SeaBAM Algorithm Evaluation

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ABSTRACT

The SeaBAM data set and a variety of statistical and graphical criteria were used to evaluate the performance of two semi-analytical and fifteen empirical chlorophyll/pigment algorithms. The Carder semi-analytical algorithm generally performed better than the Garver/Siegel semi-analytical algorithm. Neither semi-analytical algorithm performed as well as several of the empirical algorithms. The CalCOFI Cubic (Rrs490/Rrs555) and Morel 3 (Rrs443/Rrs555), both cubic polynomials, were generally superior to other empirical algorithms evaluated.

Pigment estimates made with the Gordon switching algorithm (GPs), widely used for the global processing of CZCS, were very highly correlated (R^2=0.923) with *in situ* pigment, and the regression slope of model vs. *in situ* was close to 1. However, the GPs generally underestimated pigment values in the SeaBAM data set (bias = -0.23).

We also devised and evaluated several empirical algorithms which were tuned to the SeaBAM data set to illustrate the relative merits of different formulations, beginning with a simple power regression model and progressively escalating model complexity (number of coefficients) to capture more of the detail in the co-distribution of C and Rrs490/Rrs555. The Ocean Chlorophyll 2 algorithm (OC2), a modified cubic polynomial which uses Rrs490/Rrs555, well simulates (R^2=0.918, RMS=0.172) the sigmoidal distributional pattern between radiance ratios and C. It captures the lowest values of C, where radiance band ratios asymtotically approach the limit expected for clear water. Improved performance (R^2=0.932, RMS=0.156) was obtained using the Ocean Chlorophyll 4 algorithm, a 4-band MCP formulation which uses the greater of Rrs443, Rrs490, Rrs510 in the numerator and Rrs555 in the band ratio denominator. However, additional testing of OC4 is required before it may be considered for use by SeaWiFS.

Finally, two strategies were explored to develop a pigment algorithm from the SeaBAM dataset. Different approaches were required because approximately half of the observations in the SeaBAM dataset lack pigment measurements.

Based on our evaluations and other considerations specific recommendations are made regarding chlorophyll algorithms suitable for use by SeaWiFS and CZCS.

As described in Maritorena *et al.* (This volume) the SeaBAM data set has relatively few C values above 4 ug/l. Therefore, our evaluations of model performance above this value must be considered preliminary, and should be confirmed after more measurements from chlorophyll-rich waters and other areas not well represented in the dataset (e.g. polar waters) are added to the SeaBAM global dataset.

INTRODUCTION

Since the Coastal Zone Color Scanner (CZCS) mission a variety of bio-optical algorithms have been developed to relate measurements of ocean radiance to *in situ* concentrations of phytoplankton pigments. The initial aim of the SeaBAM workshop was to identify which would be the operational SeaWiFS chlorophyll a and pigment [C+P] algorithms. The characteristics such algorithms should have are closely dictated by the objectives they are expected to achieve. One major goal of the SeaWiFS project is to achieve "chlorophyll concentrations to within 35% over the range of 0.05-50.0 mg m^{-3}" (Hooker *et al.* 1992). Thus, the operational SeaWiFS algorithms are expected to encompass accurately a large diversity of bio-optical conditions since they will be used to routinely process data at global scale. It should, however, be kept in mind that the universality of any ocean color algorithm will be limited, in one way or another, since the precision and accuracy of an algorithm designed for studies at global scale may not be adequate for more focused local or regional investigations.

In addition to the identification of algorithms suitable for application to SeaWiFS, the SeaBAM workshop provided an opportunity to evaluate and compare algorithms from past (CZCS), current (OCTS, POLDER) and near future (MODIS) sensors. Therefore, our analysis incorporated algorithms for these other sensors and provides a useful basis for the coming satellite intercomparison studies (SIMBIOS).

During the last decade, various theoretical studies and new parameterizations of some optical properties have yielded better knowledge of the marine light field and provided priceless tools for the modeling of ocean color. The emergence and development of semi-empirical (or semi-analytical) ocean color algorithms derives, at least partly, from these theoretical improvements. Semi-empirical models have the potential to allow the assessment of various optical properties from *in situ* or remotely sensed data. It is noteworthy that it was beyond the scope of the SeaBAM workshop to assess the accuracy of the retrieval of parameters other than chlorophyll a or pigments (e.g. CDOM or backscattering) so the full potential of the semi-analytical algorithms has not been evaluated in this study.

Thanks to the experience acquired with the CZCS sensor, a lot has been learned about Ocean Color empirical algorithms. The strengths and weaknesses of various approaches have already been documented and the following evaluation has been conducted and designed to check for most of the known possible shortcomings or limitations (artifacts caused by switching algorithms, non-linearity, functional form not adapted to describe the actual *in situ* data, etc.).

We used various statistical and graphical methods to check the accuracy, precision, and robustness of the algorithms under evaluation. This chapter describes these methods and the results of our evaluation of 17 semi-analytical and empirical algorithms, and discusses the relative merits of the various algorithm formulations.

METHODS

Algorithms

Two semi-analytic models, Carder (Carder *et al.* ; This volume) and Garver/Siegel (Garver and Siegel; this volume) and 15 empirical models (**Table 1**) were evaluated using the SeaBAM *in situ* dataset Maritorena *et al.* (This volume). The Global Processing (GPs), Clark 3-band, Aiken *et* *al.* Chl *a* (Eq. 21 and 23 in TM 29), Aiken *et al* Pigment (Eq. 22 and 24 in TM 29), CalCOFI 2-band, CalCOFI 4-band, OCTS-C (Chl *a*), OCTS_CP (Pigment), Morel1 and both semi-analytical algorithms were evaluated during the Santa Barbara workshop with an earlier version of the SeaBAM global dataset. Following the workshop, the Carder semi-analytical algorithm has been updated. New coefficients for CalCOFI 2-band and CalCOFI 4-band were submitted to us as well as additional equations: CalCOFI 2-band Cubic, CalCOFI 3-band, POLDER, Morel -2, -3 and -4. This chapter describes the results from the latest versions of each model or equation that were provided to us for evaluation.

Most algorithms tested estimate chlorophyll *a* (hereafter C), but some of them were designed to estimate chlorophyll *a* plus phaeophytin *a* [C+P] hereafter called pigment (Table 1). Measurements of phaeophytin were lacking in 462 of the 919 *in situ* global records. Therefore, for pigment algorithms, the missing in situ pigment data was estimated using a regression equation which relates *in situ* C to pigment. The conversion formula was derived from 2262 pairs of SeaBAM and SEABASS data (Maritorena *et al.* This volume).

