A COMPARISON OF EMPIRICAL ALGORITHMS FOR CHLOROPHYLL CONCENTRATION IN SINGAPORE REGIONAL WATERS

Md. Monirul Islam
Research Fellow
Tropical Marine Science Institute
National University of Singapore
14 Kent Ridge Road, Singapore 119223
Tel: +65 874 4649, Fax: +65 872 4067
E-mail: tmsmmi@nus.edu.sg

Chan Weng Tat
Associate Professor
Department of Civil Engineering
National University of Singapore
10 Kent Ridge Road, Singapore 119260
Tel: +65 874 2576, Fax: +65 779 1635
E-mail: cvecwt@nus.edu.sg

ABSTRACT: The subject of this study is ocean color monitoring of the regional waters around Singapore. Remote sensing reflectance measurements were used to evaluate the performance of several published ocean color chlorophyll algorithms for use with SeaWiFS (Sea-viewing Wide Field-of-view Sensor) data. The radiance-chlorophyll data were assembled from various SeaWiFS images spanning over a one - year period. Using the default chlorophyll algorithm (OC4-v4) used in SeaDAS (SeaWiFS Data Analysis System) as the basis of comparison, the study examined the characteristics of fifteen empirical chlorophyll/pigments algorithms. The results obtained in the study indicated that the chlorophyll-a concentration predictions could be categorized roughly into three regions: the first region ranges from 0.1 to 1 mg/m^3, the second from 1 to 5mg/m^3 and the last region for chlorophyll-a concentrations greater than 5.0 mg/m^3. The algorithms Aiken-C, Aiken-P, CalCOFI-1, OC1a, OC1b, OC2-V2 and OC2-v4 show nominal divergence for the three regions; CalCOFI-2, OC1c, OC1d, OC2 and OC2c show nearly the same profile for the first region, nominal divergence in the second region but show the greatest amount of divergence compared with SeaDAS default chlorophyll concentration calculated by OC4-v4 in the third region. The Morel 4 algorithm shows much higher divergence of chlorophyll concentration for all three regions, whilst CAL-P6 shows nominal deviation for the second and third regions. In the third region, the values estimated by all algorithms show much more deviation from the SeaDAS default values, especially at higher chlorophyll-a concentrations. Aiken-P shows the least root mean square value (0.290691) of the divergence from the SeaDAS default algorithm, followed by OC2-v2 (0.59598), Aiken-C (0.855854), OC2-v4 (0.979607) and so on.

1. INTRODUCTION

Satellite ocean color research began in the late 1970s with the coastal zone color scanner (CZCS) aboard the Nimbus 7 satellite which acquired data from October 1978 to June 1986 (Evans and Gordan, 1994; Acker, 1994). More than a decade after the end of the pioneer coastal zone scanner mission, a new generation of ocean color sensor SeaWiFS has emerged. Since the launch of the SeaWiFS aboard the SeaStar satellite in August 1997 (Chuanmin *et al*., 2000), global ocean color data has been available to scientists on a regular basis. SeaWiFS is superior to the original Coaster Zone Color Scanner (Hovis *et al*., 1980; Chuanmin *et al*., 2000). It has much more higher radiometric sensitivity and additional spectral bands to aid in atmospheric correction and bio-optical applications. This new sensor has more wave bands and higher precision and is designed to avoid some of the limitations of the CZCS (Hooker *et al*., 1993, Kahru and Mitchell, 1999). Satellite ocean color data provides the only practical means for monitoring the spatial and seasonal variation of near surface phytoplankton, information essential for the study of oceanic primary production, global carbon and other biological cycles, as well as for fisheries research. The influence of phytoplankton on the ocean color of seawater has been studied for several decades. It is well understood that chlorophyll-a, the primary photosynthetic pigment in phytoplankton, absorbs relatively more blue and red light then green, and the spectrum of backscattered sunlight or color of ocean water progressively shifts from deep blue to green as the concentration of phytoplankton increases (O,Reilly *et al*, 1998). In this study, SeaWiFS data was used to view the ocean color in the regional seas around Singapore. Data sets were downloaded from NASA Goddard Space Flight Centre and analysed using the SeaDAS software developed by NASA.

We briefly review the fifteen algorithms, derived from two band ratios: band 3 (490nm) and band 5 (555nm) for chlorophyll concentration, and we also present their suitability for operational use compared with the default SeaDAS algorithm. Most of the algorithms were developed by using SeaBAM (SeaWiFS Bio-optical Algorithm Mini-Workshop) and CalCOFI (the California Cooperative Oceanic Fisheries Investigations) data sets (O'Reilly et al., 1998; Kahru and Mitchell, 1999).

