Three improved satellite chlorophyll algorithms for the Southern Ocean

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[1] Remote sensing of Southern Ocean chlorophyll concentrations is the most effective way to detect large-scale changes in phytoplankton biomass driven by seasonality and climate change. However, the current algorithms for the Sea-viewing Wide Field-of-view Sensor (SeaWiFS, algorithm OC4v6), the Moderate Resolution Imaging Spectroradiometer (MODIS-Aqua, algorithm OC3M), and GlobColour significantly underestimate chlorophyll concentrations at high latitudes. Here, we use a long-term data set from the Southern Ocean (20°–160°E) to develop more accurate algorithms for all three of these products in southern high-latitude regions. These new algorithms improve in situ versus satellite chlorophyll coefficients of determination (r^2) from 0.27 to 0.46, 0.26 to 0.51, and 0.25 to 0.27, for OC4v6, OC3M, and GlobColour, respectively, while addressing the underestimation problem. This study also revealed that pigment composition, which reflects species composition and physiology, is key to understanding the reasons for satellite chlorophyll underestimation in this region. These significantly improved algorithms will permit more accurate estimates of standing stocks and more sensitive detection of spatial and temporal changes in those stocks, with consequences for derived products such as primary production and carbon cycling.

1. Introduction

[2] Ocean color remote sensing is our most effective tool for understanding ocean ecology and biogeochemistry at basin to global scales. Within this context, high-latitude oceans are of particular interest as they are the most remote and difficult to sample by other means, yet also potentially the most sensitive to climate change [*Intergovernmental Panel on Climate Change*, 2007]. The Southern Ocean is characterized by extreme weather, strong seasonality and unique photophysiology, nutrient regimes, and microbial communities. It therefore presents a challenge for both in situ and remote observations. The Sea-viewing Wide Field-of-view Sensor (SeaWiFS) and the Moderate Resolution Imaging Spectroradiometer (MODIS) use(d) empirically derived algorithms to estimate in situ total chlorophyll concentration from remotely sensed radiometry. Algorithms like these have been used to estimate chlorophyll from space since the first dedicated ocean color satellite, the Coastal Zone Color Scanner, was launched in 1978 [*Hovis et al.*, 1980]. Current satellite chlorophyll algorithms are heavily weighted toward in situ data from temperate and tropical regions, and their performance at high latitudes is notoriously poor [*Kahru and Mitchell*, 1999; *Dierssen and Smith*, 2000; *Cota et al.*, 2003; *Gregg and Casey*, 2004; *Strutton et al.*, 2011].

[3] Since the Southern Ocean has distinctive bio-optical properties [*Szeto et al.*, 2011], developing regional algorithms for SeaWiFS, MODIS, and GlobColour satellite chlorophyll should improve our ability to detect the response of phytoplankton to climate change, a long-term goal of NASA's ocean color project.

[4] Southern Ocean regional algorithms have previously been proposed, but almost all of this work focused on the Antarctic Peninsula, and used fluorometric chlorophyll measurements [*Mitchell and Holm-Hansen*, 1991; *Dierssen and Smith*, 2000; *Gregg and Casey*, 2004; *Garcia et al.*, 2005; *Marrari et al.*, 2006; *Mitchell and Kahru*, 2009; *Kahru and Mitchell*, 2010; *Szeto et al.*, 2011]. This manuscript builds on that body of work but is focussed on Southern Ocean algorithms applicable at the basin scale.

[5] In this manuscript, our goals are to:

[6] 1. Quantify the accuracy of existing satellite chlorophyll algorithms for SeaWiFS (OC4v6), MODIS (OC3M), and GlobColour in the Southern Ocean, from the Indian to the Pacific sectors.

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[7] 2. Improve algorithms for satellite estimation of chlorophyll in the region, enhance the dynamic range and reduce the underestimation of current algorithms.

[8] 3. Test the sensitivity of the improved algorithms to changes in phytoplankton community composition, as indicated by ratios of photosynthetic marker pigments (Fp index) [*Claustre*, 1994].

[9] We compared chlorophyll estimates from each satellite product with a database of >1300 in situ surface phytoplankton pigment measurements and were able to significantly improve both the accuracy and dynamic range of satellite chlorophyll algorithms. Further, we show that differences between satellite estimates and in situ measurements are related to phytoplankton community composition.

2. Data and Analysis

2.1. Current Algorithms

2.1.1. SeaWiFS

[10] SeaWiFS, like all ocean color sensors, used an empirically derived algorithm to calculate chlorophyll from band ratios of remote sensing reflectance (Rrs). The current chlorophyll algorithm used for SeaWiFS processing is OC4v6 [*O'Reilly et al.*, 1998, 2000].

$$Chl_{SW} = 10^{\left(0.3272 - 2.9940 R_{SW} + 2.7218 R_{SW}^2 - 1.2259 R_{SW}^3 - 0.5683 R_{SW}^4\right)} \quad (1)$$

where $R_{SW} = \log10(Rrs_{(443/555)} > Rrs_{(490/555)} > Rrs_{(510/555)})$. The log10 argument indicates that the algorithm uses the maximum of the three ratios. The subscript in the R_{SW} term refers to the platform (SeaWiFS). Chl_{SW} denotes the calculated chlorophyll concentration in mg m^{-3}.

2.1.2. MODIS-Aqua

[11] The current chlorophyll algorithm used for MODIS-Aqua processing is OC3M (http://oceancolor.gsfc.nasa.gov/ANALYSIS/ocv6/).

$$Chl_{MA} = 10^{\left(0.2424 - 2.7423 R_{MA} + 1.8017 R_{MA}^2 + 0.0015 R_{MA}^3 - 1.2280 R_{MA}^4\right)} \quad (2)$$

where $R_{MA} = \log10(Rrs_{(443/547)} > Rrs_{(490/547)})$. The log10 argument indicates that the algorithm uses the maximum of the two ratios. The subscript in the R_{MA} term refers to the platform (MODIS-Aqua). Chl_{MA} denotes the calculated chlorophyll concentration in mg m^{-3}.

2.1.3. GlobColour

[12] GlobColour has two chlorophyll algorithms: a weighted average empirical algorithm, which is derived from SeaWiFS, MODIS-Aqua and MERIS, and the semi-analytical Garver Siegel Maritorena (GSM) algorithm [*Pinnock et al.*, 2007; *Durand*, 2007; *Maritorena and Siegel*, 2005]. The GSM algorithm will not be discussed here. Because the GlobColour team disseminates the merged normalized water-leaving radiance data, the improved GlobColour algorithm presented here uses these as input after conversion to Remote Sensing Reflectance (Rrs) based on NASA SeaDASv7.0 with the SeaWiFS Nominal Band Solar Irradiances.

