lambda)$, $b_{bp,2}^*(\lambda)$ and $b_{bp}^k(\lambda)$ from fitting
 503 Eq. 13 to the $b_{bp}(\lambda)$ and C data, the remaining parameters (γ_1 , γ_2 and γ_k) were
 504 obtained by fitting a wavelength-dependent power function to $b_{bp,1}^*(\lambda)$, $b_{bp,2}^*(\lambda)$
 505 and $b_{bp}^k(\lambda)$. Retrieved parameters for Eq. 14 are provided in Table 1 together
 506 with their 95% confidence intervals and plotted in Fig. 3b.

507 In general, assemblage 2 has a higher (and better constrained) chlorophyll-

508 specific particulate backscattering than assemblage 1 at most wavelengths (Fig.
509 3b), with assemblage 1 having a steeper power exponent than assemblage 2, con-
510 sistent with the expectation that smaller particles have a steeper power exponent
511 than larger particles (Loisel et al., 2006; Kostadinov et al., 2009). However, it
512 is worth noting that the background component γ_k is flatter than that observed
513 by Brewin et al. (2012a) and that γ_1 is also very high (close to that of molecular
514 scattering by pure-water, see Table 1). It is likely that more data at very low
515 chlorophyll concentrations would help to separate better the spectral shape of
516 backscattering by the background component and that by assemblage 1 when fit-
517 ting Eq. 14. Nonetheless, Eq. 14 is seen to capture most of the variability in b_{bp}
518 as a function of chlorophyll (C) with reasonable error statistics (Table 2). The
519 model captures the general trend in $b_{bp}(443)$ with increasing chlorophyll, and is
520 in good agreement with that proposed by Brewin et al. (2012a) using a global
521 dataset that did not contain any measurements from the Red Sea (Figure 3e).

522 3.4. CDOM absorption model

523 Considering that no direct measurements of CDOM absorption were taken
524 during Tara, we used satellite match-ups between *in situ* chlorophyll and satellite
525 OC-CCI R_{rs} to develop a dataset of CDOM absorption (a_g) and chlorophyll,
526 from which we could parameterise a model. Using the 185 OC-CCI match-
527 ups for Tara, we first converted $R_{rs}(\lambda)$ to $R(\lambda)$ (see Appendix B of Morel and
528 Gentili, 2009b) and implemented the Morel and Gentili (2009b) 2D lookup table
529 to obtain ϕ . Of the 185 match-ups, there were 157 realistic estimates of ϕ with
530 28 ϕ estimates falling outside the realistic range (Morel and Gentili, 2009b). The

531 values of ϕ were found to vary between 1.29 and 8.76, with a median value of
532 2.11 and a standard deviation of 1.25, and indicate that absorption by CDOM
533 per unit chlorophyll during Tara was on average twice that of standard Case-
534 1 relationships. Absorption by CDOM at 400 nm ($a_g(400)$) was computed for
535 each *in situ* sample using *in situ* chlorophyll data and the estimate of ϕ (Morel,
536 2009; Morel and Gentili, 2009b), such that

$$a_g(400) = \phi 0.065C^{0.63}. \quad (15)$$

537 To estimate $a_g(\lambda)$ from $a_g(400)$, Morel and Gentili (2009b) used a fixed value of
538 0.018 nm^{-1} for the exponential slope of CDOM with wavelength (S_g). Whereas
539 the 2D lookup table used to obtain ϕ implicitly includes this hypothesis, a sen-
540 sitivity study in Morel and Gentili (2009b) indicates the choice of the S_g is not
541 crucial when deriving ϕ . Recent evidence from *in situ* and satellite inversion data
542 indicates S_g is negatively correlated with a_g at a reference wavelength (Bricaud
543 et al., 2012; Swan et al., 2013), likely related to the selective bleaching of some
544 CDOM components by sunlight (Whitehead et al., 2000), and possibly important
545 in regions exposed to high doses of solar radiation such as the Red Sea. Using
546 data from the NASA NOMAD dataset (Werdell and Bailey, 2005), from only
547 Case-1 waters, following Lee and Hu (2006), and data from the Bermuda Bio-
548 Optics Project (Siegel et al., 2001), S_g was found to be significantly correlated
549 with $a_g(400)$ following a non-linear relationship ($S_g = 0.0086a_g(400)^{-0.2024}$,
550 $r = 0.61$, $p < 0.0001$, see Supplementary Fig. S1). This relationship was used

551 to estimate spectral a_g from the 157 estimates of $a_g(400)$, such that

$$a_g(\lambda) = a_g(400) \exp[-0.0086a_g(400)^{-0.2024}(\lambda - 400)]. \quad (16)$$

552 For the 157 measurements, S_g was found to vary between 0.011 and 0.020 nm⁻¹,
553 with a median value of 0.018 nm⁻¹ and a standard deviation of 0.002 nm⁻¹, and
554 was consistent with the value of 0.018 nm⁻¹ originally used by Morel and Gentili
555 (2009b).

556 Having developed this dataset of inferred $a_g(\lambda)$ and C characteristic of con-
557 ditions in the Red Sea during the Tara Expedition, this dataset was used to de-
558 velop a Red Sea model that related $a_g(\lambda)$ directly to C , given that no direct mea-
559 surements of CDOM absorption were available. For consistency with the two-
560 component model of particulate absorption (Eq. 12), we used a similar approach
561 to describe the relationship between chlorophyll (C) and $a_g(\lambda)$, where

$$a_g(\lambda) = C_1^m [a_{g,1}^*(\lambda) - a_{g,2}^*(\lambda)] [1 - \exp(-S_1 C)] + a_{g,2}^*(\lambda) C, \quad (17)$$

562 and $a_{g,1}^*(\lambda)$ and $a_{g,2}^*(\lambda)$ represent the chlorophyll-specific absorption coefficient
563 by CDOM of assemblage 1 and 2 respectively. Equation 17 was fitted using
564 the 157 corresponding $a_g(\lambda)$ and C measurements from the Tara Expedition to
565 derive $a_{g,1}^*(\lambda)$ and $a_{g,2}^*(\lambda)$ using the same fitting procedure as that used in Eq. 12
566 and setting C_1^m and S_1 according to Brotas et al. (2013) (Table 1). Statistically,
567 the performance of Eq. 17 was similar to that of a traditional power function
568 fitted to the same dataset (Z-test at 443nm, $p=0.95$; Cohen and Cohen, 1983).

569 Since C_1^m and S_1 were prescribed (Brotas et al., 2013), there are two unknown
 570 parameters in Eq. 17, which is the same as the number of parameters required to
 571 fit a power function. Given the exponential function (Eq. 16) that $a_g(\lambda)$ follows,
 572 Eq. 17 can be expressed according to

$$a_g(\lambda) = a_{g,1}^*(\lambda_0) \exp[-S_{g,1}(\lambda - \lambda_0)] \{C_1^m [1 - \exp(-S_1 C)]\} + \quad (18)$$

$$a_{g,2}^*(\lambda_0) \exp[-S_{g,2}(\lambda - \lambda_0)] \{C - C_1^m [1 - \exp(-S_1 C)]\},$$

573 where $S_{g,1}$ and $S_{g,2}$ represent the exponential slopes of CDOM for each assem-
 574 blage, and $\lambda_0 = 443$ nm. Having obtained the values of $a_{g,1}^*(\lambda)$ and $a_{g,2}^*(\lambda)$ at
 575 every wavelength from fitting Eq. 17, the parameters $S_{g,1}$ and $S_{g,2}$ were then
 576 obtained by fitting the exponential function to $a_{g,1}^*(\lambda)$ and $a_{g,2}^*(\lambda)$. The retrieved
 577 parameters for Eq. 18 are provided in Table 1 together with their 95% confidence
 578 intervals and are plotted in Fig. 3c.

579 From the resulting parameterisation of Eq. 18, waters where assemblage 2
 580 reside are seen to have higher CDOM absorption for a given chlorophyll concen-
 581 tration, at most wavelengths, than waters where assemblage 1 reside, and a lower
 582 exponential slope (Fig. 3c). The model is seen to capture the trend in $a_g(443)$
 583 with increasing chlorophyll (Fig. 3f, see also Table 2 for statistical tests). How-
 584 ever, the Red Sea model estimates a significantly higher amount of $a_g(443)$ for
 585 a given chlorophyll concentration (Fig. 3f) when compared with standard global
 586 relationships (Morel, 2009; Morel and Gentili, 2009b).

