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Information content of *in situ* and remotely sensed chlorophyll-*a*: learning from size-structured phytoplankton model

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Keywords: satellite oceanography; remote sensing; ocean colour; data assimilation; primary production; biogeochemical model.

ABSTRACT

Chlorophyll-*a* measurements in the form of *in situ* observations and satellite ocean colour products are commonly used in data assimilation to calibrate marine biogeochemical models. Here, a two size-class phytoplankton biogeochemical model, with a 0D configuration, was used to simulate the surface chlorophyll-*a* dynamics (simulated surface Chl-*a*) for cyclonic and anticyclonic eddies off East Australia. An optical model was then used to calculate the inherent optical properties from the simulation and convert them into remote-sensing reflectance (R_{rs}). Subsequently, R_{rs} was used to produce a satellite-like estimate of the simulated surface Chl-*a* concentrations through the MODIS OC3M algorithm (simulated OC3M Chl-*a*). Identical parameter optimisation experiments were performed through the assimilation of the two separate datasets (simulated surface Chl-*a* and simulated OC3M Chl-*a*), with the purpose of investigating the contrasting information content of simulated surface Chl-*a* and remotely-sensed data sources. The results we present are based on the analysis of the distribution of a cost function, varying four parameters of the biogeochemical model. In our idealised experiments the OC3M algorithm underestimates the simulated chlorophyll-*a* concentration in offshore eddies off East Australia (Case I waters), because of the weak relationship between large-sized phytoplankton and remote-sensing reflectance. Although Case I waters are usually characteristic of oligotrophic environments, with a photosynthetic community typically represented by relatively small-sized phytoplankton, mesoscale features such as eddies can generate seasonally favourable conditions for a photosynthetic community with a greater proportion of large phytoplankton cells. Furthermore, our results show that in mesoscale features such as eddies, *in situ* chlorophyll-*a* observations and the ocean colour products can carry different information related to phytoplankton sizes. Assimilating both remote-sensing reflectance and measurements of *in situ* chlorophyll-*a* concentration reduces the uncertainty of the parameter values more than either data set alone, thus reducing the spread of acceptable solutions, giving an improved simulation of the natural environment.

1. INTRODUCTION

Satellite sensors measuring radiance in the visible range such as MERIS, OLCI, SeaWiFS and MODIS provide useful ocean color data to support the marine sciences community (McClain, 2009; Antoine et al., 2014). Such datasets can be used to estimate surface ocean circulation patterns (Barton, 2002; Pegau et al., 2002), phytoplankton primary production (Longhurst et al., 1995; Carr et al., 2006) and to investigate upwelling regions (Poulain et al., 2004; Farikou et al., 2015). Furthermore, the satellite ocean color data can be used to estimate chlorophyll-*a* concentrations (Chl-*a*), which is often used to calibrate biogeochemical models, optimizing their biological parameters (Hemmings et al., 2003; Laiolo et al., 2016).

Radiance measured at the satellite sensor comprises the combination of surface-reflected radiance, water-leaving radiance and atmospheric radiance (Robinson, 2004). The only component that provides information on ocean properties, such as Chl-*a* concentration, is the water-leaving radiance; therefore corrections are applied to remove atmospheric and surface-reflected radiance components from the water upwelled signal (e.g. Schroeder et al., 2007). The intensity and spectral characteristics of the water-leaving radiance are determined by the scattering and absorption properties of the water, dissolved matter, and particulates in the water, including organic and inorganic components (e.g. Kirk, 1983; Gordon et al., 1988; IOCCG, 2006). The optical properties of all these elements define the inherent optical properties (IOPs) of the water column (Dickey et al., 2006). Specifically, light can be absorbed or scattered: while scattering is the physical process that deviates the angle of the photon path, absorption removes photons permanently from their path (Dickey et al., 2006). The absorption process is fundamental for phytoplankton photosynthesis, allowing phytoplankton to synthesize organic compounds from inorganic carbon dioxide (CO_2) and nutrients, providing organic matter, directly or indirectly, for almost all marine life (Falkowski, 2012). The measures of absorption and scattering commonly used are absorption (a) and scattering (b) coefficients. The relationship between the scattering coefficient in a backward direction (backscattering coefficient, b_b) and absorption coefficient is used to estimate remote-sensing reflectance (R_{rs}) (i.e., $R_{rs} \propto \frac{b_b}{a + b_b}$).

Phytoplankton absorption spectra vary in magnitude and shape due to the

different pigment composition and packaging (Bidigare et al., 1990; Bricaud and Stramski, 1990; Hoepffner and Sathyendranath, 1991; Ciotti et al., 2002; Lewis, and Cullen, 2002; A. Bricaud et al., 2004). The increase in cellular pigment concentration and cell size, i.e. packaging effect, flattens the specific absorption spectra (Duysens, 1956; Kirk, 1976; Morel and Bricaud, 1981). Due to strong absorptive properties and high water content in phytoplankton cells, their scattering coefficients are relatively low (Aas, 1996). Because of the high ratio between cell size and wavelength, forward scattering dominates over scattering in the backward direction (Volten et al., 1998). Scattering and backscattering coefficients of phytoplankton are highly dependent on size, shape and refractive index of components of the phytoplankton cell (Jonasz and Fournier, 2007; Sullivan and Twardowski, 2009; Volten et al., 1998; Witkowski et al., 1998).

Marine biogeochemical models are useful tools that help to understand, conceptualize and predict marine environmental processes, including phytoplankton dynamics, represented in the basic Nutrient, Phytoplankton, Zooplankton and Detritus (NPZD) structure of these models (Fennel and Neumann, 2004). Marine biogeochemical models usually comprise numerous parameters and estimating their values is a non-linear problem (Matear, 1995; Athias et al., 2000; Jones et al., 2016). Thanks to their continuous acquisition and spatial coverage, ocean color data are particularly suitable for data assimilation in marine biogeochemical models, with most studies using remotely-sensed Chl-*a* as the product to assimilate.