2.2. In Situ Data Set

[13] A total of 1388 High Pressure Liquid Chromatography (HPLC) pigment samples, recorded from <5 m depth, were obtained from 29 austral summer Southern Ocean expeditions (40° − 70°S, 20° − 160°E, 2001–2008, Figure 1), mostly from the French vessel MV *L'Astrolabe* and the Australian vessel RSV *Aurora Australis*. Two of the 29 voyages were sourced from the NASA SeaWiFS Bio-optical Archive and Storage System (SeaBASS) database. L'Astrolabe and Aurora Australis pigment samples were collected by filtration of 2 L of surface seawater under low vacuum (≤50 kPa) onto 13 mm diameter GF/F filters (Whatman, Gottingen, Germany) in low light conditions. The filters were immediately frozen in liquid nitrogen for later analysis. Pigment extraction and HPLC analysis were conducted at the Australian Antarctic Division, Kingston Tasmania, and followed *Mock and Hoch* [2005], along with the modifications described in *Wright et al.* [2010].

2.3. Initial Comparison of Satellite Estimates to In Situ Data

[14] NASA SeaWiFS Level 3, 9 km, NASA MODIS-Aqua Level 3, 9 km, and ESA GlobColour 4 km sea surface chlorophyll data were evaluated against the in situ data set, in a standardized manner so as to allow intercomparison.
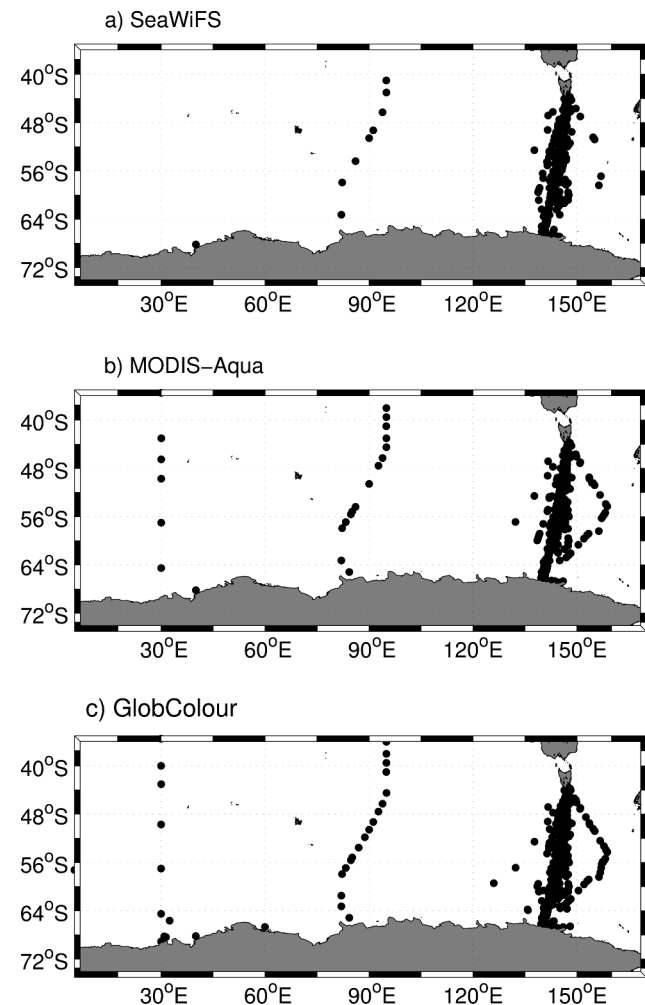

Figure 1. Maps of geographical distribution of coincident in situ HPLC and satellite chlorophyll measurements ("match ups") for each satellite data product: (a) SeaWiFS, (b) MODIS-Aqua, and (c) GlobColour.

Initial match ups were conducted using three different time averaged data products (daily averages, 8 day averages and monthly averages), in order to determine the maximum usable temporal resolution and minimize cloud interference. Spatial averaging was applied to increase probability of a satellite to in situ match. Both 3 × 3 and 5 × 5 pixel averaging of satellite data around each in situ observation were performed. To ensure homogeneity of the pixel averaging window, any pixel window with a standard deviation >0.15 mg m^{-3} among valid pixels was removed from the analysis [*Bailey and Werdell*, 2006]. The worst case, MODIS-Aqua, resulted in a loss of 2.5% of match ups, when this criterion was applied.

2.4. Creating New Models

[15] We used an optimization routine that requires a starting point algorithm as this reduces the likelihood of diverging from the relationship we wish to model. The original algorithm was used as a starting point from which to run optimization routines for SeaWiFS. The original MODIS-Aqua algorithm did not describe the Southern Ocean maximum band ratio to chlorophyll relationship well enough to use as an optimization starting point. Instead the optimized SeaWiFS algorithm was used as the MODIS-Aqua optimization starting point. All algorithm coefficients were modified for our Southern Ocean data set using the optimization toolbox in Mathworks MATLAB 2011a. The optimization process attempted to achieve a slope of 1, a *y* intercept of 0, and a large r^2 for algorithm predicted chlorophyll versus in situ chlorophyll. Increasing and decreasing the degree of the polynomial was allowed in order to obtain the best possible fit. The GlobColour data were treated with the same optimization method except that the SeaWiFS OC4v6 algorithm was used as a starting point for the optimization process, as there is no existing empirical chlorophyll algorithm for GlobColour.

2.5. Phytoplankton Pigment Contribution

[16] Pigment composition is considered to be a driving factor in the absorption profile of phytoplankton and therefore impacts satellite chlorophyll retrievals. In order to best describe the changing pigment composition across such a vast geographic scale, an index of the key diagnostic pigments was investigated using a pigment biomarker index developed by *Claustre* [1994]. The index is:

$$Fp = \left(\sum Fucoxanthin + \sum Peridinin\right) \times \left(\sum Fucoxanthin\right.$$
$$+ \sum Peridinin + \sum 19'HexFucoxanthin$$
$$+ \sum 19'ButFucoxanthin + \sum Zeaxanthin$$
$$\left. + \sum Chlorophyll - b + \sum Alloxanthin\right)^{-1} \quad (3)$$

where $\sum pigment$ is the summation of that pigment's HPLC derived concentration in mg m^{-3}.