587 *3.5. Remote sensing reflectance (R_{rs}) model*

588 Once the IOPs of a_p , a_g and b_{bp} are known, they can be combined with pure
589 seawater IOPs to estimate total absorption (a) and backscattering (b_b), such that

$$a(\lambda) = a_p(\lambda) + a_g(\lambda) + a_w(\lambda), \quad (19)$$

590 and

$$b_b(\lambda) = b_{bp}(\lambda) + b_{bw}(\lambda), \quad (20)$$

591 where $a_w(\lambda)$ and $b_{bw}(\lambda)$ are pure water IOPs for absorption and backscattering
592 respectively. For the Red Sea model, pure water a_w from Pope and Fry (1997)
593 and b_{bw} from Zhang and Hu (2009) and Zhang et al. (2009) were used. The
594 b_{bw} values were computed assuming a salinity of 40 psu and a water tempera-
595 ture of 27°C, typical of the northern oligotrophic waters of the Red Sea (Raitsos
596 et al., 2013; Triantafyllou et al., 2014; Yao et al., 2014b) where b_{bw} has a high
597 contribution to b_b .

598 Various methods have been proposed to relate $a(\lambda)$ and $b_b(\lambda)$ to $R_{rs}(\lambda)$ (e.g.
599 Gordon et al., 1988; Lee et al., 2002). Here we used the approach of Lee et al.
600 (2009, 2010a,b, 2013) that explicitly separates the phase-function of molecular

601 and particle scattering, such that

$$R_{rs}(\lambda, \Omega) = \left(G_0^w(\Omega) + G_1^w(\Omega) \frac{b_{bw}(\lambda)}{a(\lambda) + b_b(\lambda)} \right) \frac{b_{bw}(\lambda)}{a(\lambda) + b_b(\lambda)} + \left(G_0^p(\Omega) + G_1^p(\Omega) \frac{b_{bp}(\lambda)}{a(\lambda) + b_b(\lambda)} \right) \frac{b_{bp}(\lambda)}{a(\lambda) + b_b(\lambda)}, \quad (21)$$

602 where parameters $G_0^w(\Omega)$, $G_1^w(\Omega)$, $G_0^p(\Omega)$, $G_1^p(\Omega)$ were derived from Hydrolight
603 simulations (Lee et al., 2009) for various Sun angles and viewing geometries,
604 with Ω collectively representing these geometries. Parameters are provided in
605 Table 1 for a solar zenith angle in air equal to zero, sensor nadir-view angle in
606 air equal to zero, and a sensor azimuth angle in relation to the solar plane equal
607 to zero (i.e. fully-normalised). Equations 12, 14, 18, 19, 20 and 21 can be used
608 together with model parameters in Table 1 and pure water IOPS (Pope and Fry,
609 1997; Zhang and Hu, 2009; Zhang et al., 2009) to reconstruct $R_{rs}(\lambda)$ as a function
610 of chlorophyll (C).

611 4. Results

612 4.1. Performance of the Red Sea ocean-colour model

613 The Red Sea ocean-colour model was first evaluated using the 185 OC-CCI
614 satellite R_{rs} and chlorophyll match-ups during Tara. Using *in situ* chlorophyll,
615 R_{rs} from 412-555 nm was reconstructed using the model (Eq. 12, 14, 18, 19, 20
616 and 21). Reconstructed R_{rs} are compared with observed R_{rs} from satellite data
617 (OC-CCI) in Figure 4. The top row of plots show the reconstructed and observed
618 absolute values of R_{rs} . Between 412-510 nm there is good agreement between

619 model and observations, with correlation coefficients (r) exceeding 0.8 and low
620 errors ($\Psi < 0.001 \text{ sr}^{-1}$, $\Delta < 0.0009 \text{ sr}^{-1}$). There is a slight tendency for the
621 model to underestimate $R_{rs}(412)$ at larger values (Fig. 4), and for $R_{rs}(555)$ the
622 model is relatively invariant and struggles to reproduce the variability shown in
623 the OC-CCI observations.

624 Whereas the magnitude of $R_{rs}(412)$ is important for deriving IOPs, it is the
625 shape of the R_{rs} (the spectral values of R_{rs} normalised to the corresponding value
626 at a single wavelength) that is particularly sensitive to changes in chlorophyll
627 (O'Reilly et al., 2000). The bottom row of plots in Fig. 4 compares the R_{rs}
628 from the model, normalised at 555 nm, with the corresponding R_{rs} from OC-
629 CCI. In general, there is good agreement between model and observation at all
630 wavelengths, with high correlation coefficients ($r > 0.94$), low errors ($\Psi < 0.49$,
631 $\Delta < 0.45$) and biases (δ) close to zero. Similar conclusions can be drawn when
632 comparing the Colour Index (ξ , see Eq. 6) reconstructed from the model with
633 the observed ξ from OC-CCI (Fig. 4).

634 4.2. Performance of satellite chlorophyll algorithms

635 In general, all four algorithms performed reasonably at estimating chloro-
636 phyll when compared with *in situ* values ($r > 0.60$ and $\Psi < 0.29$, Fig. 5). Ac-
637 cording to the objective classification, two empirical algorithms (OC4 and OCI)
638 have the best overall performance (highest points score in the bar chart in Fig.
639 5). This is mainly due to a combination of a higher correlation coefficient (r) for
640 these two algorithms when compared with GSM and OC4-MG, a lower centre-
641 pattern (or unbiased) root mean square error (Δ), a Type-2 regression slope (S)

642 close to one, the maximum percentage of possible retrievals (η), and high confi-
643 dence in the retrieved bias (δ) and intercept bias (I). However, despite the better
644 performance of OC4 and OCI according to the classification, both algorithms
645 systematically overestimate chlorophyll, as indexed by a positive bias signifi-
646 cantly different from zero (δ , Fig. 5), which was not observed for the GSM and
647 OC4-MG algorithms.

648 *4.3. Tuning of empirical satellite chlorophyll algorithms*

649 Consistent with previous ocean-colour models (e.g. Gordon et al., 1988;
650 Morel, 1988; Sathyendranath et al., 2001; Morel and Maritorena, 2001) as the
651 chlorophyll concentration decreases the Red Sea ocean-colour model predicts an
652 increase in R_{rs} at blue wavelengths and a slight decrease in green and red wave-
653 lengths (Fig. 6a). Figure 6b shows a plot of chlorophyll (C) as a function of the
654 maximum band-ratio ($R_{rs}(443 > 490 > 510)/R_{rs}(555)$) using output from the
655 Red Sea ocean-colour model with the OC4 algorithm overlain. For a given max-
656 imum band-ratio of R_{rs} , the Red Sea ocean-colour model predicts significantly
657 lower chlorophyll than the OC4 algorithm. Similarly, when we plot chlorophyll
658 (C) as a function of the Colour Index (ξ) using output from the Red Sea ocean-
659 colour model (Fig. 6c) with the relationship used in the OCI algorithm overlain,
660 we observe that the Red Sea ocean-colour model predicts a higher ξ than the OCI
661 algorithm at chlorophyll concentrations less than 0.3 mg m^{-3} .

662 To investigate if the bias observed in the OC4 and OCI algorithms (Fig.
663 5) can be explained using the Red Sea ocean-colour model, we reparamete-
664 rised the OC4 and OCI algorithms using output from the Red Sea ocean-

665 colour model (hereafter denoted OC4-RG and OCI-RG respectively, where RG
666 refers to regionally-tuned). The Red Sea ocean-colour model was run for 2560
667 logarithmically-space bins between 0.01 and 10.0 mg m⁻³ chlorophyll to derive
668 corresponding $R_{rs}(\lambda)$ values.

669 4.3.1. OC4-RG

670 For the OC4-RG algorithm, Eq. 5 was fitted to output from the Red Sea
671 model and the tuned parameters are provided in Table 3. As the Red Sea
672 ocean-colour model outputs at a variety of wavelengths representative of recent
673 and future ocean-colour sensors (NASA, 2010), parameters for standard band-
674 ratio algorithms that function at slightly different wavelengths (for application
675 to MODIS, MERIS, OLCI and VIIRS) are also provided in Table 3. Note that
676 for these algorithms Eq. 4 is modified depending on the R_{rs} ratio provided in
677 Table 3, and Eq. 5 is then used along with corresponding values for q_0 , q_1 , q_2 ,
678 q_3 and q_4 provided in Table 3. The OC4-RG algorithm is overlain in Fig. 6b and
679 matches the relationship between chlorophyll (C) and the maximum band-ratio
680 with which it was parameterised (Red Sea forward model).

681 4.3.2. OCI-RG

682 Figure 6c shows that for ξ values between -0.005 and -0.001, the relation-
683 ship between \log_{10} chlorophyll (C) and ξ in the Red Sea forward model is linear,
684 however, above -0.001 ξ this relationship breaks down. Using radiative transfer
685 modelling, Hu et al. (2012) showed that above a ξ value of -0.0005 sr⁻¹, assuming
686 a linear relationship between \log_{10} chlorophyll (C) and ξ results in a significant
687 underestimation in chlorophyll. For the Red Sea, the forward model predicts that

688 the ξ value above which the linear relationship breaks down is slightly lower at
689 around -0.001 sr^{-1} (Fig. 6c). Therefore, Eq. 7 was tuned using output from the
690 Red Sea forward model for ξ values lower than -0.001 sr^{-1} , and the resulting pa-
691 rameters are provided in Table 4. In comparison to the original parameters of Hu
692 et al. (2012), where $A = -0.491$ and $B = 191.66$, there was a significant decrease
693 in A (-0.802) and a slight increase in B (197.74). A reduction in the A parameter
694 is consistent with the results of Brewin et al. (2013a), using a dataset entirely in-
695 dependent of any measurements used to parameterise the Red Sea ocean-colour
696 model.