Data assimilation (DA) is a useful process that combines observations and models to estimate variables. In the biogeochemical modelling space there are two uses of DA, state estimation and parameter estimation. In state estimation, DA is performed to improve the predictive power of models. In this approach the state variables are modified to fit the observations and produce a more realistic evolution of the ocean state (e.g. Shulman et al., 2013; Teruzzi et al., 2014; Ciavatta et al., 2016). A more common application of DA in biogeochemical modeling is related to optimization of parameters. In this case the model parameters are modified to fit the constraints (e.g. Doron et al., 2013; Laiolo et al., 2016; Gharamti et al., 2017). The parameter optimization involves usually three main steps: (1) running the model forward in time, (2) comparing simulation results with the observations through a cost function to quantify the differences between the two datasets, and (3) modifying the parameter values accordingly until the best fit to the data is obtained (i.e. minimize

the cost function value). Ocean color DA is a field in development that can improve the accuracy of biological variables in marine biogeochemical models. While analyzing or assimilating ocean color data is feasible, it is essential to consider the complexity and variability of the bio-optical properties that comprise the water-leaving radiance and the derived Chl-*a* data (Babin et al., 2003; Oubelkheir et al., 2006). Indeed, in open ocean waters (i.e. Case I waters), the complexity and variability of bio-optical properties decrease the accuracy of satellite data products of up to ± 5% for water-leaving radiance and ± 35% for the corresponding Chl-*a* product (McClain, 2009). Furthermore, on a global scale, there is a non-uniform distribution of accuracy in the derived Chl-*a* concentration, with a significant error increase in coastal waters (i.e. Case II waters, Odermatt et al., 2012). Marine biogeochemical DA is now moving beyond the assimilation of Chl-*a* derived from remotely sensed ocean colour. Jones et al. (2016) have already shown that in a coastal domain (Case II water), assimilating a combination of remote-sensing reflectance wavebands leads to a significant improvement over assimilating ocean colour derived Chl-*a*.

1.1. Model simulations to understand observation platforms

In this study, we exploit the recent development of optical models linked to phytoplankton dynamics (e.g. Dutkiewicz et al., 2015; Baird et al., 2016; Jones et al., 2016), presenting an idealized study for East Australia open ocean (Case I) waters. Specifically, we used a two phytoplankton size class dependent biogeochemical model (Environmental Modeling Suite, EMS), with a 0D configuration, to simulate Chl-*a* dynamics from a published set of parameter values (hereafter 'original parameter set', Table 2; Laiolo et al., 2016) in cyclonic and anticyclonic eddies off East Australia. We called the obtained synthetic dataset "simulated surface Chl-*a*" (Fig. 1a). We then use the same output from EMS to obtain the IOPs and the corresponding R_{rs} through an optical model (Appendix; Baird et al., 2016). R_{rs} was converted to Chl-*a* concentration through the OC3M algorithm (Moderate Resolution Imaging Spectroradiometer or MODIS, three band Chl-*a* algorithm; https://oceancolor.gsfc.nasa.gov/atbd/chlor_a/#sec_2; O'Reilly et al., 1998), obtaining a satellite-like Chl-*a* product that we called "simulated OC3M Chl-*a*" (Fig. 1a). We explore the properties of the synthetic datasets obtained evaluating a defined cost function in a DA parameter optimization problem. Twin experiments were performed (Fig. 1b) in which, with perturbed parameter values, we investigated the ability of the

DA system to recover the parameter values from an unperturbed EMS simulation.

2. MATERIALS AND METHODS

2.1. Study Region and Biogeochemical Model Description

The region selected for this study is located in the eastern Australian ocean, between 30° and 40°S and 150° and 160°E (Fig. 2). This area is crucial for Australia's marine ecology and economy, fisheries and tourism (Hobday and Hartmann, 2006; Brieva et al., 2015). Furthermore, it is strongly influenced by the major western boundary current of the South Pacific, the Eastern Australian Current (EAC) (Mata et al., 2000; Ridgway and Dunn 2003). The EAC originates from the warm oligotrophic waters of the Coral Sea and during its southward flow forms eddies that stimulate phytoplankton growth and enhance primary production (Falkowski et al., 1991; Hassler et al., 2010; Doblin et al., 2016). These phenomena are particularly intense in the area we selected (Ridgway and Dunn, 2003).

A marine Nutrient, Phytoplankton, Zooplankton and Detritus (NPZD) biogeochemical model, EMS, was used in this study. It was developed to couple physical, chemical, and biological processes (CSIRO Coastal Environmental Modelling Team, 2014; http://www.emg.cmar.csiro.au/www/en/emg/software/EMS.html). For this study, EMS was set up with the same structure as used in Laiolo et al. (2016), with a 0D configuration, two phytoplankton and zooplankton size dependent classes characterized by a variable C:Chl-*a* ratio (Baird et al., 2013). Forcing functions driving the phytoplankton dynamics, and therefore the total Chl-*a*, were the temperature within the mixed layer and nutrients below the mixed layer, both acquired from the CSIRO Atlas of Regional Seas dataset (CARS; http://www.marine.csiro.au/~dunn/cars2009/; Ridgway et al., 2002). Surface incident irradiance was obtained from the seasonal climatology of the selected study area (Large and Yeager, 2008). EMS was configured as 0D, representing a well-mixed mixed layer depth; therefore, biological components were considered as concentrations equally distributed within this layer.

2.2. Simulated surface Chlorophyll-*a* and simulated OC3M Chlorophyll-*a* synthetic dataset

To obtain the simulated surface Chl-*a* synthetic dataset two distinct EMS simulations were carried out. Following Laiolo et al. (2016), EMS was configured with two phytoplankton size classes (2 μm and 40 μm diameter), to simulate the typical Chl-*a* seasonal dynamics in a cyclonic (CE) and anticyclonic eddy (ACE) off East Australia (Table 2; Fig. 3a, b). CE and ACE are two ideal case studies as they represent two distinct environments with different phytoplankton dynamics and concentrations (Fig. 3a, b; Angel and Fasham, 1983; Moore et al., 2007; Laiolo et al., 2016). Once the CE and ACE Chl-*a* time-series were extracted from the EMS simulations, it was possible to calculate the corresponding R_{rs}, based on optical model presented in Baird et al. (2016). The optical model performance has been previously assessed with MODIS R_{rs} in an area adjacent to the East Australia study region (i.e., Great Barrier Reef; Baird et al., 2016). First, the IOPs were computed from the state variables (e.g. Chl-*a* concentration) and model parameters (e.g. cell dimension). Then the apparent optical properties (AOPs) including R_{rs} were calculated through the relationship with backscattering and absorption coefficients (i.e., $R_{rs} \propto \frac{b_b}{a + b_b}$) (Fig. 1b; Baird et al., 2016). Additional details about the optical model calculations of IOPs and R_{rs} are given in the Appendix. To explore the relationship between EMS phytoplankton biomass and corresponding R_{rs}, we set up the optical model to take into account both absorption and scattering for pure seawater and phytoplankton cells. Because our study area covers only Case I waters, where phytoplankton is the main component responsible for variations in optical properties (Gordon and Morel 1983; Morel and Prieur 1977; Mobley et al., 2004), other optically significant seawater constituents such as coloured dissolved organic matter (CDOM), non-algal particulates (NAP) and benthic reflectance were not considered.