[17] The Fp Index was originally derived from the knowledge that variations in chlorophyll standing stocks on a global scale are mainly due to variation in stocks of diatoms and dinoflagellates with respect to other taxa [*Claustre*, 1994]. Fucoxanthin is a key diagnostic pigment of diatom species and Peridinin is a key pigment for dinoflagellates, so large Fp values represent high concentrations of diatoms or dinoflagellates or both, relative to other phytoplankton groups [*Claustre*, 1994; *Jeffrey et al.*, 1997].

2.6. Independent Evaluation

[18] In situ data were broken down into a development data set and a validation data set. The validation data set contained a random selection of 1/3 the available in situ measurements and the development data set consisted of all remaining in situ data. In order to assess the validity and performance of the new algorithms, each satellite chlorophyll product was reprocessed using our newly developed algorithms and then compared against the validation data set.

3. Results

3.1. Initial Comparison of Satellite Estimates to In Situ Data

[19] Our in situ data set consisted of 1388 in situ HPLC chlorophyll concentrations that ranged from 0 to 3.97 mg m^{-3}, mean = 0.37 mg m^{-3}. The number of successful match ups for each temporal and spatial averaging strategy for SeaWiFS is summarized in Table 1. Case 3 (8 day data and 3 × 3 pixel averaging, Table 1) was subjectively determined as the optimum combination. This choice was based on a marked increase in the number of matches obtained by using 8 day data compared with daily data, and the relatively small difference between 3 pixel averaging and 5 pixel averaging across all products. It was thought that monthly data would average over too much of the seasonal variability. SeaWiFS data products showed the fewest match ups to the in situ data set and GlobColour the most, as can be seen from the increasing density of data points in Figure 1—greater matches to GlobColour were to be to be expected, due to it being a merged satellite data product. All three algorithms showed considerable scatter, systematic underestimation at chlorophyll >0.1 mg m^{-3} and considerably reduced dynamic range when compared to in situ data (Figure 2). There were poor correlation coefficients ($r^2 = 0.25$–0.27), poor slopes (0.23–0.26), and also significant offsets (*y* intercepts = 0.15–0.16 mg m^{-3}) that produced significant overestimates when in situ chlorophyll concentrations were below approximately 0.1 mg m^{-3} (Table 2, left columns of each pair).

[20] Histograms of the log 10 ratio of satellite chlorophyll to in situ chlorophyll show the scatter in a different way (Figure 3). For developing the new algorithms, the

Table 1. Summary, for SeaWiFS, of All Temporal and Spatial Averaging Techniques Trialed During the In Situ to Satellite Chlorophyll Match-Up Process

Case	Temporal Averaging	Pixel Averaging	% Matches[a]	Adjusted r^2
1	Daily	3	10.5%	0.18
2	Daily	5	13.1%	0.28
3	8 Day	3	42.7%	0.27
4	8 Day	5	48.6%	0.30
5	Monthly	3	63.2%	0.29
6	Monthly	5	64.2%	0.31

[a]% Matches represents the proportion of the 1388 in situ data points that matched to coincident satellite data points under each scenario.
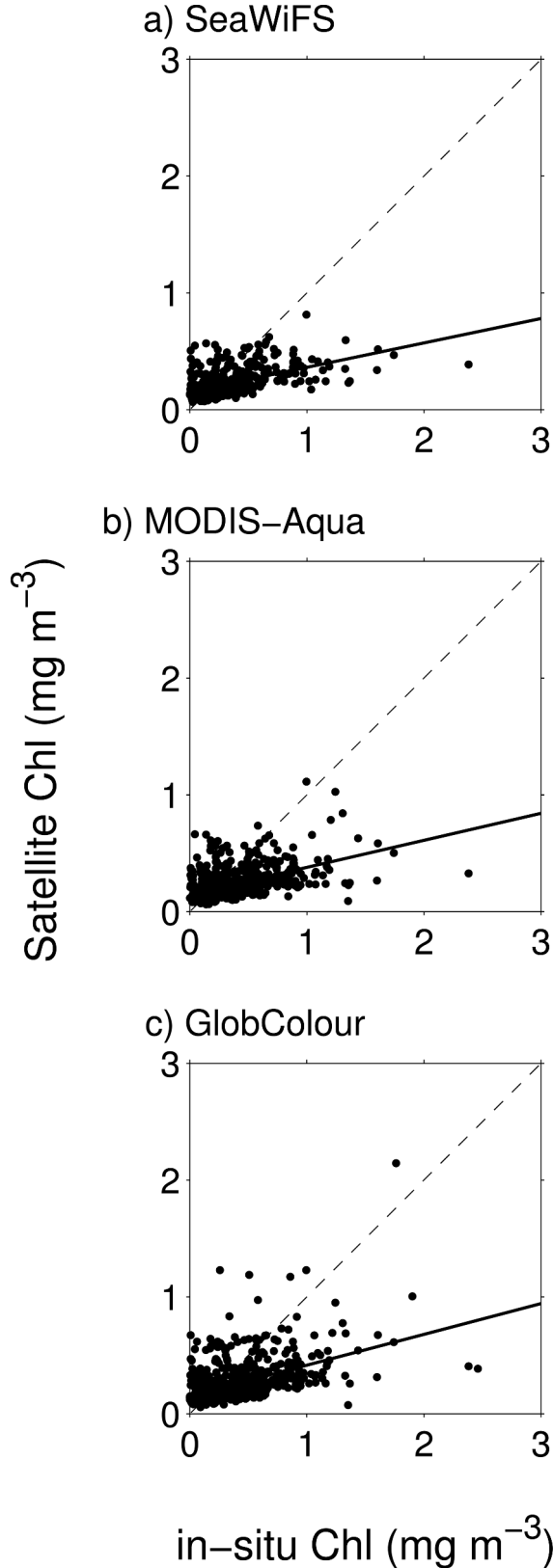
a) SeaWiFS

b) MODIS–Aqua

c) GlobColour

Figure 2. Plot of satellite chlorophyll versus in situ HPLC chlorophyll measurements for each satellite data product: (a) SeaWiFS, (b) MODIS-Aqua, and (c) GlobColour merged data product.