2. DATA PREPARATION AND SELECTED ALGORITHMS

2.1 SeaDAS software for data preparation and deriving chlorophyll concentration

SeaWiFS LIA data was collected from NASA. The data files contain the reflectance data obtained for each of the eight SeaWiFS electromagnetic bands. Metadata like time of scanning, position of the scanned areas, characteristic of sensor during the scanning session *etc.* are also included in these files. The large size of each full scene file (70-100 MB) puts a strain on processing time and physical storage space. To alleviate this, only the required portion corresponding to the area of interest was extracted. This area covered the whole of Singapore, part of Malaysia, Sumatra, Straits of Malacca and the South China Sea and is generally between latitude $6\sim-2^{o}$ and longitude $98\sim109^{o}$.

SeaDAS software was used to prepare the SeaWiFS data. The L1A SeaWiFS data only gives the reflectance measurements for each of the eight bands. An atmospheric correction procedure is first carried out to reduce the errors of both the water-leaving radiance and the chlorophyll concentration estimates (Chuanmin *et al*., 2000). Bio-optical algorithms are then employed to create a level 2 end products. There are 176 level 2 products available for selection in the SeaDAS software. Any combination of these 176 products may be selected for output and written to physical files. The output products include 8 bands across 17 radiance categories like normalized water leaving radiance (Lnw), water leaving radiance (Lw), Rayleigh radiance, aerosol radiance, ozone transmittance (sun to ground, and ground to sensor), total oxygen transmittance, *etc*. There are also 40 additional miscellaneous products like chlorophyll concentration (using various algorithms like OC2, OC4-v4, Neural Net Pigment *etc*), pigment concentration (derived from chlorophyll concentration products), sensor and solar zenith, and azimuth angle. One of the products, L2_flags, allows certain flags to be used as masks. Processing is bypassed for masked pixels and the output value is set to zero. This product can be applied for land, sun glint, total radiance greater than the knee value, large sensor zenith angle, clouds, etc.

Using the SeaDAS OC4-v4 algorithm, chlorophyll concentrations were estimated for several images for the selected areas. Similarly, Lwn files for band 3 and band 5 were prepared for the corresponding images.

2.2 Selected Algorithms

Many empirical models, with varying degrees of complexity, have been proposed within the last two decades to relate the backscattering properties observed to the concentration of dissolved substances in the water column. These models may use information in single or multiple bands, and employ different functional forms like the power function, multiple regression hyperbolic, second-order and third-order polynomials, or most commonly the log-transformation. NASA convened a small working group at the SeaWiFS Bio-optical Algorithm Mini-Workshop (SeaBAM) with the goal of identifying suitable algorithms for the estimation of chlorophyll a (C) and chlorophyll a plus phaeo-pigments (C+P) from SeaWiFS data on an operational basis (Fireston and Hooker, 1998; O'Reilly *et al*., 1998). Altogether, fifteen empirical algorithms (Table 1) identified during the workshop, as well as others suggested by S. Maritorena, and Kahru and Mitchell (Kahru and Mitchell, 1999) were evaluated in this study on the area of interest. Some of the algorithms require remote sensing reflectance, Rrs, and others require normalized water leaving radiance, Lwn.

The formulae for Aiken-C, Aiken-P, CalCOFI-1 (two band power), CalCOFI-2 (two band cubic), Morel 2, Morel 4, OC1a, OC1b, OC1c, OC1d, OC2, OC2-v2, OC2c, OC2-v4 and CAL-P6 are shown in Table 1. The Aiken hyperbolic models estimates chlorophyll (C) and the combination of chlorophyll and pigments (C+P) by the combination of a hyperbolic function up to 2 μmL^{-1} with a power function at higher concentrations (Aiken *et al*., 1995) using a 2-band ratio Lwn490/Lwn555. The CalCOFI algorithms were derived from CalCOFI data (Mitchell and Kahru, 1998) and estimate chlorophyll using a power equation of a 2-band ratio Rrs490/Rrs555. The Morel-2 algorithm uses the band ratio Rrs490/Rrs555 and Morel-4 is a cubic polynomial with Rrs490/Rrs555, which was derived from in situ measurements and an updated version of the Morel (Morel 1988) semi analytic model (O'Reilly, 1998). The empirical chlorophyll algorithms OC1a to OC1d and OC2 were tuned to the SeaBAM data.