697 As the ξ value at which the linear relationship between \log_{10} chlorophyll (C)
698 and ξ breaks down is slightly lower for the Red Sea (Fig. 6c), the boundaries at
699 which the algorithm switches from a band-difference (ξ) to a band-ratio (OC4-
700 RG) were modified accordingly, such that the OCI-RG algorithm is expressed
701 as

$$C = \begin{cases} 10^{A+B\xi} & \text{if } [10^{A+B\xi}] \leq 0.10 \text{ mg m}^{-3} \\ \alpha[10^{(q_0+q_1X+q_2X^2+q_3X^3+q_4X^4)}] + (1 - \alpha)[10^{A+B\xi}] & \text{if } 0.10 < [10^{A+B\xi}] \leq 0.15 \text{ mg m}^{-3} \\ 10^{(q_0+q_1X+q_2X^2+q_3X^3+q_4X^4)} & \text{if } [10^{A+B\xi}] > 0.15 \text{ mg m}^{-3}, \end{cases} \quad (22)$$

702 where $\alpha = (10^{A+B\xi} - 0.10)/(0.15 - 0.10)$. The parameters for A and B are provided
703 in Table 4 and corresponding values for q_0 , q_1 , q_2 , q_3 and q_4 are provided in Table
704 3. The model parameters for wavelengths relevant to MODIS, MERIS, OLCI

705 and VIIRS are also provided in Table 4. Note that for implementation of these
706 algorithms, Eqs. 6 and 22 are used with the R_{rs} band-difference (Table 4), values
707 for A and B (Table 4), and the band-ratio algorithm (Table 3) that are appropriate
708 for the sensor used. The linear relationship between \log_{10} chlorophyll and ξ
709 tuned to the Red Sea (denoted ξ_{RS}), is laid over the forward model and the ξ
710 model of Hu et al. (2012). We see that the forward model and the Red-Sea-tuned
711 ξ model match each other very well for ξ values less than -0.001 sr^{-1} , for which
712 it was parameterised (Fig. 6c).

713 To verify further that the OC4-RG and OCI-RG algorithms reproduce the re-
714 lationships between R_{rs} and chlorophyll in the Red Sea model, we conducted a
715 sensitivity analysis (Supplementary Fig. S2). For chlorophyll concentrations
716 ranging from $0.01\text{-}10.0 \text{ mg m}^{-3}$ we used the Red Sea ocean-colour model to
717 estimate R_{rs} and then applied the OC4-RG and OCI-RG algorithms to the R_{rs}
718 compute chlorophyll concentration. If both algorithms were parameterised cor-
719 rectly, initial chlorophyll should agree with chlorophyll derived from the empiri-
720 cal models, as confirmed by the results in Supplementary Fig. S2 for both OC4-
721 RG and OCI-RG. We also introduced random noise into the R_{rs} values prior to
722 applying OC4-RG and OCI-RG algorithms, whereby for a given R_{rs} value, wave-
723 length independent random noise between $\pm 10\%$ (or $\pm 20\%$) was applied to the
724 R_{rs} estimated from the Red-Sea ocean-colour model, then this spectrum was used
725 to estimate chlorophyll using OC4-RG and OCI-RG and compared with initial
726 chlorophyll values. Results are shown in Supplementary Fig. S2 and indicate
727 both OC4-RG and OCI-RG cope well with the addition of random noise in R_{rs}

728 up to 20%.

729 4.4. Performance of tuned empirical satellite chlorophyll algorithms

730 The two tuned algorithms perform significantly better, as indexed by higher
731 scores than for the other algorithms (Fig. 7). The systematic overestimation
732 in chlorophyll observed in the untuned OC4 and OCI algorithms is no longer
733 apparent in the tuned algorithms (Fig. 7). The Red Sea ocean-colour model
734 used to parameterise OC4-RG and OCI-RG relates changes in a_p , b_{bp} and a_g to
735 changes in chlorophyll concentration. The relationships between a_p and chloro-
736 phyll and the relationships between b_{bp} and chlorophyll from the Tara dataset
737 (Fig. 3) were found to be similar to those observed using globally representative
738 datasets (Bricaud et al., 1998; Brewin et al., 2012a). However, the relationship
739 between a_g and chlorophyll (Fig. 3f) was significantly different, with the Red
740 Sea model requiring a higher amount of a_g for a given chlorophyll concentra-
741 tion when compared with standard global relationships (Morel, 2009; Morel and
742 Gentili, 2009b), possibly suggesting an excess of CDOM absorption per unit
743 chlorophyll in the Red Sea as the possible cause of the systematic overestima-
744 tion in chlorophyll observed in the original OC4 and OCI algorithms.

745 To test this hypothesis, we replaced Eq. 18 with the a_g model of Morel (2009)
746 in our Red Sea model (see Fig. 3f) and re-parameterised the OC4 algorithm (Eq.
747 5, denoted OC4-RG-M09) where $q_0 = 0.4010$, $q_1 = -2.9973$, $q_2 = 3.6843$,
748 $q_3 = -4.6653$ and $q_4 = 1.6263$. Figure 8 shows a comparison of scatter plots of
749 modelled and *in situ* chlorophyll for OC4, OC4-RG-M09 and OC4-RG. The sys-
750 tematic overestimation in chlorophyll observed in OC4 (positive bias (δ)) is also

751 observed with OC4-RG-M09, clearly emphasising that a higher-than-average
752 CDOM absorption per unit chlorophyll in the Red Sea ocean-colour model (Eq.
753 18) appears to explain why the bias (δ) is closer to zero for OC4-RG and why it
754 performs better in the algorithm evaluation than OC4 (Fig. 7).

755 *4.5. Application to OC-CCI satellite images*

756 The OC4, OCI, OC4-RG and OCI-RG algorithms were run on daily OC-
757 CCI data for the year 2010 and used to produce monthly composites (after \log_{10}
758 transformation), which were then used to produce annual chlorophyll compos-
759 ites (Fig. 9). The spatial patterns in the 2010 annual chlorophyll composites
760 are consistent with the description of Raitsos et al. (2013) using MODIS-Aqua
761 data. The northern Red Sea is the most oligotrophic with higher chlorophyll
762 values in the southern regions, and around coral reef-bound coastal waters (Fig.
763 1a). The \log_{10} differences between annual chlorophyll composites of OC4 and
764 OC4-RG, and OCI and OCI-RG, are also plotted in Fig. 9. Differences be-
765 tween empirical algorithms are roughly systematic (positive bias) over the entire
766 chlorophyll range, and similar for both the band-ratio (OC4 and OC4-RG) and
767 band-difference (OCI and OCI-RG) algorithms. Differences are slightly larger at
768 higher chlorophyll concentrations, around shallow regions (<200m, see Fig. 1a)
769 in the southern Red Sea and near coral reefs. In very shallow waters, estimates
770 of chlorophyll using empirical algorithms have high uncertainty, due to the po-
771 tential influence of bottom reflectance on the shape of the R_{rs} spectrum. In more
772 oligotrophic waters, such as the northern Red Sea, differences are slightly larger
773 between the OCI and OCI-RG algorithms, when compared with differences be-

774 tween OC4 and OC4-RG.

775 Figure 10 shows two OC-CCI daily images of chlorophyll concentration for
776 11th January and 31st May 2010 produced using the OCI-RG algorithm. The
777 percentage contribution of assemblage 1 and 2 (denoted A_1 and A_2 respectively)
778 are also plotted for each daily image, by using the OCI-RG algorithm (Eq. 22)
779 and Eqs. 9 and 10. Note that the use of Eq. 9 and 10 with OCI-RG derived
780 chlorophyll is consistent with the framework of the Red Sea model, considering
781 OCI-RG was parameterised using the Red Sea model in which Eq. 9 and 10 are
782 embed explicitly. The 11th January 2010 shows a clear OC-CCI image during
783 the period of Tara. The geographical distribution of chlorophyll on the 11th Jan-
784 uary 2010 is similar to the annual composites shown in Fig. 9. The percentage
785 contribution of assemblage 1 and assemblage 2 to total chlorophyll indicates as-
786 semblage 1 dominates the northern waters of the Red Sea and assemblage 2 the
787 southern waters (Fig. 10). However, comparison with the 31st May 2010 illus-
788 trates just how dynamic the patterns in chlorophyll concentration can be in the
789 Red Sea. During this day, blooms of phytoplankton, dominated by assemblage
790 2 (P_2) and likely influenced by enhanced meso-scale eddy activity during this
791 period (Pegau et al., 2002; Raitzos et al., 2013; Acker et al., 2008; Zhan et al.,
792 2014), or wind-driven upwelling and downwelling (Labiosa et al., 2003), swirl
793 around the northern half of the Red Sea (Fig. 10).