Note that the evaluated algorithms required two types of input radiance data: normalized water-leaving radiance (Lwn), and remote sensing reflectance (Rrs). When Lwn was required, Rrs values in the SeaBAM data were converted to Lwn by multiplying the Rrs by the mean extraterrestrial Solar Irradiance corrected for the spectral sensitivity of the relevant sensor (SeaWIFS, POLDER, OCTS).

Most empirical models evaluated require radiance measurements at 555nm, except OCTS C and POLDER, which use the 565nm channel. Two subsets of the SeaBAM dataset, BBO1 and WOCE, had radiance values for 565nm but not for 555nm. For these subsets (n= 142), Rrs555 was estimated from Rrs565 using a conversion equation derived from regression analysis of BBOP *in situ* radiance profiles where concurrent measurements of Rrs555 and Rrs565 were made (Maritorena *et al.* This volume). For the OCTS C and Polder algorithms we used Rrs555 measurements, when the preferred Rrs565 was not available. Similarly, for algorithms requiring 520nm, data from 510nm were used as input to the model when 520nm data were not available, and vice versa. The consequences of these substitutions are described in a later section of this report.

Each of the empirical algorithms was coded using Interactive Data Language (IDL). These computer programs are available from the authors on request and are available on the SeaBAM Home Page.

Statistical and Graphical Evaluation Criteria

We used a variety of statistical and graphical criteria to evaluate the agreement between the various models and *in situ* C. All reported statistics are based on log-transformed data. This was done in part to encompass the several orders-of-magnitude variation in C, because log-transformed C was more normally distributed than un-transformed data (Maritorena et al. this volume), and because evidence is accumulating that C is frequently log-normally distributed (Campbell, 1995). Since the SeaBAM is not a randomly sampled dataset, but instead a deliberate mix of data from a variety of oceanic waters, we would not expect the SeaBAM set to be exactly log-normally distributed.

The first order statistics are the slope and intercept from linear regression of Log-transformed *in situ* and model C. Since it is arbitrary whether *in situ* or model data are assigned to the x or y axis because neither is 'dependent' or 'independent', a Type II (least squares x,y) functional regression model (Reduced Major Axis; Ricker, 1973; Laws and Archie 1981; Press and Teukolsky 1992) was used to compute slope and intercept instead of the Type I (least squares y) model.

The Pearson product-moment correlation coefficient r and the coefficient of determination (R^2) indicate the overall degree of **linear** association between *in situ* and model. For instance, a high R^2 (e.g. >.9) indicates a strong association between variables and provides an estimate of the fraction of total variance explained by the linear regression equation relating model estimates to *in situ* data.

The root mean square error (RMS) provides a useful estimate of the precision between model and *in situ* data. Note, however, that its interpretation is confounded when there is a bias (offset) between measured and model data. The RMS statistic is most useful in comparing precision of several models which, when regressed against *in situ* data, have linear regression slopes and intercepts very near 1 and 0, respectively. The formula for RMS statistic used here is:

$$\mathrm{RMS} = \sqrt{\frac{\sum_{i=1}^{n}\left(\log(Xi_{mod.}) - \log(Xi_{meas.})\right)^2}{n}}$$

where Xi is either C or C+P for station i and n is the number of stations in the Global dataset.

Statistics such as slope, intercept, R^2 and RMS, while providing a numerical summary of model performance, do not indicate non-linear trends, undesirable patterns, or other important features in the relationship between model and *in situ* data. Moreover, these 'bulk' statistics can not indicate model performance over portions of the data range. This is an important aspect in our evaluation since we are interested in assessing model performance throughout a large range in C (0.02-50ug/l). For instance, we note, as others have, that although R^2 may exceed 0.9, very obvious non-linear trends are evident in scatter plots of model vs. measured, such as curvature in the mid-range or tails. Some examples appear in the following sections of our report. Conversely, R^2 may be markedly reduced by a few outliers, in an otherwise highly coherent and co-related distribution of data.

Therefore, several complementary graphical portrayals were used to reveal more detailed information about model performance. These included standard scatter plots of model vs. *in situ*, histograms of the model/*in situ* ratio (not shown), empirical quantile-quantile plots (Chambers *et al.* 1983) , and graphs comparing the relative frequency distributions of *in situ* and model C. Additionally, a graph of the model vs. radiance ratio was constructed for algorithms using two-band radiance ratios.

Scatter plots show all data, and reveal local areas with high or low data density, outliers, and general distributional patterns. However, with large datasets such as SeaBAM, similar values are obscured (overplotting), and non-linear trends may be difficult to discern. The empirical quantile-quantile plot, hereafter abbreviated as qq, reveals this aspect of the data (Chambers *et al.* 1983). The qq plot is useful for making detailed comparisons of the distribution of two datasets because all paired quantiles are plotted and visible, and overall trends are obvious, including non-linear trends or departures from a 1:1 line. The qq plot, when both sets have the same number of observations, as is our case, is simply a plot of the sorted, in situ C against the sorted model C. **Table 2** summarizes the statistical and graphical criteria we used to define a 'good' model. The agreement of the results of the models to these criteria is the basis of this evaluation.

RESULTS: ALGORITHM EVALUATION

The following highlights the major features of the performance of algorithms tested using the SeaBAM global dataset (Maritorena *et al.* This volume). Keep in mind that differences exist among data sets comprising the global dataset, that the global dataset encompasses these differences and therefore has more variability than is present in the individual sets. Consequently, the performance of some algorithms, when subjected to the SeaBAM dataset, may be less than the performance with datasets used by the algorithm developer to tune their algorithms. In order to limit the number of figures, only the results obtained with the Global dataset are presented below. However, it is noteworthy that our analysis also included the results for each of the eleven subsets included in the SeaBAM global dataset.

Semi-Analytic Algorithms

<u>Carder</u>

The Carder model is a semi-analytic algorithm based on the bb/a+bb to Remote-sensing reflectance relationship (Gordon *et al.*, 1988). It uses the remote sensing reflectances at five SeaWIFS wavelengths to derive the absorption coefficient of phytoplankton at 675nm, $a_{ph}(675)$, and the absorption coefficient of colored dissolved organic matter (CDOM) at 400 nm, ag(400). The chlorophyll a concentration is then calculated from an empirical relationship between $a_{ph}(675)$ and chlorophyll a. A default, two-wavelengths empirical algorithm (Rrs490/Rrs555) is used when aph(675) is outside of a predetermined search range (aph675 = .0001 to .06). Complete details of the model are presented in Carder *et al*. (This volume).