Table 2. Linear Fit Statistics for Both the Original Satellite Chlorophyll Algorithms and the New Optimized Chlorophyll Algorithms for Each Satellite Data Product to the Development Data Set

Parameter	SeaWiFS		MODIS-Aqua		GlobColour	
	OC4v6	New	OC3M	New	Original	New
r^2	0.27	0.46	0.26	0.51	0.25	0.50
Slope	0.25	0.76	0.23	0.90	0.26	0.46
y Intercept	0.16	0.13	0.15	0.05	0.15	−0.06
Dynamic range increase		172%		138%		1.3%

scatter (at least partly derived from our relaxed match up criteria) was reduced by only considering data within one standard deviation of the mode of $\log 10(Chl_{sat}/Chl_{insitu})$ for each product. A 20% (134 of 641), 18.1% (128 of 705), and 25% (119 of 464) reduction in match ups was observed for MODIS-Aqua, GlobColour, and SeaWiFS, respectively. The underestimation by current algorithms is evident by the negative mode of all panels in Figure 3. The standard deviation and mode, respectively, were 0.41 and −0.20 mg m^{-3} for SeaWiFS, 0.38 and −0.24 mg m^{-3} for MODIS-Aqua, and 0.39 and −0.42 mg m^{-3} for GlobColour.

3.2. Creating New Models

[21] The relationship between the maximum band ratio and in situ chlorophyll is poorly described by all original algorithms (dashed lines in Figure 4). The original algorithms for all satellite products show an underestimation of up to 1 mg m^{-3} (see slopes <1 in Figure 2). The original MODIS-Aqua algorithm did not describe the maximum band ratio to chlorophyll relationship well enough to use as an optimization starting point and this is illustrated by the fact that the dashed line for the original algorithm barely intersects the data in Figure 4b. The new chlorophyll algorithms are presented below and as solid lines in Figure 4, and their performance against the in situ data set is described in Table 2 and Figure 5.

[22] SeaWiFS:

$$Chl_{SW} = 10^{\left(0.6736 - 2.0714 R_{SW} - 0.4939 R^2_{SW} + 0.4756 R^3_{SW}\right)}$$
$$R_{SW} = \log 10\left(Rrs_{(443/555)} > Rrs_{(490/555)} > Rrs_{(510/555)}\right) \quad (4)$$

[23] MODIS-Aqua:

$$Chl_{MA} = 10^{\left(0.6994 - 2.0384 R_{MA} - 0.4656 R^2_{MA} + 0.4337 R^3_{MA}\right)}$$
$$R_{MA} = \log 10\left(Rrs_{(443/555)} > Rrs_{(490/555)}\right) \quad (5)$$

[24] GlobColour:

$$Chl_{GC} = 10^{\left(0.3205 - 2.9139 R_{GC} + 8.7428 R^2_{GC} - 16.1811 R^3_{GC} + 9.0051 R^4_{GC}\right)}$$
$$R_{GC} = \log 10\left(Rrs_{(443/555)} > Rrs_{(490/555)} > Rrs_{(510/555)}\right) \quad (6)$$

[25] The optimization and data refinement process improved the fit (r^2) of all chlorophyll algorithms: Sea-WiFS from 0.27 to 0.46, MODIS-Aqua from 0.26 to 0.51, and GlobColour from 0.25 to 0.50 (Table 2). The solid lines in Figures 4 and 5 show that the improved satellite
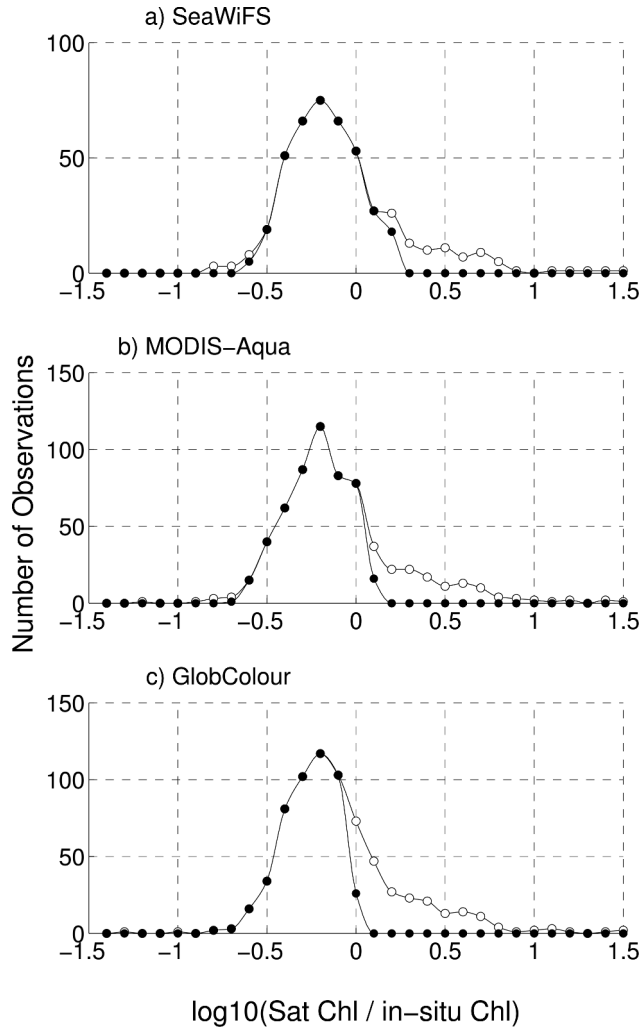
Figure 3. Histograms of the $\log10(Chl_{sat}/Chl_{insitu})$ for each satellite data product: (a) SeaWiFS, (b) MODIS-Aqua, and (c) GlobColour. Open circles represent the full in situ data set, while filled circles show the refined (± 1 standard deviation of the mode of $\log10(Chl_{sat}/Chl_{insitu})$) data set.
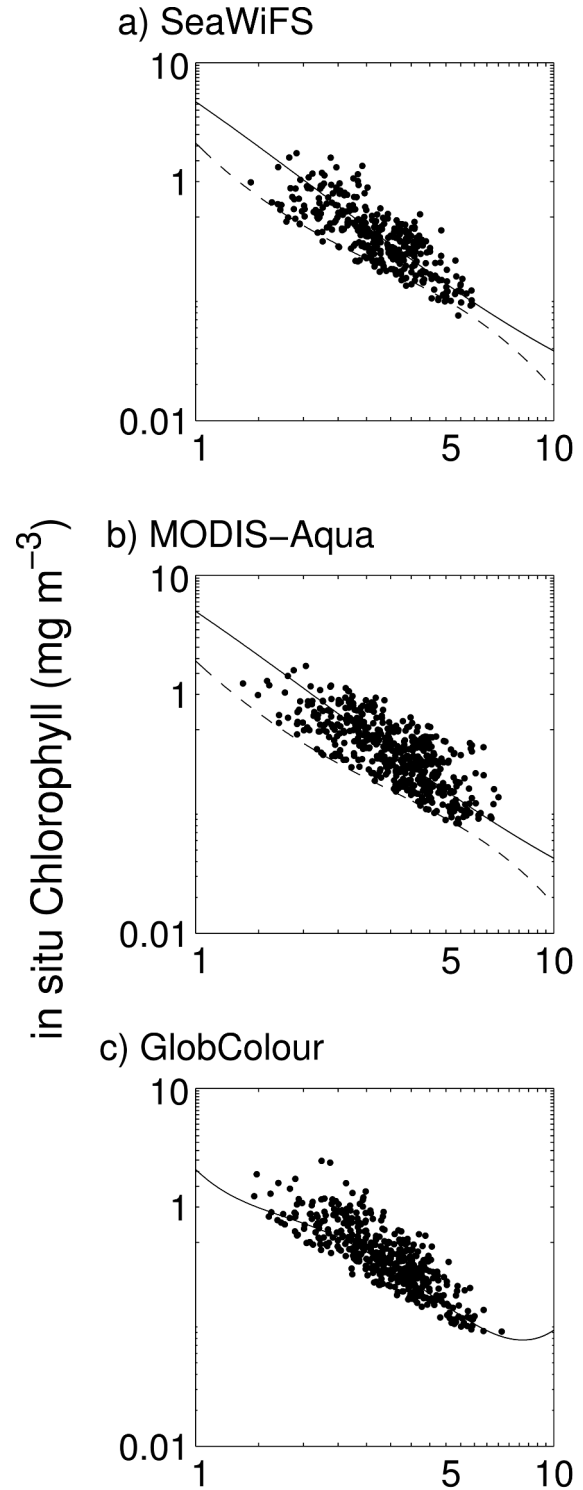
chlorophyll algorithms represent in situ chlorophyll much more accurately than the originals.