794 Seasonal climatologies of chlorophyll concentration and the percentage con-
795 tribution of assemblage 1 (A_1) and assemblage 2 (A_2) to total chlorophyll, pro-
796 cessed using the OCI-RG algorithm over the entire OC-CCI time-series (1997-

797 2012), are shown in Fig. 11 to illustrate the typical seasonal succession. The
798 temporal variations in chlorophyll in open ocean regions of the Red Sea are con-
799 sistent with those described by Raitzos et al. (2013), with higher concentrations
800 during the winter and lower concentrations during the summer. However, coral
801 reef-bound coastal waters (Fig. 1a) display equal or higher chlorophyll during
802 the summer period relative to that in winter (Racault et al., 2015). Over the
803 majority of the northern Red Sea, assemblage 1 (A_1) contributes highly to the
804 chlorophyll concentration in summer and autumn with a lower contribution dur-
805 ing spring and winter. The southern Red Sea and coral reef-bound coastal wa-
806 ters are dominated by assemblage 2 (A_2) all year around, with coral reef-bound
807 coastal waters having a lower contribution of A_2 in spring, and open-ocean wa-
808 ters having a lower contribution of A_2 in autumn.

809 **5. Discussion**

810 *5.1. Uncertainties in the analysis*

811 *5.1.1. In situ chlorophyll data*

812 Chlorophyll data used in the study came from three different sources, *in vivo*
813 fluorescence, Lidar fluorescence, and particulate absorption line height. Each of
814 these methods are subject to uncertainties. *In vivo* fluorescence in surface waters
815 can be affected by daytime-fluorescence quenching (Cullen and Lewis, 1995).
816 The fluorescence yield can also vary among species (Strickland, 1968; Kiefer,
817 1973b) and within a single species, subjected to different environmental con-
818 ditions (Kiefer, 1973a; Slovacek and Bannister, 1973). Using the same *in vivo*

819 fluorescence data, Brewin et al. (2013a) observed a positive bias in the OCI algo-
820 rithm using MODIS-Aqua, in both high- and low-light samples, suggesting that
821 the positive bias in OC4 and OCI observed in the *in vivo* fluorescence data in this
822 study (Fig. 5) was not related to daytime-fluorescence quenching. Nonetheless,
823 despite the fluorometer being laboratory calibrated prior to each cruise, it was
824 not field calibrated as no independent measurements of chlorophyll (e.g. from
825 HPLC or from *in vitro* fluorometry) were taken during the three RSRC cruises.

826 Lidar fluorescence is also subject to similar issues as *in vivo* fluorescence.
827 The method assumes a linear regime for the laser excitation and a low chro-
828 mophore density for all the species present, accurate calibration of fluorescence
829 signal against concurrent Raman signal from water, and accurate calibration of
830 Raman units to chlorophyll concentration (Barbini et al., 2001a). During the
831 MIPOT oceanographic campaign, conventional analyses were performed accord-
832 ing to the spectrofluorometric technique and the fluorescence-to-Raman ratio and
833 absolute concentrations were found to be well correlated (Barbini et al., 2004),
834 lending some confidence to the MIPOT data.

835 Of the three chlorophyll methods, the use of absorption line height to esti-
836 mate chlorophyll concentration is likely to be the most reliable. It is effective in
837 removing the contributions to a_p by a_g and a_d (detrital absorption), and is rela-
838 tively insensitive to instrument drift, incident irradiance and non-photochemical
839 quenching (Roesler and Barnard, 2014). The method has also been found to
840 perform well when compared with discrete *in situ* HPLC chlorophyll data and
841 diverse phytoplankton cultures (Dall’Olmo et al., 2009, 2012; Westberry et al.,

2010; Chase et al., 2013; Boss et al., 2014; Roesler and Barnard, 2014). Nonetheless the method is still subject to uncertainties: for instance, Eq. 2 was calibrated using concurrent HPLC data and $a_p(\lambda)$ taken during the entire Tara Oceanographic campaign in a wide range of bio-optical environments over the global ocean. Measurements of HPLC were taken at 4m depth (similar to underway sampling) at four stations in the Red Sea, three of which had concurrent measurements of $a_p(\lambda)$ (± 1 min) from the WET Labs AC-S. When comparing chlorophyll from HPLC with chlorophyll estimated from AC-S (Eq. 1 and 2), one measurement was in good agreement, but the other two observations showed higher chlorophyll from HPLC ($\delta \sim 0.3$), similar to the average bias between OCI and *in situ* chlorophyll (Fig. 5). Conclusions cannot be drawn from only three HPLC observations, which themselves are subject to uncertainty (Claustre et al., 2004), but the result emphasises the importance of taking concurrent observations of chlorophyll from difference sources, to reduce ambiguity and quantify uncertainty.

When considering the uncertainties in all three sources of *in situ* chlorophyll data, one may question whether standard algorithms do in fact systematically overestimate chlorophyll in the Red Sea, and whether this overestimation is instead an artefact of uncertainty in the *in situ* data itself. At this stage it is worth emphasising that the systematic overestimate of OC4 and OCI was observed individually for all three sources of *in situ* chlorophyll data (Fig. 5), thus lending support to their reliability and to the tuning of the algorithms (Fig. 7). To further illustrate this point, and to emphasise further the consistency and inter-

865 compatibility of the three *in situ* datasets, we created a satellite OC4 composite of
866 chlorophyll (OC-CCI data) over the duration of each cruise, and compared satel-
867 lite chlorophyll estimates with *in situ* data spatially (see Supplementary Figure
868 S3). Results show that: i) there is good agreement in spatial variability between
869 *in situ* data and satellite chlorophyll for all three datasets; and ii) that there is
870 a consistent overestimate (positive bias) in satellite OC4 chlorophyll across all
871 three *in situ* datasets.

872 Labiosa et al. (2003) compared SeaWiFS-derived chlorophyll concentrations
873 (OC4v4) with *in situ* chlorophyll, derived fluorometrically (*in vitro*), at Eilat
874 located at the northern tip of the Gulf of Aqaba, at a pier close to the shore
875 (Genin et al., 1995). Consistent with our findings, they observed that standard
876 SeaWiFS algorithms overestimated chlorophyll at high concentrations (bloom
877 periods). However, at lower concentrations they observed a slight underestima-
878 tion of SeaWiFS derived chlorophyll. This underestimation was likely related
879 to differences in the location of the satellite data (just offshore of Eilat) with re-
880 spect to the *in situ* data (taken from a Pier), considering Labiosa et al. (2003)
881 observed a small positive bias between chlorophyll data collected from the Pier
882 with that 1 km offshore, despite very good correlation (see Fig. 2d of Labiosa
883 et al., 2003). Additional datasets on *in situ* chlorophyll concentration in the Red
884 Sea are clearly required to scrutinise our findings further.

885 5.1.2. *In situ* measurements of IOPs used for bio-optical modelling

886 Measurements of particulate absorption (a_p) and attenuation (c_p), taken us-
887 ing the flow-through set-up of Slade et al. (2010), have been well validated over

888 a variety of oceanographic environments (Slade et al., 2010; Dall’Olmo et al.,
889 2009, 2011, 2012; Westberry et al., 2010). Boss et al. (2014) analysed a_p and
890 c_p data over the entire Tara Oceanographic campaign and found the data to be
891 consistent with other published data. Following the method of Werdell et al.
892 (2014a), b_{bp} was estimated from a_p and c_p using the method of Twardowski
893 et al. (2001), which assumes the scattering-to-backscattering ratio varies as func-
894 tion of chlorophyll (Eq. 3). Whereas the scattering-to-backscattering ratio has
895 been shown to vary consistently according to trophic conditions (Twardowski
896 et al., 2001; Whitmire et al., 2007; Dall’Olmo et al., 2012), the reported vari-
897 ability around the relationship is high, and it remains to be established whether
898 the Twardowski et al. (2001) relationship holds in the Red Sea. Validation of
899 this approach would require concurrent measurements of a_p , c_p and b_{bp} along
900 with chlorophyll, currently not available for the Red Sea. Direct measurement
901 of b_{bp} and chlorophyll at large scales are clearly preferable, though some com-
902 fort can be taken from the good agreement between b_{bp} estimated using Eq. 3
903 and independent satellite observations of b_{bp} (Werdell et al., 2014a). When com-
904 paring Tara Red Sea match-ups of \log_{10} -transformed $b_{bp}(443)$ estimated using
905 GSM with \log_{10} -transformed $b_{bp}(443)$ estimated using Eq. 3, we found a low
906 bias ($\delta \sim -0.08$) and root mean square error ($\Psi \sim 0.25$), but the GSM model did
907 struggle to reproduce the variability in $b_{bp}(443)$ primarily as a consequence of a
908 few outliers and a low range of variability in the match-ups.