When comparing only *in situ* CARD data with model (not shown), there is a high R^2 (0.919), slope close to 1, and intercept close to zero. The model underestimates C (bias=~0.27) for subsets COFI, BBO1,BB02, and AMT. Some Case II waters from Chesapeake Bay are strongly underestimated likely because of low Rrs(443)/Rrs(412) and high Rrs(555)/Rrs(443) values in this dataset. The default band ratio algorithm is used 47 times (~5%), at C values above 2-3ug/l. The scatter plot and the histogram of Log (Model/*in situ*) indicate the model generally underestimates *in situ* C (**Fig. 1**). The qq plot shows that the model approaches *in situ* C between 0.2 and 3ug/l, but underestimates C below and above this range. The modes of the relative frequency distribution of model vs. *in situ* are similar (0.2ug/l) but the model generates relatively more values below 0.1ug/l.

<u>Garver/Siegel</u>

The Garver/Siegel model is a semi-analytic algorithm also based on the bb/a+bb to Rrs relationship but in its quadratic form. The model uses pre-defined shapes for specific absorption and backscattering coefficients to derive the Chl a concentration, the absorption coefficient due to phytoplankton at 441 nm, $a_{ph}(441)$, the absorption coefficient due to other particulate and dissolved matter at 441 nm, $a_{dm}(441)$, and the backscattering coefficient of particles at the same wavelength, $b_{bp}(441)$, (Garver and Siegel, this volume; Garver and Siegel, 1997).

The correlation between model and in situ is quite high ($R^2 = 0.896$); However, this model generally overestimates C in the SeaBAM dataset (**Fig. 1**). There is a strong positive bias (0.269), and the slope between model and in situ is much less than 1 (0.776). This bias is evident in the histogram of Log (Model/*in situ*). The overall shapes in the relative frequency of model and in situ C are similar, except for an offset in the modes. The scatter plot and qq plot indicate congruence between model and in situ at values of ~3ug/l. The algorithm seems to be very sensitive to the model which is chosen for the specific absorption of phytoplankton and the slope of the detrital (particles and dissolved) absorption (see Garver and Siegel, this volume).

Empirical Algorithms

Gordon Global Processing Switching Algorithm (GPs)

Most CZCS-Pigment estimates have been made using the Gordon Global Processing switching bio-optical algorithm (GPs) (Gordon *et al.* 1983; Feldman *et al* 1989; Evans and Gordon 1994,) which uses the ratio Lwn443:Lwn550 at Pigment concentrations below ~1.5 *u*g/l and switches to Lwn520/Lwn550 above 1.5 *u*g/l. The equations relating radiance ratios to Pigment [C+P] for the GPs are provided in **Table 1**). Keep in mind that this algorithm was derived using linear regression of only 49 pairs of log-transformed *in situ* Pigment vs. water-leaving radiance measurements. Pigment computed using GPs is very highly correlated with *in situ* pigment ($R^{2=}$0.927, **Fig. 1**) . The regression slope is near 1 (1.021); however the model significantly underestimates *in situ* pigment (bias=-0.237) except at very low concentrations (0.03ug/l) and between 1.5-7ug/l, when the Lwn520/Lwn550 ratio is used. The relative frequency plot reveals that modal values for GPs and *in situ* coincide but GPs generates a surplus of values below 0.1ug/l and a deficit of values above 2ug/l. The qq plot reveals the overall negative bias in the model, non-linear trends (curvature) at the extremes. The qq plot also reveals a discontinuity at 1.5ug/l (y-axis) resulting from the switch in band ratios used (note that the switching discontinuity is suggested in the scatter plot but is more obvious in the qq plot.) The artifacts generated by the GS algorithm switch (bimodality, frequency discontinuity and consequences on pigment statistics) have been discussed elsewhere (Muller-Karger et al. 1990; Denman and Abbott, 1988; Campbell 1995).

Clark 3-band

The Clark 3-band (C3b) (Muller-Karger *et al.* 1990; D. Clark) avoids band switching and estimates Pigment concentration as a continuous function of normalized water-leaving radiances in three sensor channels (**Table 1**). The benefit of summing the 443 and 520 channels is to compensate for the weakness of the 443 nm band at high pigment concentrations. R^2 (0.907) is lower than GPs. The C3b tends to underestimate pigment except at lowest concentrations (**Fig. 1**). The rf plot indicates that the C3b and *in situ* modes coincide but the C3b generates too many values below 0.07 ug/l and not enough above 2ug/l.

Aiken Hyperbolic Chlorophyll

The Aiken hyperbolic model (A21+23) combines a hyperbolic function (their equation #21) with a power function (their equation #23) to estimate C (Aiken *et al.* 1995). The hyperbolic equation is employed up to 2ug/l; at higher concentrations the model switches to the power function (**Table 1**). Aiken *et al.* (1995) noted that an insufficient number of high chlorophyll values in their calibration dataset prevented them from fitting a single hyperbolic equation to the entire set. The model generates good agreement with *in situ* data between 0.1 and 0.7ug/l; but outside this range the model severely underestimates *in situ* C in the SeaBAM dataset. There is a distinct curvature evident in the scatter and qq plots (**Fig. 2**). Note that only 877 of the 919 points are shown because the model calculated negative C for 42 stations. These stations had Lwn490/Lwn555 ratios larger than 5.29, which is the model parameter set to be the reflectance ratio expected for clear water (essentially no chlorophyll). The use of a larger clear water parameter derived from recent values for the absorption coefficient of sea-water (see below) would reduce the frequency of negative values computed by the model. The qq plot shows a sharp discontinuity in the distribution of C at 2ug/l, the point at which the model switches from the hyperbolic to power equation.

Aiken Hyperbolic Pigment

The Aiken Hyperbolic pigment model (A22+24) is similar in construction to the hyperbolic A21+23 model (**Table 1**) (Aiken *et al.* 1995). In general, comments about the performance of the hyperbolic chlorophyll model apply to the hyperbolic pigment model (not shown).

OCTS C

The OCTS model estimates C using Lwn490, Lwn520, and Lwn565. Our evaluation of this model is only approximate because we substituted Lwn510 for Lwn520 when the former was lacking in the database. The consequences of this substitution are discussed below. R^2 is high (0.895), the slope is slightly greater than 1 (1.065), bias and RMS are low. The qq plot shows a good agreement between modeled and in situ C below 0.2 ug/l but as can be seen on the scatter plot, the dispersion around the 1:1 line is important. The OCTS model overestimates C from 0.3 to 5ug/l and underestimates *in situ* C above ~10ug/l (**Fig. 2**). The qq plot also reveals a large curvilinear trend above 2ug/l; below this value the OCTS model and *in situ* data appear linearly related. The rf plot indicates that the mode for the model coincides with the *in situ* mode.

OCTS P

This OCTS model estimates pigment using three bands: Lwn443, Lwn490, and Lwn520. The use of Lwn520 in the denominator of the band ratio (**Table 1**) represents a departure from the usual practice of using Lwn555, the relatively stable 'hinge' point in spectral distribution of radiance. There is reasonable agreement between model and *in situ* pigment between ~2ug/l and ~8 ug/l, and poor agreement outside this range (**Fig. 2**). The relatively low R^2 (0.817) results from the pronounced curvilinearity evident in the scatter and qq plots.