3.3. Spatial Anomaly Maps

[26] The spatial distribution of the underestimation by the original algorithms is of considerable importance. Summer climatological comparison maps are presented in Figure 6. These maps represent the difference between the original satellite chlorophyll products and the new algorithms as applied to climatological Austral summer data. There is a general underestimation by the original algorithms throughout the open ocean regions of the Southern Ocean, increasing at higher latitudes. The original MODIS-Aqua and SeaWiFS algorithms showed some isolated regions of overestimation near continental margins during summer (Figure 6).

3.4. Phytoplankton Pigment Contribution

[27] Full HPLC pigment data are available for 94% (1307 of 1388) of the in situ samples used in this analysis.

Figure 4. HPLC in situ chlorophyll measurements versus maximum band ratio of remotely sensed radiance for each satellite data product, with original algorithms presented as dashed lines and new algorithms as solid lines: (a) SeaWiFS, (b) MODIS-Aqua, and (c) GlobColour. Figure 4c has no dashed line as there is no existing empirical chlorophyll algorithm for GlobColour.
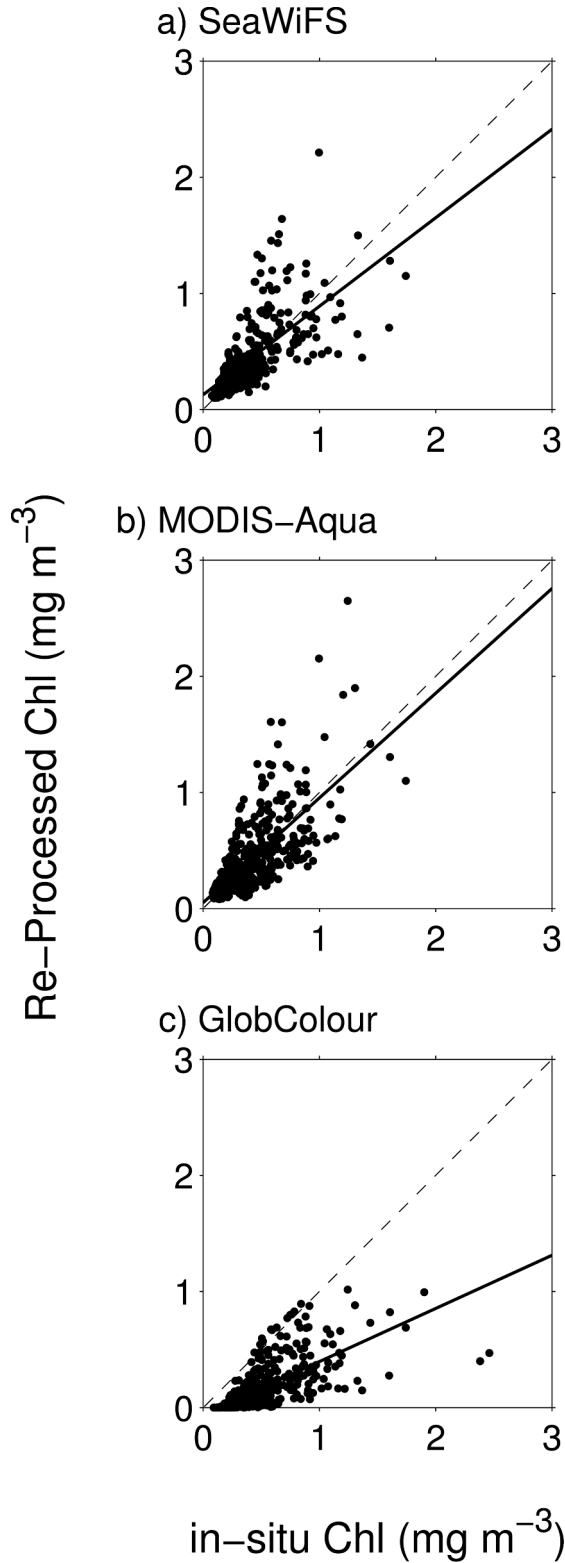
Figure 5. Plot of reprocessed and optimized satellite chlorophyll versus HPLC in situ chlorophyll measurements, for each satellite data product: (a) SeaWiFS, (b) MODIS-Aqua, and (c) GlobColour. Dashed lines represent the 1:1 satellite chlorophyll versus in situ chlorophyll relationship we aimed for in optimization and the solid lines represent the actual obtained satellite chlorophyll versus in situ chlorophyll performance.
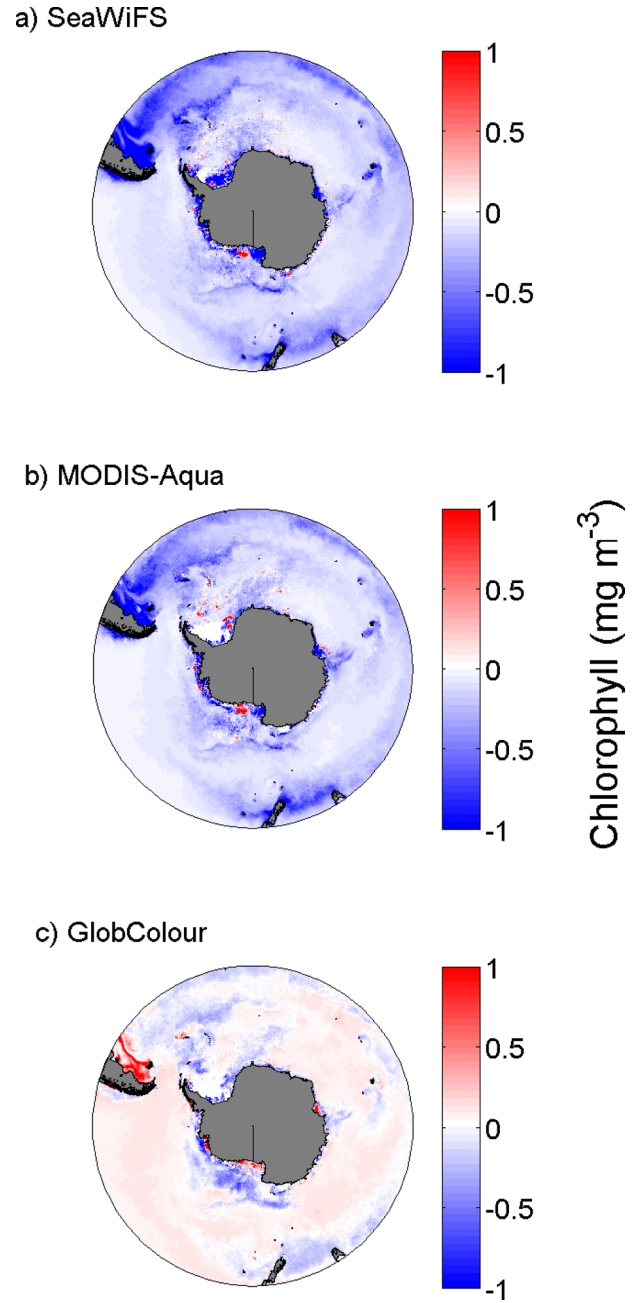