Table 1. Empirical Algorithms

Algorithm	Type	Equations	Band ratio (R) & Coefficients (a)
Aiken-C	Hyperbolic +power	$C_{21} = \exp(a0 + a1 * \ln(R))$ $C_{23} = (R + a2)/(a3 + a4 * R)$ $C = C_{21}; if\ C < 2.0 mgL^{-1}\ then\ C = C_{23}$	$R = Lwn490/Lwn555$ $a = [0.464, -1.989, -5.29,$ $0.719, -4.23]$
Aiken-P	Hyperbolic +power	$C_{22} = \exp(a0 + a1 * \ln(R))$ $C_{24} = (R + a2)/(a3 + a4 * R), [C + P] = C_{21}$ $If\ [C+P] < 2.0 mgL^{-1}\ then\ [C+P] = C_{24}$	$R = Lwn490/Lwn555$ $a = [0.696, -2.085, -5.29,$ $0.592, -3.48]$
CalCOFI two band	Power	$C = 10^{(a0 + a1 * R)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.444, -2.431]$
CalCOFI two band	Cubic	$C = 10^{(a0 + a1 * R + a2 * R^2 + a3 * R^3)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.450, -2.86, 0.996, -0.3674]$
Morel 2	Power	$C = \exp(a0 + a1 * R)$	$R = \ln(Rrs\ 490/Rrs555)$ $a = [1.077835, -2.542605]$
Morel 4	Cubic	$C = 10^{(a0 + a1 * R + a2 * R^2 + a3 * R^3)}$	$R = \log(Rrs\ 490/Rrs555)$ $a = [1.03117, -2.40134$ $0.3219897, -0.291066]$
OC1a	Power	$C = 10^{(a0 + a1 * R)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.3734, -2.4529]$
OC1b	Geometric	$C = 10^{(a0 + a1 * R)} + a2$	$R = \log(Rrs490/Rrs555)$ $a = [0.3636, -2.350, -0.010]$
OC1c	Quadratic polynomial	$C = 10^{(a0 + a1 * R + a2 * R^2)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.3920, -2.8550, 0.6580]$
OC1d	Cubic polynomial	$C = 10^{(a0 + a1 * R + a2 * R^2 + a3 * R^3)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.3335, -2.9164, 2.4686, -2.5195]$
OC2	Modified cubic polynomial	$C = 10^{(a0 + a1 * R + a2 * R^2 + a3 * R^3)} + a4$	$R = \log(Rrs\ 490/Rrs\ 555)$ $a = [0.341, -3.001, 2.811,$ $-2.041, -0.04]$
OC2-v2	Modified cubic polynomial	$C = 10^{(a0 + a1 * R + a2 * R^2 + a3 * R^3)} + a4$	$R = \log(Rrs\ 490/Rrs\ 555)$ $a = [0.2974, -2.2429, 0.8358$ $-0.0077, -0.0929]$
OC2c	MCP	$C = 10^{(a0 + a1 * R + a2 * R^2 + a3 * R^3)} + a4$	$R = \log(Rrs490/Rrs555)$ $a = [0.341, -3.001, 2.811, 2.041, -.040]$
OC2-v4	MCP	$C = 10^{(a0 + a1 * R + a2 * R^2 + a3 * R^3)} + a4$	$R = \log(Rrs490/Rrs555)$ $a = [0.319, -2.336, 0.879, -.135, -.071]$
CAL-P6	Sixth order polynomial	$C = 10^{(a0 + a1 * R + a2 * R^2 + a3 * R^3 + a4 * R^4 + a5 * R^5 + a6 * R^6)}$	$R = Log(Lwn490/Lwn555)$ $a = [0.565, -2.561, -1.051,$ $-0.294, 5.561, 3.130, -10.816]$