909 Considering that no direct measurements of $a_g(\lambda)$ were used in the study,
910 and that $a_g(\lambda)$ was estimated using *in situ* chlorophyll (Eq. 15), corresponding

911 estimates of ϕ from satellite data (Morel and Gentili, 2009b) and assuming a
912 relationship between $a_g(400)$ and S_g derived from measurements outside Red
913 Sea waters (Eq. 16), uncertainty in the derivation of $a_g(\lambda)$ requires particular
914 attention. The inverse relationship between $a_g(400)$ and S_g used in Eq. 16 is
915 consistent with satellite observations of S_{dg} (where the subscript “dg” refers to
916 combined CDOM and detrital absorption) derived by Bricaud et al. (2012), and
917 values of S_{dg} observed from satellite (between 0.01-0.02 nm⁻¹ in the Red Sea,
918 see Fig. 1 of Bricaud et al., 2012) are consistent with values of S_g used in this
919 study. Estimates of ϕ , used in Eq. 15, are the primary source of data describing
920 region-specific CDOM absorption content in the Red Sea, and thus are given
921 particular attention in the next section.

922 5.1.3. Satellite measurements of ϕ

923 Values of ϕ were estimated from satellite observations (OC-CCI) using the
924 method of Morel and Gentili (2009b). As discussed by Morel and Gentili
925 (2009b), see also Morel and Gentili (2009a), the quality of retrieved $R_{rs}(412)$
926 is crucial for accurate estimation of ϕ , and yet estimation of $R_{rs}(412)$ is difficult,
927 and match-ups based on satellite and *in situ* R_{rs} data often find this wavelength
928 to have the highest errors (e.g. Mélin and Zibordi, 2007; Mélin et al., 2011).
929 Retrievals of $R_{rs}(412)$ rely to a certain degree on accurate vicarious calibration,
930 and errors can increase when the sun zenith angle and viewing angle increase
931 (IOCCG, 2010, though sun zenith angle is perhaps not such a problem in the
932 Red Sea, due to its close proximity to the tropics). *In situ* measurements of $R_{rs}(\lambda)$
933 over large areas are currently not available for the Red Sea, but are required to

934 ascertain potential biases in ϕ , and validate any region-specific bio-optical rela-
935 tionship based on $R_{rs}(\lambda)$.

936 Additional uncertainties in satellite measurements of ϕ might arise from the
937 unique atmospheric properties of the region. The Red Sea is surrounded by
938 deserts and frequently influenced by dust storms (Edwards, 1987), common dur-
939 ing spring and summer. Whereas cloud cover is generally low in the region, dust
940 aerosols make atmospheric correction difficult, cause a reduction in ocean-colour
941 retrievals (Acker et al., 2008; Steinmetz et al., 2011) and may systematically in-
942 fluence $R_{rs}(412)$. Desert dust has also been shown to influence the retrieved
943 $R_{rs}(\lambda)$ spectrum, leading to biases in the retrieval of the chlorophyll concen-
944 tration (Moulin et al., 2001; Claustre et al., 2002). When absorbing aerosols are
945 present in the atmosphere, atmospheric correction in the blue bands becomes less
946 accurate (Moulin et al., 2001). Claustre et al. (2002) demonstrated that Saharan
947 dust deposition can lead to enhanced absorption in the blue and backscattering in
948 the green parts of the visible spectrum, directly resulting in an over-estimation of
949 chlorophyll concentration in oligotrophic waters, and likely, a high ϕ index. The
950 influence of dust on the observed systematic overestimation of chlorophyll by
951 OC4 and OCI (Fig. 5), and on the high estimates of ϕ in the Red Sea bio-optical
952 model (Eq. 18), cannot be ruled out.

953 Whereas (to our knowledge) no direct measurements of $a_g(\lambda)$ are available
954 at large spatial scales in the Red Sea, two recent cruises, conducted by RSRC of
955 KAUST university in March and November 2013, made measurements of coinci-
956 dent fluorometric-CDOM concentration (FCDOM, in ppb) and chlorophyll con-

957 centration (*in vivo* fluorescence), using a WET Labs, Inc. Eco Sensor mounted
958 onto a CTD profiler, in the central-northern Red Sea (see Fig. 12a). Conversion
959 from measured FCDOM concentration in ppb to $a_g(\lambda)$ is difficult (Xing et al.,
960 2012). Differences in sensor calibrations used to convert FCDOM output values
961 (counts) into ppb units vary, as do conversions from ppb to $a_g(\lambda)$, even in sim-
962 ilar regions (Xing et al., 2012). However, values of FCDOM in ppb may give
963 some indication as to whether CDOM is relatively high or not. A total of 107
964 profiles were made during the two cruises (70 in March and 37 in November). A
965 detailed description of the processing of the March and November 2013 cruises
966 is provided in the Supplementary material.

967 For both the March and November cruises FCDOM was positively correlated
968 with chlorophyll ($p < 0.001$, Fig. 12b). However, for the March cruise the
969 amount of FCDOM per unit chlorophyll was higher than the November cruise,
970 likely as result of the March cruise sampling close to the coastline of Jeddah,
971 near coral reefs and anthropogenic influence (Fig. 12a). When comparing the
972 ratio $R(412)/R(443)$ to $R(490)/R(555)$ derived from a MODIS-Aqua composite
973 computed over the period of each cruise and related ϕ values, the March match-
974 ups show a significantly lower $R(412)/R(443)$ for a given $R(490)/R(555)$ than
975 the November match-ups, and thus higher ϕ values (see Fig. 12c). Whereas
976 the absolute ϕ values derived from MODIS cannot be verified, results from this
977 analysis suggest that the ϕ index captured the relative changes in FCDOM among
978 the March and November cruises, lending support to the use of the Morel and
979 Gentili (2009b) ϕ index in the Red Sea.

980 Another way to verify relative changes in the ϕ index proposed by Morel and
981 Gentili (2009b) is to check whether seasonal variations in ϕ (and hence CDOM)
982 are consistent with knowledge of interactions between CDOM and marine phys-
983 ical processes. The November 2013 cruise was located primarily in offshore
984 waters in the central Red Sea (see Fig. 12a and Supplementary Fig. S4a), away
985 from the coastline of Jeddah (unlike the March 2013 cruise). Supplementary
986 Fig. S4b shows the average vertical profile of FCDOM for the November cruise
987 and the average mixed layer depth (MLD), computed as the depth at which the
988 temperature changed by 0.5°C relative to the surface temperature (Monterey and
989 Levitus, 1997; Raitso et al., 2013). Consistent with other regions in the global
990 ocean (Nelson and Siegel, 2013), FCDOM concentration increases below the
991 mixed layer. Assuming no effect of horizontal advection or changes in light, an
992 increase in MLD is likely to result in an increase in the average FCDOM con-
993 centration in the mixed-layer, as deep CDOM-rich waters will become entrained
994 to the surface mixed layer. Consistent with this hypothesis, we observed a sig-
995 nificant ($p < 0.05$) positive correlation between MLD and average FCDOM con-
996 centration in the mixed-layer (see Supplementary Fig. S4c) during the November
997 cruise.

998 To test whether seasonal variations in the ϕ index are coupled to seasonal
999 variations in MLD, we focused on the Northern Red Sea (above 24°N) as this
1000 region is controlled primary by seasonal variations in vertical convection (Sofi-
1001 anos and Johns, 2003; Triantafyllou et al., 2014; Yao et al., 2014a). When
1002 comparing average monthly climatological values of the ϕ index above 24°N ,

1003 derived from the SeaWiFS sensor (downloaded from the NASA ocean-colour
1004 website <http://oceancolor.gsfc.nasa.gov/>), with modelled seasonal variations in
1005 MLD from Yao et al. (2014a), we find a significant ($p < 0.05$) positive corre-
1006 lation ($r = 0.85$, $p = 0.003$, Fig. 13a). Furthermore, average monthly climato-
1007 logical values of the ϕ index above 24°N are significantly negatively correlated
1008 ($r = 0.88$, $p = 0.002$, Fig. 13b) with climatological values of sea surface tem-
1009 perature (SST) derived from MODIS-Aqua, consistent with the assumption that
1010 increases in MLD bring deep, cooler CDOM-rich water into the surface mixed
1011 layer. The CDOM index is also significantly negatively correlated ($r = -0.76$,
1012 $p = 0.002$, Fig. 13c) with monthly climatological values of photosynthetically
1013 available radiation (PAR) above 24°N derived from SeaWiFS, consistent with
1014 knowledge of bleaching of some CDOM components by enhanced sunlight (Vo-
1015 dacek et al., 1997; Whitehead et al., 2000; Nelson and Siegel, 2013). We also
1016 compared monthly climatological variations in ϕ and aerosol optical thickness
1017 (AOT) derived from SeaWiFS. Interestingly, we observed an inverse correlation
1018 ($r = -0.85$, $p = 0.003$, Fig. 13d), suggesting that when the aerosol thickness is
1019 at its lowest (during winter when skies are clearer) ϕ is at its highest, and during
1020 spring and summer when aeolian dust events are most frequent, ϕ is relatively
1021 low (Fig. 13d), though still considerably higher than one. If higher ϕ values in
1022 the Red Sea were linked with atmospheric aerosols, one may have expected ϕ to
1023 increase with increasing AOT. The results emphasise that seasonal variations in ϕ
1024 are consistent with knowledge on interactions between CDOM and marine phys-
1025 ical processes (Blough et al., 1993; Nelson and Siegel, 2013), and lend support

1026 to the use of the ϕ index (Morel and Gentili, 2009b) in the Red Sea.

