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An optimized Chlorophyll *a* switching algorithm for MERIS and OLCI in phytoplankton-dominated waters

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ABSTRACT

Productive upwelling zones such as the southern Benguela can exhibit phytoplankton biomass variability over several orders of magnitude, from near oligotrophic offshore waters to hypertrophic inshore blooms of > 100 mg m $^{-3}$. This introduces complexity for ocean colour applications such as Harmful Algal Bloom (HAB) monitoring. As low and high biomass algorithmic approaches for ocean colour differ, no single algorithm can optimally retrieve accurate Chl *a* over such a wide range of biomass. We propose a novel technique to apply and blend two different Chl *a* algorithms — an empirical blue-green algorithm for low to moderate biomass and a red-NIR band-ratio algorithm for moderate to high biomass. The blending method is based on the 708 and 665 nm reflectance wavelength ratio, where the blue-green algorithm is applied when the $\rho_w(708)/\rho_w(665)$ ratio is < 0.75, the red-NIR algorithm is applied > 1.15, whilst the two are blended using a weighted approach in between these values. When applied to *in situ* and satellite match-up data this method provides a median absolute relative difference (MARD) of 37.9 and 45.7%, respectively, and a RMSD of 0.27 and 0.35 respectively, over Chl *a* concentrations spanning three orders of magnitude. Application is demonstrated for both MERIS and OLCI sensors, providing a smooth transition between different biomass levels and algorithm Chl *a* returns.

1. Introduction

Deriving quantitative information of the biogeochemical constituents in the water column from satellite ocean colour data requires regionally or water type appropriate algorithms. As a component of all photosynthetic marine algae, Chlorophyll *a* concentration ([Chl *a*]) is often used as a proxy for phytoplankton biomass (O'Reilly et al., 1998).

Empirical algorithms that utilize relationships between reflectances in the blue and green spectral regions (e.g. O'Reilly et al., 1998; O'Reilly et al., 2000; Morel and Antoine, 2011) are often used to derive [Chl *a*] in open ocean or " Case 1" waters (Morel and Prieur, 1977; Gordon and Morel, 1983), where water constituents tend to covary with phytoplankton and its related degradation products. However, the assumptions that these algorithms are based upon can break down in productive or turbid waters (Dierssen, 2010). Algorithms utilizing the red-NIR part of the electromagnetic spectrum have often been preferred for ocean colour remote sensing of productive inland and coastal waters. This spectral region has several reflectance features that can be related to [Chl *a*], such as the height of the solar-induced Chl *a* fluorescence peak (e.g. Gower and King, 2007; Ryan et al., 2009), the reflectance peak around 700 nm which is often related to [Chl *a*] through relationships with band ratio (Gitelson et al., 2011; Gurlin et al., 2011; Yacobi et al., 2011) and spectral band difference algorithms (Gower et al., 2005; Matthews et al., 2012).

Although both blue-green and red-NIR band ratio algorithms are mostly robust in their ability to provide coherent patterns of the synoptic phytoplankton biomass variability at their respective optimal [Chl *a*] ranges, the natural variation in IOPs often necessitate regional tuning to ensure lower uncertainty in [Chl *a*] retrievals (e.g.McKee et al., 2007; Volpe et al., 2007). To date there is no single algorithm that can provide accurate quantitative information across all water types.

To overcome this hurdle, specific thresholds or flags have been used to switch between different algorithms (e.g. Matsushita et al., 2015; Smith et al., 2013); however, these techniques run the risk of causing discontinuities that may not be apparent just by looking at the [Chl *a*] image, but which may show up with more detailed analysis (e.g. Hooker et al., 1995). More holistic methods have included fuzzy classification of reflectance spectra into predefined optical water types for application and blending of water type-appropriate algorithms (Moore et al., 2001, 2014); this method has now also been included as part of the ocean colour products produced by the ESA Climate Change Initiative to apply and blend class appropriate algorithms across merged