Figure 6. The geographical distribution of the chlorophyll differences (original satellite chlorophyll product minus optimized satellite chlorophyll product) for the Austral summer climatology of each satellite data product: (a) SeaWiFS, (b) MODIS-Aqua, and (c) GlobColour. Negative differences indicate that the original algorithm underestimated chlorophyll relative to the new algorithm.

Figure 7 shows the distribution of the Fp diagnostic pigment index latitudinally across the study region and as function of the original satellite to in situ mismatch. Three distinct community types are present; the northern low Fp community (40–55°S), the middle mixed, variable Fp, community (55–60°S), and the southern high Fp community (60–70°S).
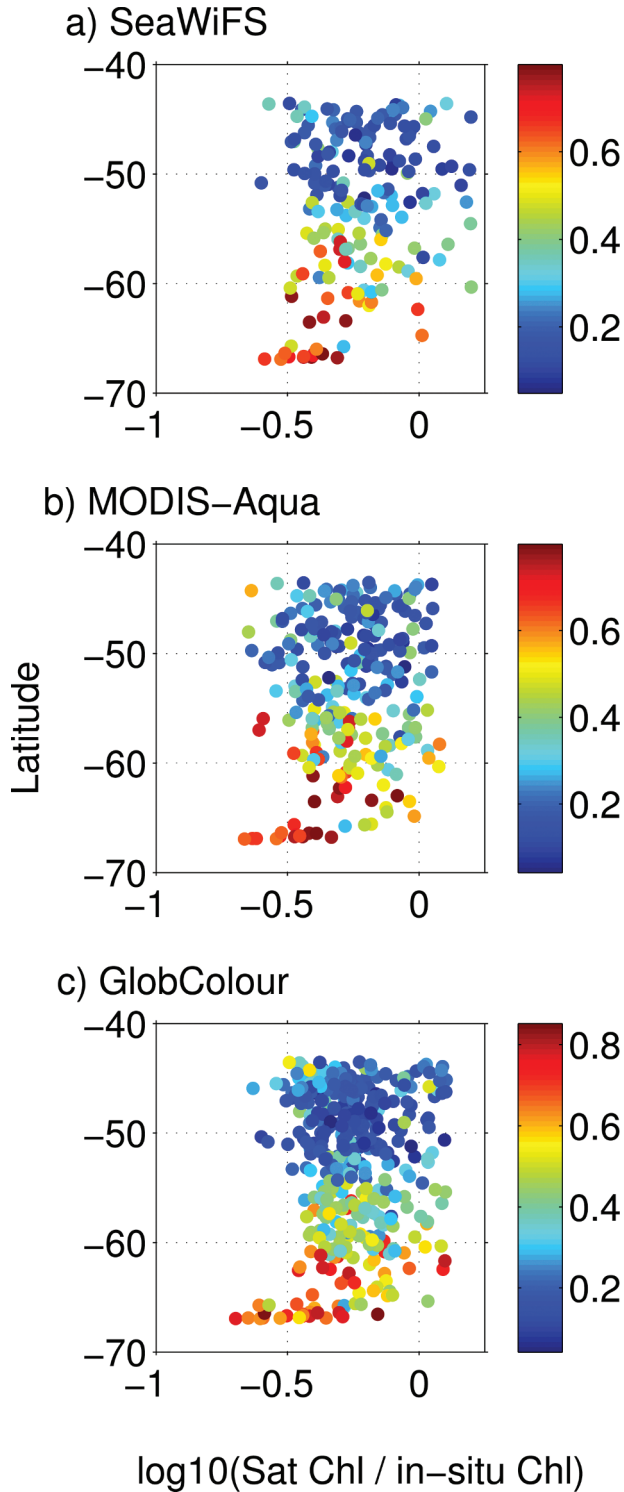
Figure 7. The latitudinal distribution of the log10 ratio of satellite to in situ chlorophyll, from Figure 3 (log10(Chl_{sat}/Chl_{insitu})) colored by the pigment biomarker index Fp for each satellite data product: (a) SeaWiFS, (b) MODIS-Aqua, and (c) GlobColour.
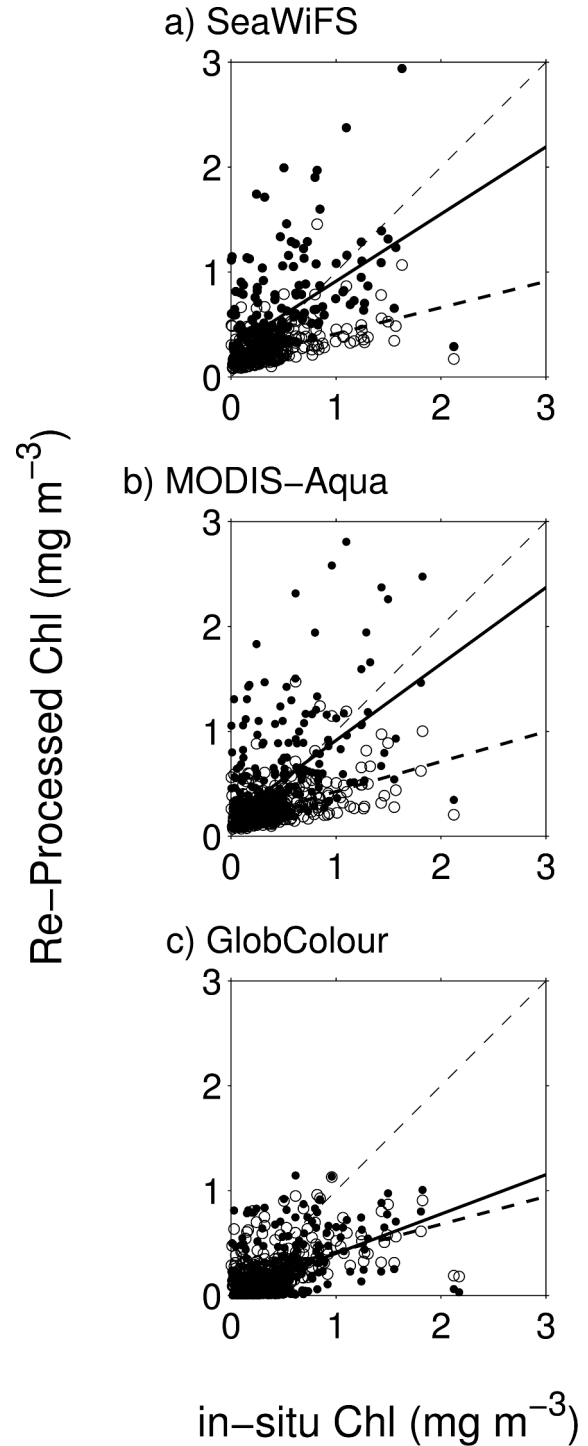
Figure 8. Plot of reprocessed and optimized satellite chlorophyll versus HPLC in situ chlorophyll from the validation data set, for each satellite data product: (a) Sea-WiFS, (b) MODIS-Aqua, and (c) GlobColour. The open circles and dashed lines represent the original satellite chlorophyll product and the filled circles and the solid lines represent the reprocessed version of the same data.