The functions for the algorithms OC1a, OC1b, OC1c, OC1d and OC2 are power, geometric, quadric polynomial, cubic polynomial and modified cubic polynomial, respectively, using the band ratio of Rrs490/Rrs555. The functions for the modified cubic polynomial algorithms OC2, OC2-v2, OC2c and OC2-v4 also use the logarithmic ratio of Rrs490/Rrs555. The OC2 chlorophyll algorithm that is used by the National Aeronautics and Space Administration in the operational processing of SeaWiFS data (Fu *et al*. 1998; Kahru and Mitchell 1999) is more fully described elsewhere (O'Reilly, 1998).
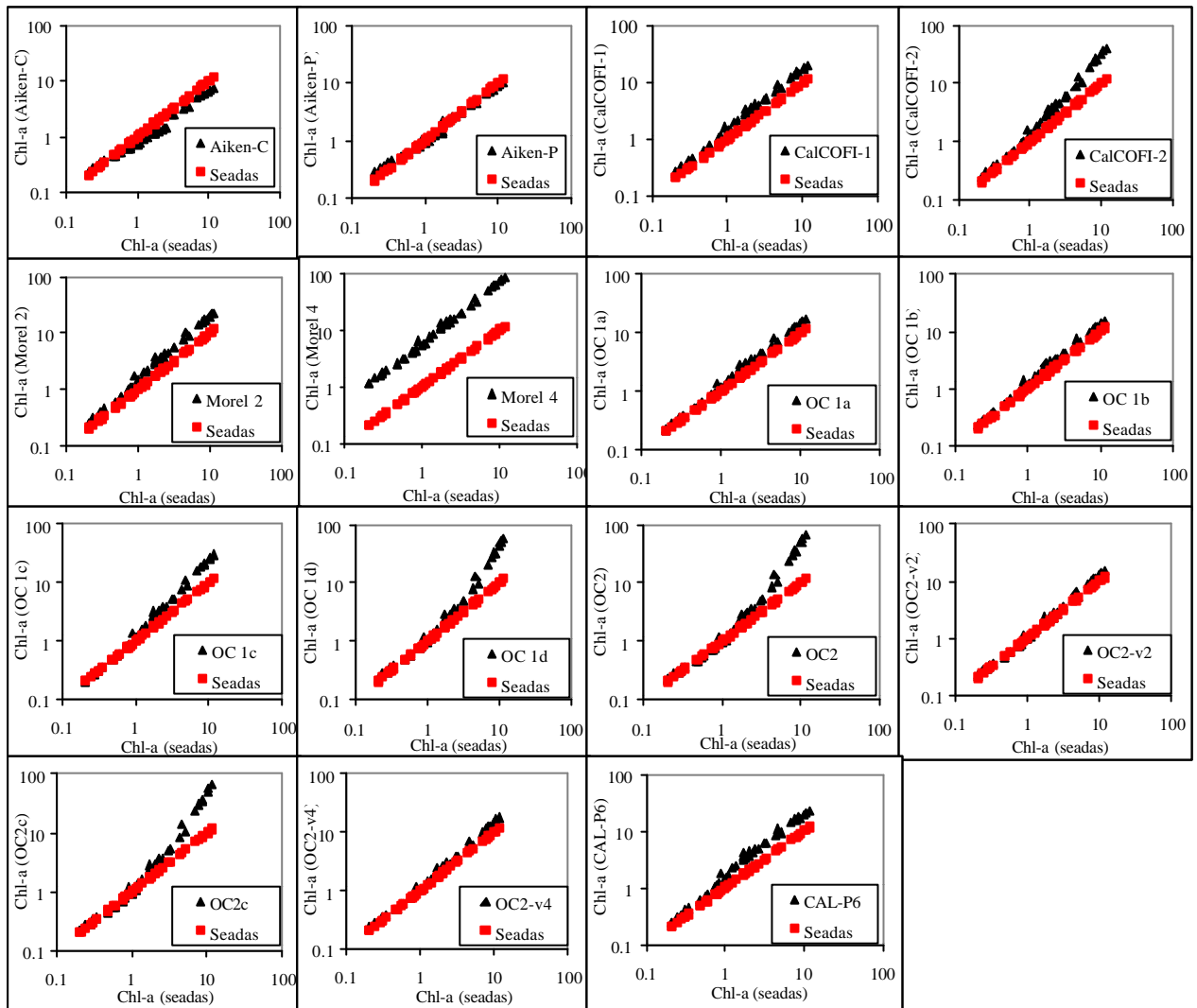
Figure 1. Comparison of chlorophyll-a predictions of selected algorithms vs. default SeaDas algorithm (OC4-v4)

The sigmoid form of the OC2 algorithm is very sensitive to small variations of low Rrs490/Rrs555, producing unrealistically high chlorophyll estimates in cases of high gelbstoff, dertrital and/or accessory pigment absorption. The new algorithm OC2-v2, is similar to OC2 accept for the values of coefficients, which have been chosen to eliminate the dramatic overestimation at high concentrations but accentuates the underestimation in the intermediate chlorophyll range for California current area (Kahru and Mitchell, 1999). The CAL-P6 algorithm, developed by Kahru and Mitchell (1999) uses a sixth-order polynomial and is formulated as a function of the ratio of Lwn490/Lwn555, which corrected the problem with OC2-v2 algorithm in the California current area.