The R_{rs} time-series was then used to obtain the simulated OC3M Chl-*a* product, following the OC3M algorithm (https://oceancolor.gsfc.nasa.gov/atbd/chlor_a/#sec_2; O'Reilly et al., 1998). The NASA OC3M algorithm consists of a fourth-order polynomial relationship between logarithms of R_{rs} ratios and Chl-*a*:

$$\log_{10}(\text{Chl-}a) = a_0 + \sum_{i=1}^{4} a_i \left(\log_{10}\left(\frac{\max(R_{rs}(443),\ R_{rs}(488)}{R_{rs}(551)}\right)\right)^i \quad (1)$$

where a_i is a sensor specific coefficient (MODIS: a_0= 0.2424, a_1=-2.7423, a_2=1.8017,

a_3=0.0015, a_4=-1.2280), R_{rs}(443), R_{rs}(488) and R_{rs}(551) represent remote sensing reflectance at 443 nm, 488 nm and 551 nm respectively.

2.3. Settings of the twin experiments

Twin experiments are used to assess the ability of a data assimilation system to recover model parameter values from model output (e.g. Kidston et al., 2011). In this study we conducted four twin experiments in total. For both ACE and CE, we recover the original parameter values from (1) the simulated surface Chl-*a* and (2) from the simulated OC3M Chl-*a* dataset (Fig. 1b). To recover the model parameter values we used a conjugate gradient algorithm, used to solve optimization problems with marine biogeochemical models (Fasham et al., 1995; Evans, 1999). The simulated surface Chl-*a* and simulated OC3M Chl-*a* datasets were assimilated in separate experiments changing two parameters simultaneously for each experiment. The purpose of these experiments was to investigate the information content of the two synthetic datasets in relation with the optimized parameters.

As Laiolo et al. (2016) showed, the information content of the Chl-*a* data is insufficient to constrain all parameters in EMS (104 in total), so we chose a sub-set of parameters to test the ability to recover the solution when uncertainty is included in the input dataset (i.e. ± 10% for simulated OC3M Chl-*a*, as we are using two wavelengths, equation (1), McClain, 2009; and ± 5% for simulated surface Chl-*a* based on Hooker et al., 2012). The key processes that control the evolution of phytoplankton concentration are phytoplankton growth, mortality and zooplankton grazing. Phytoplankton growth is generally determined from the availability of light and nutrients while the two biological parameters that largely determine the phytoplankton dynamics are the phytoplankton mortality and grazing rate (Laiolo et al., 2016). Therefore, the sub-set of parameters included phytoplankton natural mortality rate and zooplankton prey capture rate for both small and large size classes (i.e. four parameters in total). Furthermore, selecting parameters that affect the two phytoplankton size classes dynamics allowed us to explore the relation between phytoplankton sizes with simulated surface Chl-*a* and the simulated OC3M Chl-*a*.

To quantify the difference between the Chl-*a* synthetic dataset obtained with the 'original parameter set' and the Chl-*a* dynamics from the twin experiments (Fig. 1b), a cost function (x) was defined as:

$$x = \frac{1}{N}\sum_{t=1}^{T}\frac{(\ln TRUE\_MOD_t - \ln DA\_MOD_t)^2}{(\ln DA\_MOD_t \cdot (err\ \%/100))^2} \quad (2)$$

where $TRUE\_MOD_t$ represents the Chl-*a* value at day *t* of Chl-*a* dataset obtained with the 'original parameter set' which ranged from 1 to 365 (number of days in a year), DA_MOD_t the Chl-*a* value of the DA simulated data at day *t*, *err%* is the accuracy of the selected dataset and *N* represents the degrees of freedom (i.e. *N* = 364). The logarithmic transformation was applied to achieve normal distribution of the Chl-*a* concentrations around the mean seasonal value. Furthermore, to assess that the mean of the Chl-*a* dataset obtained with the 'original parameter set' and the mean of the Chl-*a* dynamics from the DA experiments were consistent, we defined (α) as:

$$\alpha = \frac{(\ln \overline{TRUE\_MOD} - \ln \overline{DA\_MOD})^2}{\frac{\delta^2}{N}} \quad (3)$$

where $\overline{TRUE\_MOD}$ and $\overline{DA\_MOD}$ represent the mean of the Chl-*a* dataset obtained with the 'original parameter set' and the mean of the DA simulated Chl-*a* dataset; *N* represents the degrees of freedom (i.e. *N* = 364) and; δ is a measure of the dataset accuracy:

$$\delta = \ln \overline{DA\_MOD} \cdot (\text{err}\ \%/100) \quad (4)$$

An acceptable fit to the dataset was considered when both (2) and (3) have values of approximately equal to one or less. To illustrate the relationship between the two datasets and the selected parameters, we plot our results in the form of cost function distribution diagrams (e.g. Dowd, 2011), with a final cost function value calculated as the sum of the quantities defined in equation (2) and (3):

$$COST = x + \alpha \quad (5)$$

To produce these diagrams, the analyzed parameters were subjected to a range of perturbations (i.e. ± 40% from the 'original parameter set' value).