1027 *5.1.4. Bio-optical modelling*

1028 The bio-optical framework of the Red Sea ocean-colour model can be traced
1029 back to the work of Sathyendranath et al. (2001) and Devred et al. (2006),
1030 whereby the absorption properties of two-component groups (or assemblages)
1031 were shown to vary with chlorophyll concentration. In our Red Sea ocean-colour
1032 model, all IOPs are tied to the chlorophyll biomass and dominant assemblage of
1033 phytoplankton, with the model assuming each assemblage resides in a distinc-
1034 tive bio-optical environment (Alvain et al., 2012). Two- and three-component
1035 models of phytoplankton absorption and backscattering, based on the work of
1036 Sathyendranath et al. (2001), have been developed and validated using data from
1037 different areas of the global ocean (Sathyendranath et al., 2001, 2004; Devred
1038 et al., 2006, 2011; Brewin et al., 2011, 2012a). In this study, we have simply
1039 taken this modelling framework and re-paramaterised it using data in the Red
1040 Sea.

1041 It has been shown that three-component models can be more representa-
1042 tive of the transition in optical properties from oligotrophic to eutrophic wa-
1043 ters when compared with two-component models (Devred et al., 2011; Brewin
1044 et al., 2011). However, a two-component model was used in the case of the Red
1045 Sea as chlorophyll concentrations rarely exceed 1 mg m^{-3} (Fig. 2), such that a
1046 three-component model is unnecessary when considering the law of parsimony.
1047 However, blooms of phytoplankton with high chlorophyll may occasionally oc-
1048 cur in the Red Sea (Genin et al., 1995), and it remains to be revealed how well the

1049 two-component model copes under such conditions. The Red Sea model is also
1050 fairly simplistic, not accounting for inelastic processes such as Raman Scattering
1051 that can impact satellite retrievals of optical constituents in oligotrophic waters
1052 (Sathyendranath and Platt, 1998; Westberry et al., 2013; Lee et al., 2013). How-
1053 ever, algorithms for deriving chlorophyll concentration (e.g. OC4 and OCI) that
1054 are empirically parameterised using *in situ* $R_{rs}(\lambda)$ and chlorophyll data include,
1055 implicitly, the Raman effects. Thus the systematic overestimation in chlorophyll
1056 observed in the Red Sea by these approaches is unlikely to be attributable to
1057 inelastic effects.

1058 The parameterisation of any bio-optical model is ultimately related to the
1059 quality of the datasets used and their inherent uncertainties. With better quality
1060 datasets model parameterisation can be improved. The Red Sea model was pa-
1061 rameterised using Tara data, collected during the month of January 2010, around
1062 the peak of the seasonal succession of phytoplankton (Raitso et al., 2013) (Fig.
1063 13). Chlorophyll-specific IOPs presented in Table 1 are likely to have seasonal
1064 (Devred et al., 2006) and even inter-annual variations. We have already demon-
1065 strated that the ϕ index has a clear seasonal cycle in the northern Red Sea (Fig.
1066 13). Retuning of OC4 and OCI algorithms for the Red Sea (OC4-RG and OCI-
1067 RG respectively) was verified using data between November and March (MIPOT,
1068 Tara and RSRC), but the performance of the algorithms during the summer
1069 (May-October) is yet to be tested. Additional data is required to evaluate the
1070 suitability of these retuned algorithms for processing summer satellite data in
1071 the Red Sea.

1072 Algorithms such as the OC4-RG and OCI-RG proposed here are empirical
1073 in nature. The inferred relationship between chlorophyll and reflectance ratios
1074 (or differences) contains implicit dependence of the relationship on the change
1075 in phytoplankton community structure with change in chlorophyll, and on the
1076 covariance of other absorbing and scattering material with chlorophyll. These
1077 algorithms are not designed to cope with changes in these relationships which
1078 may occur in a future climate. For instance, in recent years there have been an
1079 increasing frequency and intensity of *Noctiluca scintillans* blooms in the Indian
1080 Ocean and Arabian Sea (Gomes et al., 2014). Blooms of this species have also
1081 been observed in the Red Sea (Mohamed and Mesaad, 2007). If in the future, the
1082 phytoplankton community structure changes, or if associated variables change
1083 (e.g. CDOM and non-algal particle concentration), these alterations will inter-
1084 fere with the performance of empirical algorithms. On-going comparisons (and
1085 re-calibration) with *in situ* data, coupled with surveillance of other products from
1086 satellite in these regions (such as *Noctiluca scintillans* (Werdell et al., 2014b)),
1087 is required to monitor performance of these empirical chlorophyll algorithms.

1088 5.1.5. Use of OC-CCI data

1089 We chose to use OC-CCI data primarily due to improved coverage in the
1090 Red Sea region when compared with individual sensors and other merged prod-
1091 ucts, so as to maximise the number of satellite and *in situ* match-ups. However,
1092 given that this merged product is relatively new, it would seem pertinent to ver-
1093 ify whether the results found in our study using OC-CCI data are consistent with
1094 with data from individual sensors. During 2010 when the Tara Oceans expe-

1095 dition sampled in the Red Sea, SeaWiFS, MODIS-Aqua and MERIS were all
1096 operating in parallel. Supplementary Fig. S5 shows results from a comparison
1097 of match-ups of SeaWiFS, MODIS-Aqua and MERIS derived chlorophyll, us-
1098 ing standard band-ratio algorithms, OCI and the tuned algorithms (Table 3 and
1099 4), with *in situ* chlorophyll data from Tara. Consistent with OC-CCI, SeaWiFS,
1100 MODIS-Aqua and MERIS derived chlorophyll all show a systematic overesti-
1101 mation in chlorophyll when using the OC4 and OCI algorithms. When using the
1102 revised algorithms (Table 3 and 4) the systematic overestimation in chlorophyll
1103 disappears and satellite chlorophyll is in better agreement with *in situ* chloro-
1104 phyll (Supplementary Fig. S5), supporting the results using OC-CCI data.

1105 Considering OC-CCI data are merged at Level-3 processing, satellite and *in*
1106 *situ* match-ups in this study were conducted using daily Level-3 products, unlike
1107 standard NASA validation protocols (Bailey and Werdell, 2006). However, re-
1108 sults from the match-ups presented here using the RSRC data (Fig. 5) resonate
1109 with the results from Brewin et al. (2013a, see their Fig. 2) using Level 2 (1 km)
1110 MODIS-Aqua satellite data in-line with NASA validation protocols, supporting
1111 the use of Level-3 products for match-up analysis in this study.

1112 *5.2. Evidence for and against high CDOM absorption per unit chlorophyll in* 1113 *the Red Sea*

1114 Results from our analysis suggest that standard empirical ocean-colour algo-
1115 rithms, based either on a band-ratio (OC4) or band-difference (OCI), overesti-
1116 mate chlorophyll in the Red Sea, possibly due to an excess of CDOM absorption
1117 per unit chlorophyll. Knowledge on the sources and sinks of CDOM in the Red

1118 Sea remain elusive. An argument that would contradict our hypothesis is that
1119 there is very little riverine input in the Red Sea (Patzert, 1974), such that any ad-
1120 ditional CDOM is unlikely to come from terrestrial sources. A further argument
1121 against high CDOM is that the Red Sea is close to the tropics, and exposed to
1122 intense surface irradiance. Therefore, any CDOM produced would be expected
1123 to undergo rapid degradation from photo-bleaching (Vodacek et al., 1997; Nel-
1124 son and Siegel, 2013). As discussed in the previous sections, there are also other
1125 reasons that may explain an overestimation in chlorophyll from standard satellite
1126 algorithms, such as uncertainty in the performance of atmospheric-correction al-
1127 gorithms and effects of aeolian dust deposition on the optical properties of the
1128 water (Claustre et al., 2002).