The objective of this paper is present comparisons of the selected empirical algorithms for SeaWiFS data in the regional waters around Singapore. Although no calibration with ground truth data was done for the remote sensing images collected, the study presented lays the foundation for future work in integrating field data collection, remote sensing and numerical modeling for Singapore regional waters.

3. RESULTS AND DISCUSSION

The major focus of this paper is the comparison of the SeaDAS default chlorophyll-a algorithm (OC4-v4) with other developed algorithms which estimate in situ chlorophyll concentration from SeaWiFS. The analyses are based on the data collected from Singapore and its surrounding waters spanning over one year. Differences in data acquisition, methodologies, radiometric design, calibration, data processing and environmental factors are probably responsible for part of the variability observed. Moreover, measurements of chlorophyll concentration may vary with season, location, depth and concentration range of data and the way of pigments were separated and the kind of statistical analyses performed.
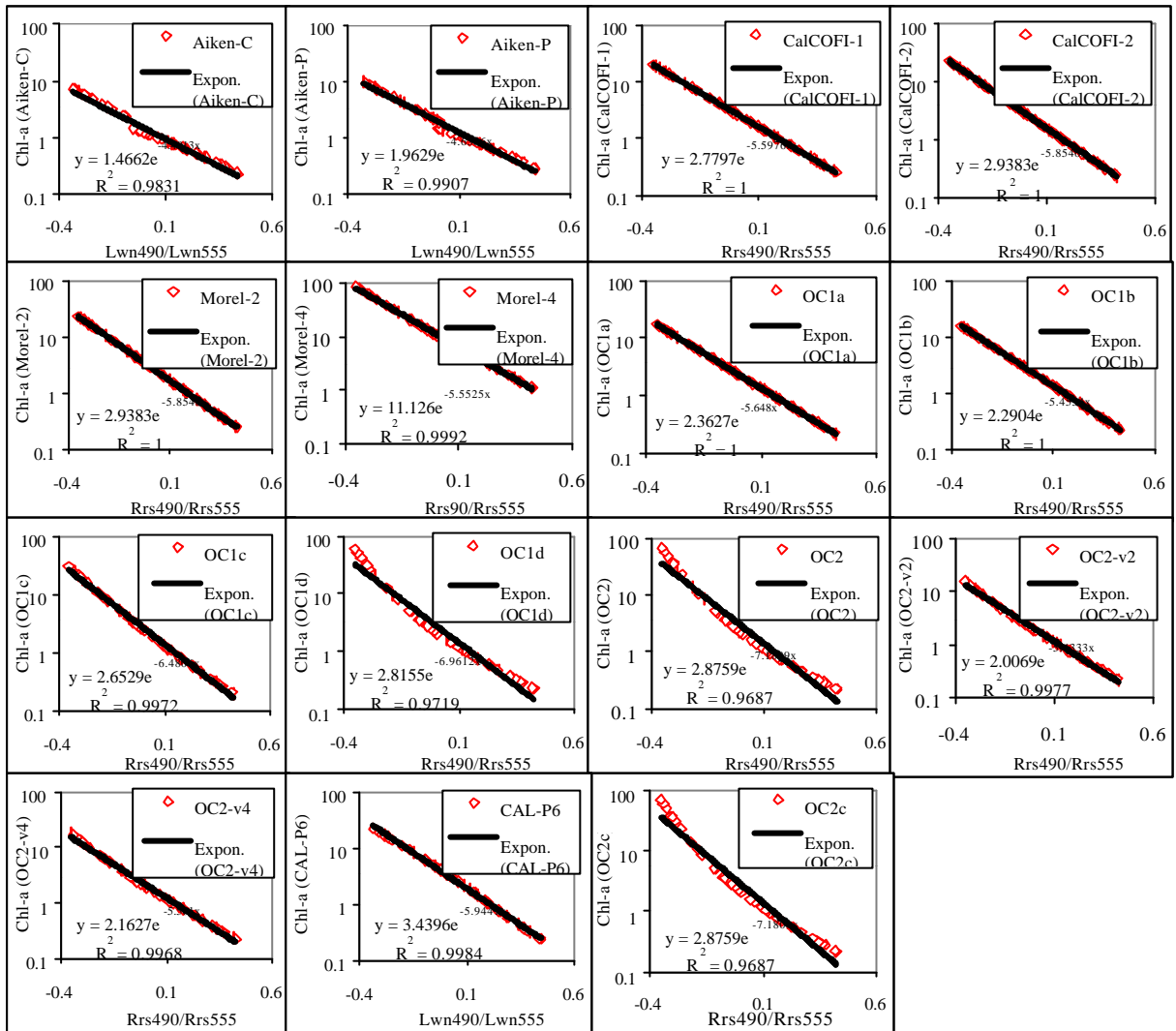
Figure 2. Comparison among the considered algorithms: scattered plots of the measured Chlorophyll concentration (mg/m^3) versus band ratio in logarithmic scale