3. RESULTS

3.1. Simulated surface Chlorophyll-*a* and simulated OC3M Chlorophyll-*a* dataset

Simulations were undertaken with environments (temperature, mixed layer depth) characteristic of cold-core eddies (CE) and warm-core eddies (ACE). As expected, the simulations produced higher total Chl-*a* in the CE compared to the ACE environment, with a generally greater Chl-*a* in the large phytoplankton class than the

small size class (Fig. 3a, b). In our idealized experiment, the comparison of the simulated surface Chl-*a* with the simulated OC3M Chl-*a* showed significant differences in their seasonal cycle: for both CE and ACE the OC3M algorithm underestimated the simulated surface Chl-*a* concentration throughout the entire year (Fig. 3a – d). To separate large and small phytoplankton signals in the simulated OC3M Chl-*a* (Fig. 3c and d) we first removed all optical factors related to only one phytoplankton size class from the EMS simulation. Then we calculate the optical properties and the R_{rs} related to the second phytoplankton class through the optical model. In the CE environment, the OC3M algorithm underestimated the mean simulated surface Chl-*a* by about a factor of three (mean simulated surface Chl-*a* = 0.27 mg m^{-3}; mean simulated OC3M Chl-*a* = 0.083 mg m^{-3}), while in the ACE environment the OC3M algorithm underestimated the mean simulated surface Chl-*a* by a factor of two (mean simulated surface Chl-*a* = 0.20 mg m^{-3}; mean simulated OC3M Chl-*a* = 0.077 mg m^{-3}). Because the simulated OC3M Chl-*a* is a poor representation of the simulated surface Chl-*a* we did not perform twin experiments between these two synthetic datasets. When contrasting simulated OC3M Chl-*a* with simulated surface Chl-*a* we determined that they are linearly correlated for the small phytoplankton but uncorrelated for the large phytoplankton (Fig. 3e and f).

3.2. Twin experiments

To assess the information content of the simulated surface Chl-*a* and simulated OC3M Chl-*a* datasets we show how the cost function (5) varied as parameter values changed. The visualization of the cost function spread around the global minimum (i.e. cost function equal to zero, using the prescribed parameter values in Table 1) allowed us to better understand the relationship between parameters as well as the information content of the two different datasets that could be used to constrain the model.

In Figure 4, as stated in the methods section 2.3, the acceptable region is based on a cost function value (5). The magnitude of the cost function was assessed in relation to several different parameter combinations. In Figure 4 the red and blue shaded areas shows the acceptable parameter values for simulated surface Chl-*a* and simulated OC3M Chl-*a* respectively; within this area, light blue and red show a cost function equal to one, highlighting local minima. Blue and red dashed lines show the simulated OC3M Chl-*a* and simulated surface Chl-*a* cost values respectively. An

acceptable solution should have a cost value that meets both (x)<1 and (α)<1, represented in the figures by values less than two for both simulated surface Chl-*a* and simulated OC3M Chl-*a* (shaded areas). The diagram axes show the parameters selected for the simulation used to evaluate the cost function and the perturbation applied to their original values (Table 2). The black circle in the centre of each panel shows the global minimum (i.e. parameter values used to generate the synthetic dataset to constrain the system, thus here the cost function equals zero).

First, the large phytoplankton mortality and large zooplankton prey capture rate show similar patterns in the cost function values for simulated surface Chl-*a* and simulated OC3M Chl-*a* (Fig. 4a). Specifically, the simulated surface Chl-*a* region of acceptable parameter values is totally included inside the simulated OC3M Chl-*a* acceptable region, showing a tighter relationship between simulated surface Chl-*a* and parameters affecting large phytoplankton growth (Fig. 4a). Second, with small phytoplankton mortality and small zooplankton prey capture rate, the two different data constraints produce overlapping regions of acceptable parameter values (Fig. 4b) for both datasets (i.e. simulated surface Chl-*a* and simulated OC3M Chl-*a*). In this case, the simulated OC3M Chl-*a* region of acceptable parameter values is included inside the simulated surface Chl-*a* region, showing the OC3M Chl-*a* better constrains parameters affecting small phytoplankton growth (Fig. 4b). The region of acceptable parameter values span similar regions and the DA would not be able to determine unique values for both parameters (Fig. 4a and b). In summary, for large phytoplankton and zooplankton parameter combinations, simulated surface Chl-*a* more tightly constrains the acceptable parameter values than simulated OC3M Chl-*a* (compare size of red shaded area to blue shaded area; Fig. 4a). In contrast, for the small plankton parameters, simulated OC3M Chl-*a* more tightly constrains the acceptable parameter spread than the simulated surface Chl-*a* data (Fig. 4b). As both eddy environments show similar cost function distribution diagrams, here we show results related to CE only.

We then explored cases where a combination of large and small plankton parameter values varied. First, we considered the case where small zooplankton prey capture rate and large phytoplankton natural mortality rate varied (Fig. 4c). The regions of acceptable parameters were different for the two datasets, with a small area of overlap that includes the global minimum (central area of Fig. 4c). Second, we considered the case where small phytoplankton natural mortality and large

zooplankton prey capture rate varied (Fig. 4d). Again the region of acceptable parameter values was different for simulated surface Chl-*a* and simulated OC3M Chl-*a* (red versus blue shaded areas, respectively), with a small region of overlap matching the global minimum (Fig. 4c and d).

In Figure 4c, to produce acceptable results that fit the simulated surface Chl-*a* (i.e. red area), the large phytoplankton natural mortality parameter value (Y axis) has to be tightly constrained (i.e. between -10% and +10%), while the parameter in the X axis (i.e. small zooplankton prey capture rate) does not have an impact on the cost function spread (its value can vary between -40% and +40% producing acceptable results). In the same subplot (Fig. 4c), if we consider the simulated OC3M Chl-*a* acceptable solution area instead (i.e. blue area), the small zooplankton prey capture rate (X axis) is more tightly constrained (between -40% and +10%) than the large phytoplankton natural mortality parameter (Y axis, between -40% and +40%). These features are consistent with all the subplots in Figure 4, suggesting that the simulated OC3M Chl-*a* better constrains the parameters affecting small phytoplankton dynamics while simulated surface Chl-*a* better constrains the parameters affecting large phytoplankton dynamics. This is consistent with the regions of acceptable parameters evident in Figure 4a and b.