3.5. Independent Evaluation

[28] In order to assess the validity and performance of the new algorithms, each satellite chlorophyll product was reprocessed using the new algorithms and compared against the validation data set (shown in Figure 8 and Table 3). The performance of reprocessed satellite

Table 3. Linear Fit Statistics for the Original Satellite Chlorophyll Algorithms and the New Optimized Chlorophyll Algorithms When Applied to an Independent Data Set for Validation

Parameter	SeaWiFS		MODIS-Aqua		GlobColour	
	OC4v6	New	OC3M	New	Original	New
r^2	0.27	0.29	0.27	0.30	0.28	0.28
Slope	0.25	0.64	0.29	0.73	0.26	0.37
y Intercept	0.16	0.27	0.14	0.18	0.15	0.03
Dynamic Range Increase		38%		114%		1%

chlorophyll to in situ chlorophyll (Figure 8), shows greatly improved slopes, close to those shown in Figure 5, for all products (increases of 0.39, 0.44, and 0.11 for SeaWiFS, MODIS-Aqua, and GlobColour, respectively; shown in Table 3).

4. Discussion

[29] Developing regional algorithms for SeaWiFS, MODIS-Aqua, and GlobColour has improved the ability of each satellite product to represent the true concentration of surface chlorophyll in the Southern Ocean. Current NASA and GlobColour chlorophyll products result in more than a 50% underestimation in our study region (Figure 2).

[30] The high-latitude oceans are characterized by strong seasonality. Blooms dominated by just a few species are not uncommon in summer while growth is limited by (micro-) nutrients or light for the rest of the year [*Bathmann et al.*, 1997]. Species-specific absorption in the 440–570 nm range of wavelengths fluctuates widely enough to cause large taxon-specific differences in chlorophyll retrievals when using the current empirical algorithms [*Stuart et al.*, 2000; *Arrigo et al.*, 1998]. This study is the first to combine a numerically large and spatially widespread in situ sample set to develop robust and reliable algorithms specific for the Southern Ocean. All three chlorophyll algorithms were optimized using similar methods. All three optimized algorithms improved chlorophyll retrievals for the Southern Ocean (Table 2 and Figures 4 and 5), but the new MODIS-Aqua algorithm was by far the best performer with a slope closest to 1.0 and y intercept effectively 0 (Table 2 and Figure 5). The instrument is currently supported and operating for the foreseeable future, unlike the now concluded SeaWiFS and MERIS missions.

[31] Along with improved chlorophyll accuracy, these new regionalized algorithms increased the dynamic range of detectable chlorophyll. The underestimation of chlorophyll by current satellite algorithms in the Southern Ocean compresses the range of chlorophyll that can be detected. This can be seen in Figure 2, where the in situ range of 0–3 mg m^{-3} is represented in a range of less than 0–1 mg m^{-3} by all three algorithms. This >50% reduction in dynamic range severely reduces the resolving power of satellite chlorophyll products, limiting their ability to detect change in both space and time. The correction of the underestimation (i.e., achieving a slope close to 1 for the satellite versus in situ chlorophyll plots) was one of the highest priorities of the optimization process, more so than improving accuracy (increasing r^2). The algorithms described here substan-

tially expand the dynamic range of detection and in the case of MODIS-Aqua by over 130% (Table 2). The ability to correctly capture the dynamic range of Southern Ocean chlorophyll is of fundamental importance when this remotely sensed data is used as validation or initialization for ecosystem models, and when determining large-scale decadal variability and trends in ecosystem dynamics [*Behrenfeld et al.*, 2006; *Arrigo et al.*, 2008].