POLDER

The POLDER algorithm relates a single band ratio (Rrs443/Rrs565) to C via a cubic polynomial regression equation (**Table 1**). Model and *in situ* C are highly correlated (R^2=0.915) and coincide between .04 and 0.2ug/l; outside this range the model overestimates C (**Fig. 2**). The qq plot reveals a non-linear trend below ~0.5ug/l. The dispersion of the modeled data is relatively limited, particularly at low and mid- concentrations. This algorithm uses the 443/565 ratio which is, most of the time, underestimated by the 555 data in the SeaBAM dataset. This may explain part of the observed overestimation (see later section of this chapter).

CalCOFI 2-band

The CalCOFI 2-band relates C to Rrs490/Rrs550 using a power equation (**Table 1**). This model is highly correlated (R^2=0.915) with *in situ* C and the slope is very close to unity. All general statistical parameters are good. There is an overall limited positive bias to the model. However, there is significant overall sigmoid curvature evident in the qq plot (**Fig. 3**). The frequency of modeled C is broadly distributed, relative to *in situ*, particularly in the region bracketing the *in situ* mode; This feature is characteristic of 2-band ratio power equations.

<u>CalCOFI cubic</u>

The CalCOFI 2-band cubic is similar in form to the POLDER: a cubic polynomial regression equation linking Rrs490/Rrs555 to C (**Table 1**). The general performances of this algorithm are good. Model data are highly correlated with *in situ* (R^2=0.918). Overall, model data are slightly positively biased (0.083) and the slope is slightly less than 1 (0.98). The RMS is low (0.190). Relative to the SeaBAM data, the CalCOFI cubic is overestimating C below 0.6, and generating a broader mode in the relative frequency distribution (**Fig. 3**).

<u>CalCOFI 3-band</u>

This equation relates C to Rrs490/Rrs555 and Rrs510/Rrs555 (**Table 1**). Relative to the SeaBAM set, the CalCOFI 3-band generally overestimates *in situ* C (**Fig. 3**). There is a significant bias (0.127) and slope (0.917). Some localized curvature of quantiles occurs between 0.1-0.3ug/l, which may be more related to limitations within the SeaBAM dataset (Rrs520 was substituted for Rrs510 when the former was not available, see later in this chapter) than to characteristics of the model.

<u>CalCOFI 4-band</u>

The functional form of this equation is similar to CalCOFI 3-band, except the CalCOFI 4-band uses Rrs443/Rrs555 and Rrs412/Rrs510 (**Table 1**). This is the only empirical algorithm tested which uses the Rrs412 band. The overall performance is quite similar but somewhat inferior to the CalCOFI 3-band; R^2 and RMS, in particular, are slightly lower and higher, respectively (**Fig. 3**).

<u>Morel 1</u>

The Morel 1 equation relates C to Rrs443/Rrs555 using a power equation (**Table 1**). It is designed for Case I waters only. The overall statistical results are good. The model is well correlated with *in situ* C (R^2=0.917) and has a low bias (0.052) and RMS (0.179). The dispersion of the modeled data is limited at low and mid concentrations, as for the POLDER algorithm. As observed for other power law equations, the qq plot reveals a general sigmoid pattern with the model overestimating low and underestimating high values of C (**Fig. 4**). As in other 2-band power equations, the frequency of modeled C is broadly distributed, relative to *in situ*, particularly in the region bracketing the modal value.

<u>Morel 2</u>

Morel 2 is similar to Morel 1 but uses Rrs490/Rrs550 (**Table 1**). Its overall performance is remarkably similar to CalCOFI 2-band, which also uses Rrs490/Rrs550 (cf **Figs 4, 3**). The major differences are that the Morel 2 algorithm is slightly less biased while the slope of CalCOFI 2-band is nearer to 1. A comparison of Morel 2 and with Morel 1 shows that the distribution of quantiles for 2-band power equations using Rrs443/Rrs555 is more sigmoid than quantiles for Rrs490/Rrs555, but data are more scattered in that later case.

Morel 3

Morel 3 is another example of a cubic polynomial, similar to POLDER in that both use Rrs443/Rrs555. The statistical results are good. The model achieves high R^2 (0.915), small RMS (0.183) and bias (0.058); slope slightly departs from 1 (0.97). The use of 443 channel in the band ratio limits the dispersion of the data, except at high concentrations. The *in situ* mode and low C concentrations are overestimated (cf **Fig 4, 3**). The performance of the Morel 3 is generally better than POLDER since the former has lower bias and a slope closer to 1.0.

Morel 4

Morel 4 is also a cubic polynomial, similar to CalCOFI cubic. Both use Rrs490/Rrs555 for the band ratio. The R^2 for the Morel 4 (0.907) is less than that for CalCOFI cubic (0.918), but the Morel 4 better captures the lowest *in situ* C concentrations (cf. **Fig. 4, 3**). The relative frequency of C estimated by Morel 4 is much broader than *in situ* C, and like the Morel 3, the Morel 4 mode is offset from the *in situ* mode.

The Influence of Wavelength Mismatches (555_565 and 510_520)

As mentioned in the Global Evaluation Dataset chapter (Maritorena *et al.* This volume), the radiometric correction applied to the 565 nm data allows all 919 stations to have 555 or proxy-555 nm Rrs instead of blended 555 and 565 nm data. This adjustment of Rrs565 data provides a better match between input Rrs and SeaWiFS wavelengths and eliminates some noise from the radiometric data. This conversion is particularly important at lowest and highest C concentrations which are of major influence in model evaluation or curve fitting. For example, because at low C concentrations the remote-sensing reflectance at 565 nm is lower than at 555 nm, a substitution of 565 nm for 555nm in the band ratio will overestimate the band ratio and underestimate C. Based on the R = f[bb/(a+bb)] relationship, and the most recent absorption coefficients for pure sea water (Pope & Fry, 1997), bbw values from Smith & Baker (1981), the 443/555 and 490/555 ratios should not exceed 16.53 and 6.13, respectively (or 21.78 and 6.66 for the R = f[bb/a] relation). If not corrected, the use of 565 nm data for the clearest waters in the global dataset yield band ratios higher than that expected for "Clear water."