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satellite datasets (Jackson et al., 2017). The Coast Colour project proposes a merged [Chl *a*] product, which blends the retrievals of a blue-green empirical algorithm and a neural network algorithm, based on the satellite retrieved concentration of total suspended matter (Brockmann, 2014). A similar method has been employed in the Yellow and East China Seas, where the height of the normalized water-leaving radiance at 555 nm was used to switch and blend between two regionally-modified algorithms for Case 1 and turbid waters, respectively (Siswanto et al., 2011). The novelty detection technique of D'Alimonte et al. (2003) uses the triplet of the logarithm of the R_{rs} at 490, 555, and 665 nm with a probability density function to blend the returns from two different neural network algorithms when satellite pixels are considered non-novel. Weighted algorithm switching and blending can also optimize retrievals in low biomass Case 1 environments; the NASA [Chl *a*] product, chlor_a, uses the colour index (CI) (Hu et al., 2012) and the standard OC3 for MODIS or OC4 for SeaWiFS (O'Reilly et al., 2000), whilst a transition between the two products occurs at CI values of 0.15 and 0.2 (Feldman and McClain, 2017). Kahru and Mitchell (2010) use both the maximum band ratio and the mean geographical position relative to the Subtropical Front to weight and blend their Southern Ocean specific algorithm with OC4, whilst Carder et al. (1999) blend semianalytical and empirical algorithms based on the phytoplankton absorption coefficient at 675 nm ($a_{\phi}(675)$) value returned by the semianalytical algorithm. Weighted algorithm blending thus offers the ability to smoothly transition between water-type appropriate algorithms to ensure optimal retrievals and minimize spatial discontinuities.

The region of interest in the current study is the southern Benguela, a highly productive and dynamic eastern-boundary upwelling system. The optical conditions can be described as phytoplankton-dominated extreme Case 1 (Matthews et al., 2012), with inorganic particulates and coloured dissolved organics contributing very little to the bulk inherent optical properties. Due to the wind-driven and pulsed nature of the system, [Chl *a*] may range from approximately < 1 to $> 30\,\mathrm{mg\,m^{-3}}$, in newly and aged upwelled water respectively (Barlow, 1982), over a matter of days; [Chl *a*] $> 100\,\mathrm{mg\,m^{-3}}$ is often reported in bloom conditions (Pitcher and Nelson, 2006). Harmful algal blooms (HABs) occur frequently from January to May in the latter half of the upwelling season (Pitcher and Calder, 2000), which have the potential to negatively impact commercial and recreational activities in the region (Pitcher and Calder, 2000; Probyn et al., 2000). Although the [Chl *a*] product cannot directly describe the type of species or toxicity of a bloom, it can be used as an indicator for high biomass blooms that could potentially lead to hypoxic events (Pitcher and Weeks, 2006).

Whilst standard empirical algorithms may be sufficient to monitor the average coastal and offshore conditions of [Chl *a*] $< 25\,\mathrm{mg\,m^{-3}}$, algorithms are also required to accurately assess the very high biomass ranges where potential harmful impacts from toxic diatom and toxic or hypoxia-causing dinoflagellate blooms may materialize. The water-leaving reflectance signal attributed to increasing phytoplankton biomass becomes dominated by features in the red part of the spectrum at around $15\,\mathrm{mg\,m^{-3}}$ (Robertson Lain et al., 2014); thus, from a remote sensing perspective, operational monitoring of this highly variable system would benefit from a dynamic approach that utilizes appropriate algorithms corresponding to the dominant spectral features and *in situ* ranges of phytoplankton biomass, whilst providing optimal blended returns. We propose that it is possible to base an algorithm switch on the ratio of the reflectance peak near 700 nm, attributed to a combination of strong phytoplankton and water absorption and elevated phytoplankton backscattering, and the reflectance trough near 675 nm, caused by a maximum in Chl-*a* absorption. This ratio is strongly related to [Chl *a*] and is often employed in red-NIR algorithms (Gurlin et al., 2011).