1129 Despite these arguments, there is some evidence that may support the hypoth-
1130 esis of higher CDOM absorption than average in the Red Sea. Firstly, the results
1131 do not imply the Red Sea is rich in CDOM, but simply that CDOM is higher than
1132 in the average oligotrophic-mesotrophic environment (i.e. for a given chloro-
1133 phyll concentration). Using satellite and *in situ* data, Morel and Gentili (2009a)
1134 found that CDOM absorption in the nearby Mediterranean Sea is twice that ob-
1135 served at the same latitude in the Atlantic Ocean. Nearby to the Red Sea, the
1136 Mediterranean Sea is also a semi-enclosed basin. It is possible that a refractory
1137 component of CDOM might have built up over time that is resistant to degrada-
1138 tion from photo-bleaching. The Red Sea is also home to a vast number of coral
1139 reefs that sustain a huge amount of biological productivity and fisheries (Munday
1140 et al., 2008). Red Sea coral reefs produce large amounts of Dissolved Organic

1141 Matter (DOC, see van Duyl and Gast, 2001; Yahel et al., 2003; Wild et al., 2010),
1142 and it may be that a component of this DOC is correlated with CDOM. Boss and
1143 Zaneveld (2003) observed enhanced concentrations of CDOM near coral reefs
1144 and near seagrass beds. It may be that benthic processes in basins with a high
1145 amount of area at boundaries relative to total area (such as the Red Sea and the
1146 Mediterranean), could influence CDOM more than in basins such as the Atlantic
1147 and Pacific.

1148 Higher CDOM per unit chlorophyll may also be related to a positive rela-
1149 tionship between enhanced metabolic processes and temperature (Taucher and
1150 Oschlies, 2011). The Red Sea is among the warmest seas on the planet, changes
1151 in microbial-loop activity with temperature (Behrenfeld, 2011) may alter pro-
1152 duction and degradation of CDOM. The Red Sea is also subject to high irradi-
1153 ance. In high light environments changes in the ratio of phytoplankton carbon
1154 to chlorophyll may result in modifications in the ratio of chlorophyll to CDOM,
1155 without any change in the ratio of phytoplankton carbon to CDOM. Ultimately,
1156 additional datasets are required to verify if the Red Sea has elevated CDOM
1157 absorption per unit chlorophyll.

1158 **6. Summary**

1159 Using an objective classification, and a dataset of satellite (OC-CCI prod-
1160 ucts) and *in situ* chlorophyll match-up data, we tested the performance of two
1161 standard ocean-colour empirical chlorophyll algorithms (one based on a blue to
1162 green band-ratio, OC4, and the other a band-difference, OCI), a semi-analytical
1163 algorithm, and an empirical algorithm that accounts for the influence of CDOM

1164 on the remotely-sensed chlorophyll estimates. We found that the two empiri-
1165 cal algorithms (OC4 and OCI) had the highest performance, but systematically
1166 overestimated chlorophyll when compared with the *in situ* data.

1167 By developing a Red Sea ocean-colour model, parameterised where possible
1168 to data from the Red Sea, we adjusted the two ocean-colour empirical algorithms
1169 for chlorophyll estimation and the systematic overestimation in chlorophyll orig-
1170 inally observed was eliminated. The relationships of particulate absorption and
1171 particulate backscattering with chlorophyll that are used in the Red Sea model,
1172 are similar to established global relationships, but the amount of CDOM ab-
1173 sorption per unit chlorophyll concentration in the model is higher than standard
1174 global relationships. An enhanced amount of CDOM absorption per unit chloro-
1175 phyll in the Red Sea was found to explain the overestimation in chlorophyll
1176 originally observed for the OCI and OC4 algorithms. A series of algorithms ad-
1177 justed for the Red Sea have been proposed, designed for a range of ocean-colour
1178 sensors, and are now available for further testing. Given the unique and under-
1179 studied marine and atmospheric environment of the region, uncertainties in the *in*
1180 *situ* data, and the potential influence of aeolian dust on atmospheric correction,
1181 additional information is required to scrutinise our findings.

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Table 1: Parameters of the Red Sea ocean-colour model

| Parameters for the 2-component assemblage model (Eq. 9 and 10) | | | |
|--|---|---|-----------------|
| Reference | C_1^m [mg m ⁻³] | S_1 [Dimensionless] | |
| Brotas et al. (2013) | 0.058 (0.054↔0.063) | 17.056 (14.693↔18.646) | |
| Parameters for Particle absorption model (Eq. 12) | | | |
| Wavelength [nm] | $a_{p,1}^*$ [m ² (mgC) ⁻¹] | $a_{p,2}^*$ [m ² (mgC) ⁻¹] | |
| 410 | 0.1823 (0.1807↔0.1840) | 0.0464 (0.0459↔0.0468) | |
| 412 | 0.1858 (0.1841↔0.1874) | 0.0472 (0.0467↔0.0477) | |
| 443 | 0.2132 (0.2120↔0.2142) | 0.0461 (0.0457↔0.0465) | |
| 486 | 0.1341 (0.1335↔0.1347) | 0.0347 (0.0345↔0.0350) | |
| 488 | 0.1313 (0.1307↔0.1319) | 0.0340 (0.0337↔0.0342) | |
| 490 | 0.1284 (0.1278↔0.1290) | 0.0332 (0.0330↔0.0334) | |
| 510 | 0.0745 (0.0740↔0.0749) | 0.0242 (0.0241↔0.0244) | |
| 530 | 0.0344 (0.0340↔0.0347) | 0.0196 (0.0195↔0.0197) | |
| 547 | 0.0195 (0.0192↔0.0198) | 0.0170 (0.0169↔0.0172) | |
| 551 | 0.0183 (0.0181↔0.0187) | 0.0154 (0.0153↔0.0156) | |
| 555 | 0.0168 (0.0166↔0.0171) | 0.0138 (0.0137↔0.0140) | |
| 560 | 0.0156 (0.0153↔0.0159) | 0.0117 (0.0116↔0.0119) | |
| 620 | 0.0110 (0.0108↔0.0112) | 0.0056 (0.0055↔0.0057) | |
| 665 | 0.0251 (0.0250↔0.0253) | 0.0173 (0.0173↔0.0174) | |
| 670 | 0.0291 (0.0290↔0.0293) | 0.0201 (0.0200↔0.0201) | |
| Phytoplankton assemblage parameters for Particle backscattering model (Eq. 14) | | | |
| Parameter | $i = 1$ | $i = 2$ | |
| $b_{bp,i}^*(\lambda_0)$ [m ² (mgC) ⁻¹] | 0.0016 (0.0003↔0.0028) | 0.0023 (0.0022↔0.0024) | |
| γ_i [Dimensionless] | 4.48 (2.59↔16.18) | 0.43 (0.38↔0.50) | |
| Background component parameters for Particle backscattering model (Eq. 14) | | | |
| | $b_{bp}^k(\lambda_0)$ [m ⁻¹] | γ_k [Dimensionless] | |
| | 0.00096 (0.00091↔0.0102) | 0.54 (0.45↔0.68) | |
| Parameters for CDOM absorption model (Eq. 18) | | | |
| Parameter | $i = 1$ | $i = 2$ | |
| $a_{g,i}(\lambda_0)$ [m ² (mgC) ⁻¹] | 0.0907 (0.0655↔0.1425) | 0.2022 (0.1791↔0.2754) | |
| $S_{g,i}$ [nm ⁻¹] | 0.031 (0.028↔0.038) | 0.014 (0.013↔0.015) | |
| Parameters of Eq. 21 of Lee et al. (2009)* | | | |
| | $G_w^0(\Omega)$ | $G_w^1(\Omega)$ | $G_p^0(\Omega)$ |
| | 0.0604 | 0.0406 | 0.0402 |
| | | | $G_p^1(\Omega)$ |
| | | | 0.1310 |

95% confidence intervals are in brackets and were estimated using a Monte-Carlo approach and $\lambda_0 = 443$ nm.

* parameters are for solar zenith angle in air equal to zero, sensor nadir-view angle in air equal to zero, and a sensor azimuth angle in relation to the solar plane equal to zero, where Ω collectively represents the three sun-sensor angular geometries.