4. DISCUSSION

The idealised twin experiments allowed us to investigate information content of two key data streams – *in situ* Chl-*a* and Chl-*a* derived from water leaving radiances. By comparing the model derived Chl-*a* with Chl-*a* computed from simulated water leaving radiances, we could investigate the resulting impact on key parameters in a biogeochemical model, and how it would impact parameter optimization using DA. By working with model simulations, as well as simulated in-water IOPs from which it was possible to calculate R_{rs} and the corresponding OC3M Chl-*a* product, the phytoplankton dynamics in two different oceanic environments (CE and ACE) could be generated in a consistent manner.

The first key point to emerge from our theoretical study was that the simulated OC3M Chl-*a* product was a poor proxy for the total simulated surface Chl-*a* concentration (Fig. 3a - d), suggesting that existing biogeochemical models that assimilate Chl-*a* from ocean colour data could have relatively large inaccuracies. For both CE and ACE simulations, the relationship between large phytoplankton Chl-*a*

and simulated OC3M Chl-*a* was poor, with the simulated OC3M Chl-*a* showing little sensitivity to the amount of simulated Chl-*a* in the large phytoplankton (Fig. 3c and d). The simulated OC3M Chl-*a* was unable to detect our large phytoplankton cells and this caused a large (up to 3 times) under-estimate of total Chl-*a*. In contrast, for the small phytoplankton cells the OC3M Chl-*a* was good estimator of simulated surface Chl-*a*.

The second key point was that the simulated surface Chl-*a* better constrained parameters affecting large phytoplankton growth while simulated OC3M Chl-*a* better constrained parameters related to small phytoplankton dynamics (Fig. 4a and b). This suggests important features about the information that could be extracted from the two data streams, highlighting a stronger relationship between simulated surface Chl-*a* with parameters affecting large phytoplankton dynamics, and simulated OC3M Chl-*a* with parameters affecting small phytoplankton dynamics.

The third key point to emerge when we tried to determine both small and large plankton parameters (Fig. 4c and d) was that simulated surface Chl-*a* and simulated OC3M Chl-*a* contained independent information and if applied together they could dramatically reduce the region of acceptable parameter solutions. Specifically, in a real world scenario, a combination between ocean colour data and *in situ* Chl-*a* concentration measurements could provide enough information for the DA to reduce the spread of acceptable solutions for both small and large plankton parameters. Indeed, for the cases considered here, the DA would find the global minimum, rejecting wide areas that could include several local minima (Fig. 4c and d).

For our model setup we chose two phytoplankton size classes, where the radius of the large phytoplankton class was 20 times greater than the small phytoplankton class (2 and 40 μm diameter, respectively). Our choice of the size phytoplankton classes was based on eddies off East Australia (Laiolo et al., 2016). Furthermore, observations of phytoplankton concentrations in similar oligotrophic regions are consistent with this study, showing large phytoplankton (mainly diatoms) occurring within CE and higher concentrations of small phytoplankton including picocyanobacteria located in the surrounding oligotrophic waters (e.g. Jeffrey and Hallengraeff, 1980; Rodriguez et al., 2003; Vaillancourt et al., 2003; Brown et al., 2008).

While use of two size classes with 20 times difference in radius may accentuate the distinctive information carried by simulated surface Chl-*a* and

simulated OC3M Chl-*a*, it is known that phytoplankton size influences the IOPs of the water column (Bricaud et al., 1995; Ciotti et al., 2002; Volten et al., 1998; Jonasz and Fournier, 2007; Mouw et al., 2012). Our theoretical study suggests a weak relationship between large sized phytoplankton (e.g., chain forming diatoms, dinoflagellates and colonial cyanobacteria) and R_{rs}, leading to an under-estimation of the satellite derived Chl-*a* concentration when large phytoplankton dominate the photosynthetic community (Fig. 3). The detected R_{rs} is a consequence of the IOPs of the water column or, in other words, the result of either light absorption and/or scattering in the water column (Dickey et al., 2006). To explore these properties in our study, we used the optical model of Baird et al. (2016) to assess how absorption and backscattering were responding to different Chl-*a* and carbon (C) ratios, while maintaining a constant Chl-*a* concentration (0.3 mg m^{-3}) for both phytoplankton size classes (small = 2 μm and large = 40 μm) (Fig. 5).

These analyses highlighted that for the small phytoplankton class, as C increases (i.e. increasing number of cells but same amount of total Chl-*a* concentration), there is a corresponding increase in both absorption (Fig. 5a) and backscatter (Fig. 5c) signals. While the increase in the backscatter signal is related to the higher C concentration (Fig. 5c), the slight increase in the absorption (Fig. 5a) is related to the packaging of pigments relative to the energy impinging on the geometric cross-section of the cell (i.e. package effect; Ciotti et al., 2002; Bricaud et al., 2004; Ciotti and Bricaud 2006; Astoreca et al., 2012). Therefore, due to the dimension of the phytoplankton cells the packing effect is less evident in the small phytoplankton class for different C:Chl-*a* concentrations. Conversely, for the large phytoplankton class different C:Chl-*a* have a smaller impact on the backscatter signal (Fig. 5d), due to the greater dimension of the phytoplankton cells, but a higher impact on the absorption coefficient (Fig. 5b), due to the reduced package effect caused by an higher number of larger phytoplankton cells. Because R_{rs} is derived from the relationship between absorption and backscatter ($R_{rs} \propto \frac{b_b}{a+b_b}$), R_{rs} for large phytoplankton was nearly independent of the C:Chl-*a* (Fig. 5f), while variable C:Chl-*a* strongly influenced the R_{rs} for small phytoplankton, particularly in the blue region of the spectrum (Fig. 5e).