The problem with the blended 510 and 520 nm data is more complicated because along the C concentration range the Rrs(510)/Rrs(520) ratio is much more variable than the Rrs(555)/Rrs(565) ratio. According to the semi-analytical models of Morel (1988) and Gordon *et al.* (1988), the Rrs(510)/Rrs(520) ratio varies from ~1.32 to ~0.95 as C increases from 0.015 to 7 ug/l (whereas for the same Chla concentration range, the Rrs(555)/Rrs(565) decreases only from ~1.13 to ~0.97). This is illustrated in **Fig. 5**. So, using 510 data in an algorithm which is designed to have 520, or inversely using 520 in an algorithm which needs 510 is likely to affect its performance. This point is also true for algorithms which do not use 555 but use 565 (e.g. OCTS and POLDER). It is noteworthy that these wavelength mismatches are easily and accurately corrected in semi-analytical algorithms by changing model spectral parameters to match input radiance wavelengths.

The following analysis is based on the reflectance ratio predicted by the semi-analytical models of Morel (1988) and Gordon *et al.* (1988). These predict the irradiance reflectance (Morel) or the remote-sensing reflectance (through the R/Q term in Gordon *et al.*) for a given pigment concentration in Case I waters. Dealing with the above mentioned band ratios, the agreement between the two models is fairly good between 0.01--~7 ug C/l (see **Fig. 5**). At higher concentrations the behavior of the two models diverges. It is beyond the scope of this analysis to determine how radiometric quantities actually or theoretically evolve at high concentrations of C; both in-situ measurements and theoretical analyses have limitations in such waters (self-shading, CDOM and terrestrial influence for in-situ measurements, spectral dependence of backscattering at high concentration in models).

The conversion of the 565 nm data to proxy-555 was made because of the good agreement between in-situ measurements and predicted theoretical values and because it concerned only a limited number of stations over a limited range in C concentration. Some of these conditions are no longer fulfilled for other possible corrections. Converting data on the only basis of model predicted ratio values did not appear desirable at that stage. This is why the algorithms were evaluated without any further data conversions. We considered that it was better to assess the impact of using wrong wavelengths (based on model predicted values) in an a posteriori analysis. Actually, only 7 of the 18 algorithms are affected by the wavelength mismatching of some of the stations in the Global dataset, namely : Gps, C3b, OCTS_C, OCTS_CP, POLDER, CalCOFI 3-band and CalCOFI 4-band).

In our analysis of the influence of wavelength mismatches, we used Rrs(510)/Rrs(520) and Rrs(555)/Rrs(565) ratios as predicted for the 0.01-50 mg.m-3 C concentration range by the model of Morel (1988). This model was preferred over the model of Gordon *et al.* (1988) because of its more monotonic behaviour at high concentrations. A polynomial fit of both predicted band ratios as a function of C was derived providing an equation to convert any wavelength to its right proxy (i.e. 555 <---> 565 and 510 <---> 520). Data were so converted to the exact wavelengths needed by each algorithm. The results obtained with these corrected data were then compared with those from non-corrected data. It is noteworthy that the method described above remains a crude correction of the data and that its aim is mainly to reduce the noise in the input data. The method is however reasonable for Case I waters at low and mid-range C concentrations (< ~10 mg.m-3). The method is much more questionable for high concentration stations (because of the above mentioned reasons) and Case II waters. Because of the limited number of high concentration and Case II stations, the conversions were applied to them anyway.

A comparison of statistical results before and after wavelength correction is presented in **Table 3**. The wavelength corrections generally yielded improved statistical agreement with in situ C, except for OCTS_CP and GPs. Actually, the GPs algorithm is only affected by the wavelength correction at high concentration when the 520/550 ratio is used to derive the C concentration. As these high concentrations represent a limited number of cases (the algorithm switches in 80 cases over 919), the statistics with the wavelength correction and without it are very similar for the Gordon_sw algorithm. The algorithms which most benefit from wavelength transformations are POLDER, CalCOFI-3, CalCOFI-4, OCTS-C and, to a lesser extent Clark-3b. POLDER algorithm improves in 4 of the 5 statistical parameters, particularly bias and intercept. The major changes are obviously observed in the low and mid-range concentrations with lower predicted concentrations than with the non-transformed data (cf**. Fig. 6,7** with **1,2,3**). This drop in the modeled concentrations at the low end results in an increased slope which is the only parameter which does not improve. Both CalCOFI algorithms improve in all 5 statistical parameters, especially the coefficients of determination (R^2) and RMS. Here again, better results are obtained for the low and mid-range data. The modeled values are less scattered after transformation of the data resulting in lower bias, RMS and better slope. OCTS-C is highly improved in R^2, RMS, intercept, and bias with the best scores of all algorithms in these 2 later parameters. Modeled concentrations are much less noisy along the whole concentration range. The transformed data result in a general drop in the predicted concentrations below ~2 ug/l. Also, the modeled vs. measured distribution tends to get a sigmoid shape. The Clark-3 algorithm is only partially improved by the transformation of the data. The general underestimation observed previously with non-corrected data is now reduced leading to lower bias and RMS. The R^2 is basically the same. The slope departs more from one, probably because of a stronger underestimation of high concentration station when using the transformed data.

These results illustrate part of the impact of using unadapted wavelengths in the models. It is clear that the 7 above mentioned algorithms were disadvantaged in our evaluation.

Comparisons of Algorithm Performance

The SeaBAM dataset and a variety of statistical and graphical criteria were used to evaluate the performance of two semi-analytical and fifteen empirical algorithms. Statistical and graphical results are summarized in Table 4a and 4b. Algorithms are sorted according to their general statistical performances. For each statistical parameter (intercept, slope, etc...), the algorithms were ranked (lowest to highest intercept, slope closest to 1, decreasing R^2). For each algorithm the rank of each statistical parameter is then summed and the algorithms are sorted according to their global rank. Information about non-linearity and discontinuities is also indicated in Table 4a**.**

The Carder semi-analytical algorithm generally performed better than the Garver/Siegel semi-analytical algorithm. Neither semi-analytical algorithm performed as well as several of the empirical algorithms. Using this ordination scheme, the Morel 1, Morel 3, CalCOFI 2-band and CalCOFI Cubic were generally superior to other empirical algorithms evaluated. Adjustment of some of the radiance data to match better the exact wavelengths expected by seven algorithms (GPs, C3b, OCTS_C, OCTS_P, POLDER, CalCOFI 3-band and CalCOFI 4-band) resulted in improved general statistical performance and most of these algorithms achieved higher rank after correction (Table 4b). With these corrections, OCTS_C shifts from the 7th to the 3rd rank with the same score as CalCOFI Cubic. However, it must be keep in mind that if OCTS_C greatly improved in RMS, R^2, bias intercept, the slope is among the highest and there is non-linear trend present in model vs. in situ. The other “radiance-corrected” algorithms did not result in better performance than the top 4 algorithms.