Table 2: Performance of Eq. 12, Eq. 14 and Eq. 18.

| Wavelength [nm] | a_p | | a_g | | b_{bp} | |
|-----------------|-------|--------|-------|--------|----------|--------|
| | r | Ψ | r | Ψ | r | Ψ |
| 410 | 0.937 | 0.079 | 0.919 | 0.122 | 0.778 | 0.091 |
| 412 | 0.937 | 0.078 | 0.919 | 0.123 | 0.778 | 0.091 |
| 443 | 0.969 | 0.050 | 0.920 | 0.142 | 0.776 | 0.091 |
| 486 | 0.979 | 0.045 | 0.920 | 0.162 | 0.787 | 0.090 |
| 488 | 0.979 | 0.045 | 0.920 | 0.162 | 0.788 | 0.090 |
| 490 | 0.978 | 0.045 | 0.920 | 0.163 | 0.790 | 0.090 |
| 510 | 0.977 | 0.051 | 0.920 | 0.168 | 0.795 | 0.090 |
| 530 | 0.970 | 0.070 | 0.920 | 0.172 | 0.796 | 0.091 |
| 547 | 0.959 | 0.092 | 0.919 | 0.177 | 0.799 | 0.090 |
| 551 | 0.957 | 0.094 | 0.919 | 0.178 | 0.800 | 0.090 |
| 555 | 0.953 | 0.098 | 0.919 | 0.180 | 0.800 | 0.090 |
| 560 | 0.948 | 0.101 | 0.919 | 0.182 | 0.799 | 0.090 |
| 620 | 0.904 | 0.129 | 0.919 | 0.226 | 0.784 | 0.094 |
| 665 | 0.994 | 0.033 | 0.919 | 0.278 | 0.763 | 0.102 |
| 670 | 0.996 | 0.026 | 0.919 | 0.284 | 0.763 | 0.102 |

r refers to the Pearson correlation coefficient and Ψ the root mean square error. All statistical tests were performed in \log_{10} space.

Table 3: Values of the coefficients for standard, empirical band-ratio chlorophyll algorithms tuned to the Red Sea ocean-color model and for a suite of ocean-colour sensor wavelengths.

| Sensor/dataset | Identifier * | R_{rs} ratio | q_0 | q_1 | q_2 | q_3 | q_4 |
|----------------|--------------|------------------------|---------|---------|--------|---------|--------|
| SeaWiFS/OC-CCI | OC4-RG | max(443, 490, 510)/555 | -0.0381 | -2.9297 | 4.6447 | -5.5384 | 1.9556 |
| MERIS/OLCI | OC4ME-RG | max(443, 490, 510)/560 | -0.0472 | -2.5860 | 3.4994 | -3.9545 | 1.2466 |
| MODIS | OC3MO-RG | max(443, 488)/547 | -0.1333 | -2.4079 | 2.7585 | -3.4081 | 1.1122 |
| VIIRS | OC3VI-RG | max(443, 486)/560 | -0.1269 | -2.1819 | 2.1972 | -2.7276 | 0.8490 |

* ME = MERIS, MO = MODIS and VI = VIIRS. The reader is also referred to NASA (2010) for more information on the algorithms. RS refers to a tuning of the algorithm to Red Sea data.

Table 4: Values of the coefficients for the band-difference algorithm of Hu et al. (2012) tuned to the Red Sea ocean-color model, and for a suite of ocean-colour sensor wavelengths.

| Sensor/dataset | Identifier * | R_{rs} band-difference (ξ) | A | B |
|----------------|--------------|---|---------|----------|
| SeaWiFS/OC-CCI | OCI-RG | $R_{rs}(555) - 0.50(R_{rs}(443) + R_{rs}(670))$ | -0.8021 | 197.7366 |
| MERIS/OLCI | OCIME-RG | $R_{rs}(560) - 0.53(R_{rs}(443) + R_{rs}(665))$ | -0.7625 | 188.2083 |
| MODIS | OCIMO-RG | $R_{rs}(547) - 0.46(R_{rs}(443) + R_{rs}(670))$ | -0.8843 | 212.5575 |
| VIIRS | OCIVI-RG | $R_{rs}(560) - 0.52(R_{rs}(443) + R_{rs}(670))$ | -0.8103 | 190.5906 |

Note that for implementation of Eq. 22, $\alpha = (10^{A+B\xi} - 0.10)/(0.15 - 0.10)$.

* ME = MERIS, MO = MODIS and VI = VIIRS. RS refers to a tuning of the algorithm to Red Sea data.

Figure 1: (a) Bathymetry of the Red Sea (using ETOPO5 sea-floor elevation data obtained from the National Oceanographic and Atmospheric Administration (NOAA) at <http://www.ngdc.noaa.gov/mgg/global/etopo5.HTML>, regridded to 4km spatial resolution) with the locations of coral reefs overlain (from the Global Distribution of Coral Reefs dataset (version 2010) compiled by the UNEP-WCMC available at <http://data.unep-wcmc.org/datasets/13>, regridded to 4km spatial resolution). Figures (b) to (d) show the distribution of the *in situ* and satellite match-up data used in the study.

Figure 2: (a) Relationship between chlorophyll and $a_p(443)$ measured during Tara and (b) the percentage contribution of assemblage 1 (A_1) and 2 (A_2) to total chlorophyll as a function of total chlorophyll (C) following the parameterisation of Brotas et al. (2013) for pico-phytoplankton.

Figure 3: Parameters of the Red Sea two-component bio-optical model: (a) chlorophyll-specific particulate absorption coefficients (a_p) as a function of wavelength, (b) chlorophyll-specific particulate backscattering coefficients (b_{bp}) as a function of wavelength and the background backscattering component (b_{bp}^k), and (c) chlorophyll-specific CDOM absorption coefficients (a_g) as a function of wavelength for the two assemblages (A_1 and A_2). Figures d-f show the relationship between $a_p(443)$ and C , $b_{bp}(443)$ and C , and $a_g(443)$ and C respectively, for the Tara data and the fitted model.

Figure 4: Comparison of reconstructed remote sensing reflectance (R_{rs}) using *in situ* chlorophyll (C) and OC-CCI observed R_{rs} . The top row of figures show the absolute values of R_{rs} and the bottom row the shape of R_{rs} , normalised at 555nm, and the colour index (ξ). Black line refers to 1:1 line.

Figure 5: Results from the chlorophyll (C) model comparison. The bar chart at the top shows results from the point classification and scatter plots of modelled and *in situ* chlorophyll are shown below for the OCI, OC4, OC4-MG and GSM. Black line refers to 1:1 line and dashed line Type-2 regression.

Figure 6: (a) $R_{rs}(\lambda)$ plotted as a function of wavelength for a variety of chlorophyll concentrations (C) using the Red Sea ocean-colour model. (b) Shows C plotted as a function of the maximum band-ratio for the OC4 model, output from the Red Sea ocean-colour model (forward model), and a tuned OC4 model, denoted OC4-RG, tuned using output from the Red Sea ocean-colour model. (c) Shows C plotted as a function of the Colour Index (ξ) using the parameterisation of Hu et al. (2012), output from the Red Sea ocean-colour model (forward model), and a tuned ξ relationship, denoted ξ_{RS} , tuned using output from the Red Sea ocean-colour model below a ξ value of -0.001 sr^{-1} .

Figure 7: Results from the chlorophyll (C) model comparison when including the two regionally tuned empirical algorithms (OC4-RG and OCI-RG). The bar chart at the top shows results from the point classification and scatter plots of modelled and *in situ* chlorophyll are shown below for the OC4-RG and OCI-RG. Black line refers to 1:1 line and dashed line Type-2 regression.

Figure 8: Scatter plots of modelled and *in situ* chlorophyll for OC4, OC4-RG-M09 and OC4-RG. Black line refers to 1:1 line and dashed line Type-2 regression.

Figure 9: Annual OC-CCI Red Sea chlorophyll (C) composites for 2010 estimated from the OC4, OCI, OC4-RG and OCI-RG algorithms. The \log_{10} differences between annual chlorophyll composites of OC4 and OC4-RG, and OCI and OCI-RG, are also plotted.

Figure 10: Two OC-CCI daily images of chlorophyll concentration for 11th January and 31st May 2010 produced using the OCI-RG algorithm. The percentage contribution of assemblage 1 (A_1) and assemblage 2 (A_2) are also plotted for each daily image, using the OCI-RG algorithm and Eq. 9 and 10.

Figure 11: Seasonal climatologies of chlorophyll concentration (C) and the percentage contribution of assemblage 1 (A_1) and assemblage 2 (A_2), over the entire OC-CCI time-series (1997-2012) processed using the OCI-RG algorithm, for Winter (December, January and February), Spring, (March, April and May), Summer (June, July and August) and Autumn (September, October and November).

Figure 12: (a) Shows the location of the samples used in two KAUST cruises (March and November 2013) of corresponding FCDOM and chlorophyll data. (b) Shows the relationship between FCDOM and chlorophyll for both cruises and (c) shows a plot of reflectance ratios $R(412)/R(443)$ versus $R(490)/R(555)$ for each sample, of each cruise, derived from the match-ups using a MODIS-Aqua composite averaged over the time period of each cruise.

Figure 13: Seasonal climatologies in the northern Red Sea (above 24°N) of the ϕ index (CDOM index, Morel and Gentili, 2009b) derived from the SeaWiFS sensor, the mixed layer depth (MLD) from Yao et al. (2014a), sea surface temperature (SST) derived from MODIS-Aqua, photosynthetically available radiation (PAR) derived from SeaWiFS and aerosol optical thickness (AOT) derived from SeaWiFS. Satellite data were downloaded from the NASA ocean-colour website <http://oceancolor.gsfc.nasa.gov/>.