As phytoplankton abundance increases, usually the proportion of larger phytoplankton cells rises (e.g. Fig. 3a and b) and both absorption and scattering

spectra are affected. Previous studies show the size of photosynthetic cells has a direct impact on the light absorption efficiency: bigger cells have a lower and spectrally flatter absorption coefficient when compared to smaller phytoplankton cells due to the packaging effect (Ciotti et al., 2002; Bricaud et al., 2004; Ciotti and Bricaud, 2006; Astoreca et al., 2012; Bricaud et al., 1995). This is consistent with results presented in Figure 5a and 5b. The package effect reduces absorption and can therefore increase the error of estimated Chl-*a* concentration from observed remote-sensing reflectance (Marra et al., 2007; Mouw et al., 2012). Much less is known about the backscattering of oceanic particles (portion of scattered photons that leave the water column and hence can be measured by satellite sensors) and its relationship with phytoplankton size (Morel and Maritorena, 2001). Factors such as cell shape and internal structure rather than cell size seem to have a bigger impact on backscattering efficiency than size alone (Vaillancourt et al., 2004). Our backscattering analyses are consistent with Stramski and Kiefer (1991), who demonstrated backscattering from Case I waters is dominated by small particles (less than 1 μm), with a much smaller backscattering contribution from cells larger than 8 μm. Our analyses therefore suggest that both absorption and scattering are involved in the weak R_{rs} signal generated from large phytoplankton cells. Lack of the other optically significant components (e.g. NAP and CDOM) in our model can also affect the results, however their influence on optical properties in the study region is minimal.

Results presented in this study suggest that Chl-*a* concentration within open ocean mesoscale features, in CE in particular, could be higher than the estimated concentration from the ocean colour product calculated through the OC3M algorithm. This reflects a phytoplankton community composed mainly of relatively large photosynthetic cells such as diatoms, with direct implications on primary production estimates and biogeochemical cycles of different elements. In oligotrophic environments, like East Australia offshore waters, picophytoplankton (e.g. *Prochlorococcus*; Partensky et al., 1999) are often an important component of the phytoplankton community, however, eddies (CE in particular) can provide a favourable environment for the growth of larger phytoplankton (e.g. diatoms) (McGillicuddy and Robinson, 1997; Rodriguez et al., 2003; Vaillancourt et al., 2003; Brown et al., 2008; Doblin et al., 2016; Laiolo et al., 2016). Indeed, eddies are hot spots of biological activity, with cyclonic eddies alone enhancing the global primary production by 20% (Falkowski et al., 1991; McWilliams, 2008). The area we selected

for this study is strongly influenced by eddies that originate from the EAC: an average of 28 eddies with a minimum lifetime of 10 weeks occur every year in our study domain (calculated from Chelton et al., 2011 eddies database). Furthermore, in the same region, climate change projections reveal a strengthening of the EAC with a consequent increase in eddy phenomena (Matear et al., 2013). Surprisingly, recent studies show similar primary production (CE= 337 mg C m^{-2} d^{-1}, ACE=272 mg C m^{-2} d^{-1}, calculated from Laiolo et al., 2016) and average Chl-*a* concentration (CE=0.30 mg m^{-3}, ACE=0.25 mg m^{-3}; Everett et al., 2012; calculated from Chelton et al., 2011 dataset) in eddies located in eastern Australian waters and the adjacent Tasman Sea, respectively. Both these studies (i.e. Everett et al., 2012 and Laiolo et al., 2016) used ocean colour data, therefore the similarities found in CE and ACE could be related to an underestimation of the Chl-*a* concentration in CE, associated with the typical higher abundance of large sized phytoplankton in these mesoscale features. Although it is well known that CE on their own enhance the global primary production by ~20% (Falkowski et al., 1991; McWilliams, 2008), published observations that compare East Australia CE and ACE *in situ* primary productivity are not available yet.

The notion that small celled phytoplankton dominate oligotrophic waters is clearly not representative of all open ocean systems. Nevertheless, all open ocean waters are categorised as Case I waters and the current MODIS OC3M algorithm converts R_{rs} from these waters to the Chl-*a* concentration product. Despite the area selected for this case study being located in open ocean waters, we focused only on mesoscale features, known to enhance phytoplankton growth in oligotrophic systems. Simulation and observational studies are consistent in showing that in oligotrophic waters, seasonal increases in Chl-*a* concentration are generally related to large-sized phytoplankton cells increasing within a background of smaller phytoplankton (e.g. McAndrew et al., 2007; Mouw et al., 2012). This behaviour is consistent with the phytoplankton dynamics in CE and ACE off East Australia (Doblin et al., 2016; Laiolo et al., 2016), suggesting that there could be an underestimation by the OC3M Chl-*a* concentration product across the global ocean (Case I waters) related to local and regional increases in the abundance of large sized phytoplankton abundance.

5. CONCLUSION

Ocean colour data play a key role in informing and calibrating marine biogeochemical models through DA methods (Hemmings et al., 2003). For this study, the development of optical models linked to marine biogeochemical models (e.g. Baird et al., 2016; Jones et al., 2016), made it possible to explore properties of MODIS ocean colour data used for DA purposes. Our idealised experiments suggest that the OC3M algorithm can underestimate the Chl-*a* concentration in open ocean mesoscale features such as cyclonic (cold core) eddies, because of the weak reflectance signal from large sized phytoplankton classes such as diatoms, that are typically found within CE boundaries. For our idealized model setup where we consider two phytoplankton groups that have contrasting size (2 and 40 μm), the simulated surface Chl-*a* and simulated OC3M Chl-*a* data streams provide distinct information for the large and small phytoplankton dynamics respectively. While our model setup may be simplified compared to natural systems in that we only have two sizes of phytoplankton, it raises an important issue about the role of size on the conversion of remotely sensed reflectance to a chlorophyll-*a* product.

Tables

Table 1: Abbreviations and symbols

Abbreviations / Symbols	Definition	Unit
EAC	East Australian Current	
CE	Cyclonic eddy	
ACE	Anticyclonic eddy	
EMS	Environmental Modelling Suite	
Chl-*a*	Chlorophyll-*a* concentration	mg m^{-3}
C	Carbon concentration	mg m^{-3}
simulated OC3M Chl-*a*	Satellite-like Chl-*a* product obtained from EMS output	mg m^{-3}
simulated surface Chl-*a*	*In situ*-like Chl-*a* measurements	mg m^{-3}
IOPs	Inherent optical properties	
AOPs	Apparent optical properties	
R_{rs}	Remote sensing reflectance	sr^{-1}
a	Absorption coefficient	m^{-1}
b_b	Backscattering coefficient	m^{-1}
OC3M	Band ratio algorithm of Chl-*a* concentration for data from MODIS radiometer - equation (1)	

Table 2: EMS 'original parameter set' for cyclonic eddy (CE) and anticyclonic eddy (ACE) used to obtain the simulated surface Chl-*a* dataset; T_{ref} refers to reference temperature (Laiolo et al., 2016). The sub-set of parameters included in this study is composed of large phytoplankton natural (linear) mortality, small phytoplankton natural (linear) mortality rate, large zooplankton natural (quadratic) mortality and small zooplankton natural (quadratic) mortality.