Using this summary of bulk statistical properties, the Morel 1 (power) is slightly better than the Morel 3 cubic polynomial. Similarly, the CalCOFI power is slightly better than the CalCOFI cubic polynomial. However, the graphical results illustrate that the cubic polynomial formulations more closely match the distribution of *in situ* C (qq and rf plots) than do the models based on power equations. Therefore we suggest that, beside any consideration on the wavelengths used, the Morel 3 and CalCOFI cubic polynomial-based algorithms are superior to other algorithms in their overall performance.

Evaluation of Algorithms Tuned to the SeaBAM Dataset

Above, we evaluated a variety of empirical equations relating single or multiple band radiance ratios to C or to pigment. The formulation and complexity of these algorithms varied. Some use single band ratios, others multiple band ratios. The complexity of equations (number of coefficients or parameters) varied from two (power) to four (cubic polynomial). Some insights into the inherent strengths and weaknesses of the various formulations were gained by comparison of algorithms using the SeaBAM dataset. However, because these algorithms were developed and tuned using data which may or may not coincide with mean trends in the SeaBAM global set, it is difficult to use these results to determine which functional equations have the highest potential merit. The following section describes the relative performance of several basic types of empirical equations which were 'tuned' to the global set to achieve a slope of 1 and intercept of 0, maximum R^2 and minimum RMS. This permits a fairer evaluation of the benefits and handicaps of the various functional forms used in empirical algorithms.

Power Equation (OC1a)

The power equation has been widely used to relate radiance ratios to C (e.g. Smith and Baker 1982; Gordon et al. 1983; Mitchell and Holm-Hansen, 1991). In part, its popularity may be due to the relative ease of derivation of model parameters using a simple linear regression of log-transformed data. Despite its simplicity, the power model captures a large fraction of the variation in radiance band ratios and the several orders-of-magnitude variation in C (**Fig. 8**); The R^2 for the power model fit (RMA) to the SeaBAM dataset is quite high (0.915). It is clear however that the power model fits the most frequent, central data but does not fit the extremes well. There is significant overall sigmoid pattern evident in the scatter and qq plots and curvature at the extremes. This pattern actually mirrors the fact that the power equation cannot capture the sigmoid shape of commonly used band ratios vs in situ C in log-log space. Additionally, the relative frequency distribution of model C is much broader than *in situ*. (This pattern also appears in comparisons of frequency distributions between *in situ* pigments and CZCS pigment retrievals based on the power equation).

Geometric (OC1b)

This equation form has not been widely used. Hojerslev (1981) describes an example of a geometric empirical algorithm: C = 54.5 (1 + 2.57*(lw447/lw521))^-3.40 . This functional form does a slightly better job of describing the low end of the C range than the power equation, but like the power, it does not capture the inherent sigmoid pattern evident in plots of band ratios vs. C. Consequently the plot of model C vs. *in situ* C contains a 'residual' sigmoid trend (**Fig. 8**).

Quadratic Polynomial (OC1c)

The fit of this quadratic polynomial (2^{nd} order) to SeaBAM data is illustrated in **figure 8**. The curvature achieved by this model provides for a better match with highest *in situ* C than the power model, but a relatively poorer match with lowest C values.

Cubic Polynomial (OC1d)

During the SeaBAM workshop, we explored an empirical algorithm formulation provided by Dennis Clark (pers. comm.) which is being developed for MODIS. The equation relates log-transformed band ratio (Rrs490/Rrs555) to log-transformed C using a cubic polynomial (3^{rd} order) equation. The POLDER, and CalCOFI 2-band cubic, Morel 3 and Morel 4 use a similar formulation, with either Rrs443 or Rrs490 in the numerator and with Rrs555 or Rrs565 in the denominator of the band ratio (**Table 1**). Our fit of a cubic polynomial equation (OC1d) to SeaBAM data is illustrated in **figure 8**. Overall, this formulation works well. It matches the mode of the *in situ* distribution (relative frequency plots) better than the power, geometric, or quadratic models, but, like these other formulations, it does not well simulate low C concentrations and the frequency distribution of C around the mode of cubic polynomials is still too broad relative to the in situ frequency distribution (**Figure 8**).

Modified Cubic Polynomial ('Ocean Chlorophyll 2')

None of the cubic polynomial models we evaluated fit the low C values very well. Similarly, we were not able to induce the cubic polynomial to capture the lowest C-highest ratios of Rrs490/Rrs555 without compromising the fit elsewhere. Inspection of scatter plots and qq plots for the cubic polynomial fit to SeaBAM (OC1d) suggests that an additional correction term (coefficient) is required which influences the shape of the curve at low C but has little effect at higher concentrations. The resulting equation, tuned to the SeaBAM dataset and named 'Ocean Chlorophyll 2' (OC2), is provided in **Table 1**. C estimated by OC2 is highly correlated (R^2=0.918) with *in situ* C, and the RMS is relatively low, 0.172 (**Fig. 9**). The qq plot illustrates close agreement between model and *in situ* throughout the range of C, and the relative frequency distribution of model and *in situ* C are highly congruent.

This model fits the mid-range of the data as well as the extremes. It captures the inherent sigmoid relationship between Rrs490/Rrs555 band ratio and C, and evident in semi-analytical models such as Gordon *et al.* 1988, and Morel, 1988 (**Fig. 10**) . Gordon *et al.* (1988), in their evaluation of their model against the NET data, suggested a sigmoid shape was superior to the power function (linear in log space). Our empirical fit (OC2) suggests that the sigmoid relationship is not symmetric about a node, but instead asymmetric, with steeper curvature at low C than at high C concentrations (more observations with C above 30 ug/l are required to confirm this). This may indicate an inherent weakness in the hyperbolic formulation, which assumes the sigmoid curve is symmetric. At low C the OC2 asymptotically approaches the expected clear water value (~6.2) for the Rrs490/Rrs555 radiance ratio.

The OC2 requires 5 parameters (constants). If this seems excessive, keep in mind that the Gordon Global Processing algorithm (Switching) uses two power equations (4 coefficients) to estimate chlorophyll. The switch between R443/550 and R520/550 is not smooth; Minimization of switching-related artifacts would likely require additional parameters (e.g. blended weighting of equations, etc.).

Modified Cubic Polynomial ('OC2a')

The Ocean Chlorophyll 2a algorithm (OC2a, Table 1; Fig. 9), a modified cubic polynomial equation tuned to the SeaBAM dataset, uses Rrs443/Rrs555. Its overall performance is just slightly less than the similarly constructed OC2 (Rrs490/Rrs555) algorithm (**Table 4**). However, above 2-3ug/l OC2a estimates of C are more variable than C estimated by OC2 (Fig 9, lower row).

Other Functional Forms

Other band ratios were explored but are not presented here. For example, cubic polynomial equations which use (Rrs443+Rrs490)/Rrs555, or (Rrs443+Rrs490+Rrs510)/Rrs555, or other combinations for the band(s) ratio did not yield improvement over the results described for OC2.