In order to optimize this approach for satellite application, the 708 and 665 nm bands were utilized respectively. With the availability of good spectral coverage in the red-NIR the Level 2 radiometric data from both the MEdium Resolution Imaging Spectrometer (MERIS) and the Ocean and Land Colour Imager (OLCI) provide the ideal sensors for application of this approach to derive quantitative [Chl *a*]. Although the MERIS time-series ended in 2012, it provides ten years of ocean colour data for time-series analysis and algorithm development and testing. OLCI was built on MERIS heritage with similar radiometric setup and quality to ensure algorithm and data time-series continuity between these sensors.

The focus of this paper is to optimally resolve [Chl *a*] over a wide range of biomass in waters where phytoplankton are the dominant optical constituent in the water column (i.e. where the contributions from absorption and backscattering of terrigenous coloured dissolved organic particles and inorganic particles to the water-leaving signal are relatively small). The goal was not to derive new algorithms, but to find the best performing existing algorithms for low to moderate ($< 10\,\mathrm{mg\,m^{-3}}$), and moderate to high ($> 10\,\mathrm{mg\,m^{-3}}$) biomass waters, and to devise a method to assign, and where necessary blend, algorithm returns.

2. Materials and methods

2.1. In situ data collection

All the *in situ* data were collected in the southern Benguela along the west coast of South Africa between 2002 and 2017. This region has been the focus of many ocean colour remote sensing studies since 2002 due to the high productivity of the upwelling system and resulting harmful algal blooms. Field campaigns have most often focussed on the upwelling or highly productive seasons (February to April) in order to capture *in situ* and satellite validation data for the phytoplankton blooms which frequently occur during this time. The available data were collected during collaborative research efforts between the Department of Agriculture, Forestry and Fisheries (DAFF), the Council for Scientific and Industrial Research (CSIR) and the University of Cape Town (UCT) and have included data collection in the St Helena Bay region near Lambert's Bay ($N = 142$), Elands Bay ($N = 25$), and the Berg River mouth ($N = 5$), as well as in Saldanha Bay ($N = 6$). The methodological details for these field studies are all similar, and are described below. Additional data collected in the Benguela region includes the Benguela Calibration (BENCAL) cruise ($N = 20$) during October 2002; details of the data collection methodology can be found in the cruise report (Barlow et al., 2003). A complete *in situ* dataset which focused on the R_{rs} and [Chl *a*] data was compiled from the aforementioned studies.

Coincident radiometric measurements and water sample collection were performed within maximum of 60 min(although usually within 30 min) of satellite overpass times, usually between 09:30 and 10:30 local time. In-water radiometric measurements were made with a hyperspectral Tethered Satlantic Radiometric Buoy (TSRB). The TSRB measures upwelling radiance ($L_u(z)$ at $z = -0.66\,\mathrm{m}\,\mu\mathrm{W\,cm^{-2}\,nm^{-1}\,sr^{-1}}$) and above surface downwelling irradiance ($E_d(0^+)$, $\mu\mathrm{W\,cm^{-2}\,nm^{-1}}$) and has two 256 channel spectrographs that cover a spectral range of 400 to 800 nm. During acquisition the instrument was floated far enough from the vessel to avoid shadowing or interference. Measurements were typically recorded for about 2 to 5 min. Raw data were processed with Prosoft 6.3d (Satlantic: Halifax, Canada); the median values of the deployment were selected and resampled to a spectral resolution of 5 nm. The measured radiometric variables were converted to remote sensing reflectance (R_{rs}) using the equivalent algal population (EAP) inversion algorithm with Ecolight-S (Mobley, 2011) (as described in Evers-King et al., 2014) to derive the upwelling radiance attenuation coefficient (K_{Lu}). Various sources of uncertainty can affect the derivation of *in situ* R_{rs}, including the cumulative uncertainty in upwelling radiance (Antoine et al., 2006), calibration uncertainty for irradiance (Zibordi and Voss, 2010), the self-shading percentage error of the TSRB (Leathers et al., 2001), and the tilt and roll of the instrument (Zibordi et al., 2012), to name a few. The cumulative uncertainty budget for these types of radiometric buoys has been