Parameter	CE	ACE	Unit
Large zooplankton growth efficiency	0.34	0.34	
Small zooplankton growth efficiency	0.30	0.29	
Large phytoplankton natural (linear) mortality rate	0.01	0.01	day^{-1}
Small phytoplankton natural (linear) mortality rate	0.02	0.02	day^{-1}
Large zooplankton natural (quadratic) mortality rate	0.8	0.35	$(mmol\ N/m^3)^{-1}\ day^{-1}$
Small zooplankton natural (quadratic) mortality rate	0.35	0.35	$(mmol\ N/m^3)^{-1}\ day^{-1}$
Large phytoplankton maximum growth rate at T_{ref}	1.8	1.8	day^{-1}
Large phytoplankton cells diameter	40	40	μm
Small phytoplankton maximum growth rate at T_{ref}	1.0	1.0	day^{-1}
Small phytoplankton cells diameter	2	2	μm
Small zooplankton maximum growth rate of at T_{ref}	0.4	0.4	day^{-1}
Small zooplankton swimming velocity	0.0015	0.0016	m/s
Large zooplankton maximum growth rate at T_{ref}	0.90	0.4	day^{-1}
Large zooplankton swimming velocity	0.053	0.055	m/s
Remineralization rate	0.10	0.10	day^{-1}
Sinking velocity	5.00	5.00	m/day

Figure captions

Figure 1. Diagrams representing how the two synthetic datasets were created (panel a) and how the twin experiments were conducted (panel b).

Figure 2. Australian region and the study area highlighted by the dashed line (150° E – 160° E; 30° S – 40° S). To illustrate the main features (cyclonic eddy CE, anticyclonic ACE, East Australian Current EAC) occurring in the study area, the satellite image of surface Chl-*a* calculated with OC3M algorithm using reflectance acquired with the MODIS radiometer (2nd April 2016) and the current pattern based on altimeter data is shown. Data source: Integrated Marine Observing System (http://oceancurrent.imos.org.au/oceancolour.php)

Figure 3. Simulated seasonal climatology of total Chl-*a* concentration (solid black line), Chl-*a* in small phytoplankton (blue dotted) and Chl-*a* in large phytoplankton (red dashed line) for CE (a) and ACE (b) off East Australia. The green line represents seasonal climatology for CE (a) and ACE (b) off East Australia (Laiolo et al. 2016) calculated from GlobColour (25 km spatial resolution, 8-day average; http://hermes.acri.fr/index.php?class=archive), while the shaded green areas represent the corresponding standard deviation. The middle panel shows for the same simulations, the corresponding simulated OC3M Chl-*a* obtained from the R_{rs} calculated from the simulated surface Chl-*a* for the two phytoplankton classes (panels a and b) for CE (c) and ACE (d). Note there is a different scale on the Chl-*a* concentration between panel a - c and b - d. The lower panel compares the simulated surface Chl-*a*, with the corresponding simulated OC3M Chl-*a* for CE (e) and ACE (f).

Figure 4. For various pairs of parameters, the region of parameter values that produced acceptable fits to the data. Here we show results for CE as similar plots were obtained for ACE. Black circles represent the global minimum, where the cost function is equal to zero. Red shaded areas represent acceptable solutions for the simulated surface Chl-*a* assimilation; within this area, light red shows cost function equal to one highlighting local minima. Red dashed lines show the simulated surface Chl-*a* cost values. Blue dashed lines and blue shaded areas show the simulated OC3M Chl-*a* cost values. Shaded blue areas represent acceptable solutions; within this area,

light blue shows a cost function equal to one, highlighting local minima. Acceptable solutions (i.e. (x)<1 and (α)<1) are represented by values less than two.

Figure 5. Absorption, backscattering and R_{rs} spectra of small (2 μm) (left column) and large (40 μm) (right column) phytoplankton classes for different ratios of phytoplankton Carbon (C) to Chl-*a*. The black lines represent a scenario with 0.3 mg m^{-3} of Chl-*a* and 6 mg m^{-3} C (C:Chl-*a* 20:1); the red lines represent a scenario with 0.3 mg m^{-3} of Chl-*a* and 15 mg m^{-3} C (C:Chl-*a* 50:1); the green lines represent a scenario with 0.3 mg m^{-3} of Chl-*a* and 30 mg m^{-3} C (C:Chl-*a* 100:1); and the blue lines represent a scenario with 0.3 mg m^{-3} of Chl-*a* and 45 mg m^{-3} C (C:Chl-*a* 150:1). The amount of Chl-*a* and C in the left and right columns are equal and entirely distributed in the small phytoplankton class (left) or large phytoplankton class (right). Panels a and b show absorption spectra, panels c and d backscattering and panels e and f the R_{rs} for the two phytoplankton classes.

ACKNOWLEDGEMENTS

This research was supported under the Australian Research Council's Discovery Projects funding scheme (DP140101340 to MD and RM). Furthermore, we would like to thank NASA for the production and distribution of the chlorophyll-*a* product as well as the OC3M algorithm. Data presented in Figure 2 were sourced from the Integrated Marine Observing System (IMOS), an initiative of the Australian Government being conducted as part of the National Collaborative Research Infrastructure Strategy and the Super Science Initiative. Finally, we would like to acknowledge the valuable reviews provide by the four anonymous reviewers, which has helped improve the clarity and focus of the manuscript.

APPENDIX

Bio-optical model

First the IOPs (i.e., absorption, scattering and backscattering) of the water column are calculated from the model state variables and parameters. Then, the optical model solves for the AOPs including the remote-sensing reflectance (R_{rs}). R_{rs} at two wavelengths can then be processed through the OC3M algorithm to obtain an estimation of the Chl-*a*.