We also explored the use of the polynomial regression model with non-transformed (raw) band ratios vs. C. This approach yielded lower R^2, higher RMS and residual curvilinear patterns in the scatter and qq plots (not shown).

Maximum band ratio ('Ocean Chlorophyll 4')

So far, the Global Processing Switching algorithm (GPs), described above, yields the highest coefficient of determination (R^2=0.927) between *in situ* and model, indicating that its scheme of equations is most effective in capturing the **linear** association between log-transformed radiance combinations and log-transformed *in situ* C. The GPs achieves this largely by switching the band ratio from Lwn443/Lwn550 to Lwn520/Lwn550 and thereby avoiding the relatively lower and noisier 443/555 ratios which characteristically accompany C values exceeding ~1.5ug/l. The strategy behind the GPs is sound and insightful but the switching between power equations leads to the artifacts described above. Note also that the highest overall precision (lowest RMS) between model and in situ C is achieved using Rrs490/Rrs555. However, scatter plots of band ratio vs. C suggest that Rrs443/Rrs555 is more precisely related to C for low values of C and Rrs510/Rrs555 is more precisely related to C at high C concentrations.

With this in mind, along with the well-known shift in the Rrs spectra with increasing C, we investigated a strategy which maximizes the precision of model/*in situ* comparisons by using three band ratios without parameterizing separate equations or terms for each. The functional form for the Ocean Color 4 algorithm (OC4) is a modified cubic polynomial relating a single band ratio to C. The significant departure here is that the single band ratio in the model varies, being determined by whichever ratio, Rrs443/Rrs555, or Rrs490/Rrs555, or Rrs510/Rrs555, is greatest (**Table 1**).

The OC4 yields an R^2 of 0.932 and RMS of 0.156 after tuning to the SeaBAM dataset to achieve a slope of 1.000 and intercept and bias of 0.000 (**Fig. 9, Table 4**). Of the three band ratios considered, Rrs443/Rrs555 was maximal from lowest C to values of approximately 0.3ug/l, Rrs490/Rrs555 dominated between 0.3 and ~1.5ug/l, and Rrs510/Rrs555 dominated when C exceeded approximately 1.5ug/l (**Fig. 11**). Note that the ranges of dominant band ratios overlap by 10-20% so there is a smooth transition from Rrs443/Rrs550 to Rrs490/Rrs555 to Rrs510/Rrs555, with decreasing band ratio (**Fig. 11c**). This is a desirable property of the model as it implies that discontinuities in frequency distributions of C estimated with OC4 are not likely. Additional testing of this aspect is currently conducted.

The OC4 algorithm might serve to define operationally three ocean realms with respect to trophic status: oligotrophic (<0.3ug/l), mesotrophic (0.3-1.5ug/l) and eutrophic (>1.5ug/l), depending on whether radiances in the 443nm, 490nm, or 510nm bands dominate. The scheme parallels that of Antoine *et al.*(1996) who suggest values of 0.1 and 1 ug/l define the limits between oligo- and mesotrophic waters and between meso- and eutrophic waters, respectively.

CONCLUSIONS AND RECCOMMENDATIONS

SeaWiFS Chlorophyll *a* algorithm

The identification of an operational SeaWIFS Chlorophyll *a* algorithm was the main objective of the SeaBAM Workshop and follow-on activities. From the graphical and statistical results presented here it is clear that all of the evaluated algorithms work fairly well, at least in some portions of the Chl *a* concentration range. The algorithm required as the operational equation for SeaWiFS must have minimum bias and errors over the widest possible concentration range and particularly in the low- and mid- range which represent most of the World Ocean waters. The best empirical algorithms evaluated were those using cubic polynomial functions to relate 2-band radiance reflectance ratios to chlorophyll (e.g. Morel 3 and CalCOFI 2-band). This is confirmed in our exploration of algorithms specifically tuned to the SeaBAM dataset. The cubic polynomial algorithms, however, do not simulate adequately low C concentrations, where the radiance ratios asymptotically approach the reflectance ratio expected for 'clear water'. To do this requires an additional model coefficient and results in the 'Modified Cubic Polynomial' formulation (MCP). The MCP simulates the asymmetrical sigmoid pattern evident in plots of band ratios vs. C (in log-log space). Two such 2-band chlorophyll algorithms, OC2 and OC2a, use radiance ratios Rrs490/Rrs555 and Rrs443/Rrs555, respectively. In part because of their formulation and in part because they are specifically tuned to the SeaBAM dataset, OC2 and OC2a give the best statistical and graphical agreement with *in situ* chlorophyll over the entire range of data available in the SeaBAM dataset.

Several algorithms which use more than two bands performed well, notably the OCTS-C, CalCOFI 3 and 4-band and the GPs algorithms, but not as well as the 2-band cubic or 2-band modified cubic polynomial algorithms. Using the SeaBAM dataset we explored several multi-band formulations. Results superior to those using OC2 and OC2a were achieved by the OC4 algorithm, which uses a MCP equation to relate the maximum band ratio (the greater of Rrs443/Rrs555, Rrs490/Rrs555, or Rrs510/Rrs555) to *in situ* chlorophyll. The OC4 capitalizes on the observation that Rrs443/Rrs555, Rrs490/Rrs555, and Rrs510/Rrs555 band ratios provide the greatest precision (and potentially the greatest radiometric sensitivity) at low, mid-range, and high chlorophyll concentrations, respectively. While the performance of the OC4 algorithm is superior to OC2 and OC2a, it seems prudent at that stage to do some more testing to determine if OC4 generates artifacts (e.g. discontinuities resulting from shifts in the dominant band ratio); These additional evaluations are currently underway. Also, from the perspective of on-orbit calibration, the evolution of calibrations in four (or more) channels is more likely to introduce unexpected complications in data processing. For these reasons, a 2-band ratio algorithm such as OC2 or OC2a is initially preferred over multi-band algorithms such as OC4.

Regarding whether OC2 is better than OC2a, there are several issues to consider. First, overall statistical results were slightly higher using OC2 than OC2a. However, at the low- and mid-range, results obtained with the 490/555 ratio (OC2) are generally slightly more scattered around the 1:1 model : *in situ* line than C estimated using 443/555 and OC2a, but the inverse is true at high chlorophyll concentrations. Thus, OC2a might satisfy all needed requirements for the major part of the World Ocean (i.e. at Chl a concentration < ~ 2-3 ug/l). However, while no assessment of the signal to noise ratio or radiometric sensitivity were conducted in the framework of the workshop, it seems unlikely that water-leaving radiances in the 443nm band can be adequately retrieved (with atmospheric correction) by passive ocean color sensors from water with high chlorophyll concentrations such as coastal water or offshore phytoplankton blooms (Gordon (1987). Problems with atmospheric corrections may also affect the use of the 443nm channel (errors in aerosols retrieval) more so than other blue-green bands. Also, in waters with high CDOM concentration, the absorption by gelbstoff would interfere more strongly with the chlorophyll absorption peak at 443 nm than at longer wavelengths (Carder et al., 1989). Based on these findings and considerations **we recommend OC2 as the most robust and suitable chlorophyll algorithm** for global coverage by SeaWiFS at launch. In addition to the satisfying required criteria, OC2 is reversible and conservative.