[32] The ability to resolve change in chlorophyll is affected not only by the algorithm's capacity to estimate chlorophyll but also by the phytoplankton community composition. Satellite chlorophyll algorithms cannot discriminate between the individual species they are observing; they merely measure the community as a whole. Phytoplankton community structure and community physiological states are broadly reflected by community pigment composition [*Higgins et al.*, 2011; *Jeffrey et al.*, 2011]. Unfortunately, there is extensive overlap in pigment composition between phytoplankton species [*Cota et al.*, 2003; *Higgins et al.*, 2011; *Jeffrey et al.*, 2011]. It is with this in mind that a pigment biomarker (Fp) developed by *Claustre* [1994] was invoked to determine the link between satellite algorithm accuracy and phytoplankton community composition.

[33] The ratio of satellite chlorophyll to in situ chlorophyll, which describes performance and therefore underestimation of satellite products, covaries with community pigment composition (Fp) in the Southern Ocean (Figure 7). Low Fp indices typically represent oligotrophic regions, high Fp indices typically represent mesotrophic or eutrophic conditions, and variable or frontal regions are often represented by a highly variable Fp index [*Claustre*, 1994]. High Fp values indicate a phytoplankton community containing high concentrations of diatoms and/or dinoflagellates relative to all other taxa. In our data set, we observed a transition from low Fp (≈ 0.2), oligotrophic conditions at around 45°S, through a mixed frontal zone community (≈ 55–60°S) into a high Fp (≈ 0.8) zone reflecting more eutrophic conditions and diatom/dinoflagellate dominance around 60–70°S. This gradient is associated with some systematic variability in satellite chlorophyll algorithm accuracy. The current ocean color satellite algorithms are most accurate in the frontal zones of 55–60°S, as seen by the $\log 10(Chl_{sat}/Chl_{insitu})$ values grouped closer to zero in Figure 7. North of approximately 50°S the scatter slightly increased, indicating poorer algorithm performance in these oligotrophic communities. The algorithm performance was poorest in the higher latitude diatom dominated region, where retrieval accuracy may have also been impacted by sea ice.

[34] The merging of independent satellite ocean color products, in order to improve spatial and temporal coverage, will improve the detection of change in areas of significant cloud cover, such as the Southern Ocean. GlobColour merges MODIS-Aqua, MERIS, and SeaWiFS chlorophyll products through an error-weighted averaging technique [*Pinnock et al.*, 2007]. For the merged product to be as representative as possible, knowledge of parent sensor errors and biases is very important. The weighted averaging techniques employed by GlobColour are error correcting in nature. They assign lower weight to high variance data during averaging, but inherent biases in the parent products are not

easily dealt with (see discussion in *Durand* [2007] and *Pinnock et al.* [2007]). The effectiveness of any bias compensation that may occur in the GlobColour merging process is diminished in the Southern Ocean. MERIS, which is included in GlobColour, is known to overestimate some nLW bands, especially 413 nm, whereas SeaWiFS and MODIS have a tendency to under estimate. We propose that, for the Southern Ocean, the merging process is compressing the dynamic range of the GlobColour product due to the different biases of the original products. This compression of GlobColour's dynamic range is evident in the maximum band ratio used to calculate chlorophyll in this manuscript. The standard deviation of SeaWiFS and MODIS-Aqua maximum band ratios were 0.97 and 1.11, respectively, whereas GlobColour had almost half the standard deviation (0.53) for a similar range of in situ chlorophyll standard deviation. This compression of variability in the *x* axis of Figure 4c made the curve fitting and optimization procedure more difficult. GlobColour is the poorest performer in the Southern Ocean, and its performance was not significantly improved by optimization (Figures 2 and 5 and Table 2). GlobColour was optimized herein by using merged water-leaving radiance data but a more robust approach, not attempted here, would be to use optimized satellite products, like the improved algorithms developed here for MODIS and SeaWiFS, and then merge the optimized data, according to the GlobColour error weighting, to produce a Southern Ocean specific GlobColour chlorophyll product. Depending on the needs of the user, the increased temporal and spatial coverage of GlobColour may not be justified given the poor accuracy and dynamic range, even after regional optimization.

[35] All algorithms require testing and validation in order to characterize accuracy and performance. As detailed in section 2, the algorithms developed here were produced using two thirds of the available data set but a randomly selected subset was reserved for validation and testing. When validated against this reserved data set, all of our new algorithms showed an improvement on standard chlorophyll products for the Southern Ocean. Figure 8 shows original product performance (open circles) and the same product when reprocessed with the new algorithms (filled circles). All products showed strong improvements in both dynamic range (slope) and correlation (r^2) that are broadly consistent with corresponding results in Figure 5 and Table 2. The new MODIS-Aqua and SeaWiFS algorithms performed particularly well in the validation, with improved final r^2 and dynamic range increases of 0.30 and 114% and 0.29 and 38%, respectively, vindicating their wide-scale application and preferential use over currently available algorithms (Figure 8 and Table 3).

[36] Atmospheric correction is a major source of uncertainty and variability in polar remotely sensed products, mainly due to large solar zenith angle [*Wang*, 2003]. The algorithm optimization process conducted here did not set out to address the issues associated with atmospheric correction but may have indirectly done so. The method described here effectively scales remote sensed reflectance so as to better describe its relationship to chlorophyll in the Southern Ocean and has therefore possibly accounted for, at least in a small way, the variance due to unsuitable or incorrect atmospheric correction. Further work on atmospheric correction at high latitudes is still needed. Improvements in this area will impact the signal-to-noise ratio and spatial coverage of many polar ocean color products [*Wang*, 2003].

[37] Provision of validated Southern Ocean satellite chlorophyll data to the wider scientific community is one of the goals of this work. We do not, however, attempt to blend our improved Southern Ocean chlorophyll with global data. Users who wish to do this are directed to *Moore et al.* [2001, 2009] and *Kahru and Mitchell* [2010]. We have reprocessed the existing SeaWiFS and MODIS-Aqua chlorophyll data sets, and will process data from the latter source on a regular basis as more data become available. These reprocessed Southern Ocean data sets are supported and hosted by Australia's Integrated Marine Observing System (IMOS: http://imos.org.au/) where they are available for download and use.

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