Inherent optical properties (IOPs)

Absorption coefficient. The absorption-cross section (α) of a spherical cell without considering internal scattering is given by (Duysens, 1956; Kirk, 1975):

$$\alpha = \pi r^2 \left(1 - \frac{2\left(1-(1+2\gamma c_i r)e^{-2\gamma c_i r}\right)}{(2\gamma c_i r)^2}\right) \quad \text{(a.1)}$$

where (r) represents the radius of cell, (γ) the pigment-specific absorption coefficient, (c_i) the homogeneous intracellular pigment concentration. πr^2 is the projected area of a sphere and the bracketed term can range from 0 for no absorption ($\gamma c_i r = 0$) to 1 when the cell is fully opaque ($\gamma c_i r \to \infty$). The total absorption ($a_{T,\lambda}$), is given by:

$$a_{T,\lambda} = a_{w,\lambda} + \sum_{x=1}^{N} n_x \alpha_{x,\lambda} \quad \text{(a.2)}$$

where $a_{w,\lambda}$ represents clear water absorption, N the number of phytoplankton classes (in our case $N \leq 2$ large and small phytoplankton), n the concentration of cells (cell m^{-3}) and α_λ the absorption cross-section (m^2 $cell^{-1}$).

Scattering coefficient. The total scattering coefficient is given by:

$$b_{T,\lambda} = b_{w,\lambda} + b_{phy,\lambda} \sum_{x=1}^{N} n_x c_{i,x} V_x \quad \text{(a.3)}$$

$b_{w,\lambda}$ is the scattering coefficient due to clear water, the phytoplankton scattering is the product of the Chl-*a* specific phytoplankton scattering coefficient ($b_{phy,\lambda}$) and the water column concentration of all classes ($\sum_{x=1}^{N} n_x c_{i,x} V_x$), where N represents the number of phytoplankton classes, n the concentration of cells (cell m^{-3}), c_i is the Chl-*a* concentration in the cell and V is the cell volume. The value for $b_{phy,\lambda}$ is set to 0.2 (mg Chl-*a* m^{-2})$^{-1}$ for all wavelengths, a typical value for marine phytoplankton (Kirk, 1994).

Backscattering coefficient. Backscattering coefficient (b_b) has a component due to pure seawater and a component due to particulates. The particulate component for phytoplankton is strongly related to cell carbon (and therefore cell size) and the number of cells (Vaillancourt et al., 2004):

$$b^*_{bphy,\lambda} = 5 \times 10^{-15} m_C^{1.002} \quad \text{(a.4)}$$

were m_C is the carbon content of the cells, here in pg cell^{-1}. The total backscatter then becomes:

$$b_{b,\lambda} = \tilde{b}_w b_{w,\lambda} + b^*_{bphy,\lambda} n \quad \text{(a.5)}$$

where the backscatter ratio of pure seawater, ($\tilde{b}_w$ is 0.5 and n is the concentration of cells.

Remote sensing reflectance (R_{rs})

To calculate the R_{rs} at the surface, we need to consider the light returning from multiple depths and the bottom. The ratio of the backscattering coefficient to the sum of backscattering and absorption coefficients for the whole water column, u_λ, is:

$$u_\lambda = \sum \frac{w_{\lambda,z'} b_{b,\lambda,z'}}{a_{\lambda,z'} + b_{b,\lambda,z'}} \quad \text{(a.6)}$$

where $w_{\lambda,z'}$ is a weighting representing the component of the R_{rs} due to the absorption and scattering at depth z'.

$$w_{\lambda,z} = \frac{1}{z_1 - z_0}\left(\int_0^{z_1} \exp(-2K_{\lambda,z'})dz' - \int_0^{z_0} \exp(-2K_{\lambda,z'})dz'\right) \quad \text{(a.7)}$$

$$= \frac{1}{z_1 - z_0}\int_{z_0}^{z_1} \exp(-2K_{\lambda,z'})dz' \quad \text{(a.8)}$$

in this case, the integral of $w_{\lambda,z}$ to infinite depth is 1. In areas where light reaches the bottom, the integral of $w_{\lambda,z}$ to the bottom is less than one, and benthic reflectance is important. Note that the weighting of the surface expression of an IOP based on twice the vertical attenuation rate has been used in semi-analytical reflectance models (Lee et al., 2002), to consider the surface expression of depth-varying Chl-*a* concentration (Moline and Prezelin, 2000). K_λ represents the vertical attenuation coefficient at wavelength λ, the factor of 2 accounts for the pathlength of both downwelling and upwelling light. When considering absorption and scattering, K_λ is given by:

$$K_\lambda = \frac{a_{T,\lambda}}{\cos\theta_{sw}} \sqrt{1 + (g_i + g_{ii}\cos\theta_{sw})\frac{b_{T,\lambda}}{a_{T,\lambda}}} \quad \text{(a.9)}$$

The term outside the square root quantifies the effect of absorption, where $a_{T,\lambda}$ is the total absorption. The term within the square root represents scattering as an extended

pathlength through the water column, where g_{i} and g_{ii} are empirical constants and take values of 0.402 and 0.180 respectively (Kirk, 1991; Mobley, 1994). For waters ranging from coastal to open ocean, the average cosine of scattering varies by only a small amount (0.86 – 0.95, Kirk, (1991)), and thus uncertainties in g_{i} and g_{ii} do not strongly affect K_{λ}.

The below-surface remote-sensing reflectance ($\mathrm{r_{rs}}$), is given by:

$$r_{\mathrm{rs},\lambda} = g_0 u_{\lambda} + g_1 u_{\lambda}^2 \tag{a.10}$$

where $g_0 = 0.895$ and $g_1 = 0.1247$ are empirical constants for the nadir-view in oceanic waters (Lee et al., 2002; Brando et al., 2012), and these constants result in a change of units from the unitless u to a per unit of solid angle, $\mathrm{sr^{-1}}$, quantity $r_{\mathrm{rs},\lambda}$.

The above-surface remote-sensing reflectance, through rearranging Lee et al. (2002), is given by:

$$R_{\mathrm{rs},\lambda} = \frac{0.52\mathrm{r}_{\mathrm{rs},\lambda}}{1-1.7\mathrm{r}_{\mathrm{rs},\lambda}} \tag{a.11}$$

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