The algorithms in Table 1 using the 490/555 band ratio were used in this study, because the 490 nm band allows reliable chlorophyll estimation over a wide range of concentrations and statistical results using the 490/555 band ratio were superior to any other two-band combination. The comparison between the results derived from different algorithms and the default SeaDAS chlorophyll-a (OC4-v4) concentrations are shown in Figure 1. The results obtained in the study indicate that the chlorophyll-a concentration predictions could be categorized roughly into three regions: the first region ranges from 0.1 to 1 mg/m^3, the second from 1 to 5mg/m^3 and the last region for chlorophyll-a concentrations greater than 5.0 mg/m^3. The algorithms Aiken-C, Aiken-P, CalCOFI-1, OC1a, OC1b, OC2-V2 and OC2-v4 show nominal divergence for the three regions, and CalCOFI-2, OC1c, OC1d, OC2 and OC2c show nearly the same profile for the first region, nominal divergence for the second region, but a much higher divergence for the third region, from chlorophyll-a concentrations estimated by SeaDAS default algorithm. The Morel 4 algorithm shows much higher divergence for all three regions whilst CAL-P6 shows only nominal divergence for the second and third regions. In the third region, the values estimated by all algorithms show much more divergence from the SeaDAS default values, especially at higher chlorophyll-a concentration level.

To find the algorithm that gives the best fit, root mean square values of the difference between of all the selected algorithms and SeaDAS default algorithm were calculated. Aiken-P shows the smallest root mean square value (0.290691) of divergence from the SeaDAS default algorithm, followed by OC2-v2 (0.59598), Aiken-C (0.855854), OC2-v4 (0.979607) and so on. Therefore, it can be conclude that the Aiken-P algorithm has the best statistical fit with the SeaDAS algorithm for Singapore regional waters.

Figure 2 shows a comparison between the selected algorithms as scatter plots of the estimated chlorophyll using the selected algorithms against the band ratio (Lwn490/Lwn555 or Rrs490/Rrs555). The band ratio

Lwn490/Lwn555 is used in the Aiken-C, Aiken-P and CAL-P6 and Rrs490/Rrs555 algorithms, whilst the band ratio of Rrs490/Rrs555 is used in the other algorithms. Therefore, this figure shows the variation and trend of the deviation and predictability of the selected algorithms. As band 490nm represents the blue-green light wave, an increase in the water leaving radiance means that there is less absorption occurring in the surface water. Similarly, band 555nm represents electromagnetic wave energy in the green light spectrum, and a decrease in the measured radiance in this band represents an increase in the absorption of the wave. Phytoplankton contains chlorophyll and absorbs electromagnetic energy in the blue and red spectrum and reflects in the green. It is reasonable to conclude that a high Lwn or Rrs ratio would correspond to a low concentration of chlorophyll.

This is a preliminary study of the use of SeaWiFS data for ocean color monitoring. Two recommendations are suggested to improve the present study. Firstly, it is obvious that all the algorithm predictions (including the SeaDAS default algorithm for Chlorophyll –a) have to be compared with ground truth data when these become available. Only then will it be possible to establish which algorithm works best for Singapore regional waters. It may be the case that a new algorithm may have to be derived to cater to local conditions. Secondly, change analysis on a set of SeaWiFS images should be performed to detect spatial and temporal trends. Such trend analysis will be central in any long term monitoring effort of chlorophyll concentrations in regional waters of Singapore. As an overall conclusion, remote sensing of ocean color using SeaWiFS satellite would greatly help in future applications of phytoplankton monitoring in regional waters.

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