SeaWiFS Pigment Algorithm [C+P]

There is keen interest in the ocean color community in assessing long term (decadal) changes in phytoplankton pigment, biomass, and primary productivity in the world oceans. The CZCS mission, from 1978-1986 (Yoder 1988; Hooker et al. 1993, McClain, 1993), established a baseline which can be compared with time series developing or anticipated from contemporary ocean color sensors such as OCTS and SeaWiFS. The rationale for a SeaWiFS Pigment algorithm is the generation of a quantity which would be compatible with the pigment product generated during the CZCS mission. CZCS pigment was defined as the sum of Chlorophyll *a* + phaeophytin *a* as generally measured by the classical fluorometric methods (Yentsch & Menzel, 1963; Lorenzen & Jeffrey, 1980).

In the SeaBAM data set only 448 of 919 records (49%) had fluorometric measurements of both chlorophyll *a* and phaeophytin *a*. This included observations from 4 of the 11 subsets in the global data set [BBOP(n=133), COFI(n=303), MOCE(n=5), and Canadian Arctic (n=7)]. Consequently, the design of the SeaBAM global data set is less suited for the construction and evaluation of pigment algorithms, particularly at concentration above 1 ug/l, where only 58 stations have both chlorophyll and phaeophytin measurements. Despite these limitations we explored the construction of a SeaWiFS pigment algorithm using two approaches. Each uses the Rrs490/Rrs555 band ratio.

The first approach involved fitting a MCP equation to the 448 pigment measurements available in the SeaBAM dataset. Comparisons between this model, Ocean Pigment 2a (OP2a), and *in situ* data are illustrated in **figure** 12. The correlation between *in situ* and model pigment is high (R^2=0.938) and the RMS is low (0.146) due to the relatively low diversity of data and subsets involved in the regression.

The second algorithm, named ‘OP2’, employs a two step procedure. First, chlorophyll is estimated from Rrs490/Rrs555 with the OC2 algorithm; Then pigment is calculated using a regression equation relating *in situ* pigment to *in situ* chlorophyll (Maritorena *et al.* this volume): **[C+P] = 1.3404*Chla$^{\wedge 0.983}$;** (n = 2262, R^2 = 0.993).

Figure 13 illustrates the relationship between pigment predicted by both models and *in situ* C in the SeaBAM evaluation dataset. Also shown, for comparison, is the relationship between *in situ* C and *in situ* [C+P]. The positive bias between model pigment and *in situ* C indicates that both algorithms globally yield pigment concentrations higher than *in situ* C concentrations. However, when pigment estimated by OP2a is plotted against chlorophyll estimated by OC2, the regression slope is positive, indicating that the chlorophyll component of pigment decreases with increasing chlorophyll concentration. This trend is opposite that observed in large pigment data sets (Morel and Berthon, 1989; Balch *et al.* 1992; Maritorena *et al.* this volume,). These results reflect the relatively limited and probably unrepresentative number of actual pigment observations available in the SeaBAM data set which were used in the regression to derive coefficients in the OP2a MCP equation.

Since there is both methodological (Trees et al. 1985) and natural sources of variability in the relationship between chlorophyll and phaeopigment concentrations, an appealing feature of the OP2 (= OC2 + chlorophyll/pigment relationship) approach to estimate 'pigment' is that it would permit (if required) regional adjustments to the chlorophyll vs. pigment regression coefficients. **Therefore, we prefer the use of OP2 over OP2a to generate a SeaWiFS pigment product.**

However, since it has been demonstrated that fluorometric pheophytin determinations are often contaminated by the presence of other forms of chlorophyll (Lorenzen & Jeffrey, 1980, Vernet & Lorenzen, 1987), the definition of 'pigment' is now confounded and imprecise. Furthermore, it is likely that recent improvements in HPLC technique and new equipment and methods for fluorometric measurements of chlorophyll *a* (e.g. Welschmeyer 1994) will make it increasingly difficult to compare new 'sea truth' chlorophyll data with earlier fluorometric pigment estimates used as 'sea truth' for the CZCS mission. We therefore **recommend that chlorophyll *a*, not pigment, be the standard ocean color satellite product from SeaWiFS and that the common product between past and new ocean color data be Chlorophyll a. This implies that the CZCS data will need to be reprocessed using a suitable chlorophyll algorithm.**

Toward compatibility between past and new ocean color data

The compatibility between products derived from past (CZCS) and new ocean color satellite data (OCTS, SeaWiFS, etc.) embraces various aspects such as sensor characteristics and the way data should be processed. The new ocean color sensors have more channels and there are differences in the center wavelengths of some of these: CZCS channels are centered at 443, 520, and 550, 670, whereas SeaWiFS's are centered at 412nm, 443nm, 490nm, 510nm, 555nm, 670, 765, and 865nm. Because it was originally built for SeaWiFS needs, the SeaBAM global data set is not well designed, in its present state, to develop a CZCS chlorophyll algorithm. Only 236 stations (NABE and EQPAC) have measurements at the first 3 CZCS bands and their representativeness is inadequate to allow the derivation of a global algorithm. As previously indicated in this chapter, Rrs(510) and Rrs(520) are not interchangeable. The correction we applied to estimate Rrs510 from measured Rrs520 illustrates the importance of small wavelength differences (10nm) in empirical model performance, and provides a fairer comparison among algorithms, but such adjustments are coarse and not recommended. Because the conversion of the SeaBAM global data set into a proxy-CZCS band data set would involve major transformations of most of the data we considered that it was unreasonable to do so.

The only CZCS chlorophyll algorithm which can be currently derived from the SeaBAM data set must use 443nm and 555 nm data (accepting the practical equivalence of Rrs550 and Rrs555). The Ocean Chlorophyll 2a algorithm (Table 1; Fig. 9), a modified cubic polynomial equation tuned to the SeaBAM dataset, uses Rrs443/Rrs555. Its overall performance is just slightly less than the similarly constructed OC2 (Rrs490/Rrs555) algorithm (Table 4). From the scatter plots (Fig. 9) it is evident that dispersion (variability) above 2ug/l is higher using OC2a than when using OC2, but below 0.3ug/l, model-in situ variability is slightly greater using OC2. Thus the OC2a algorithm provides one method for processing SeaWiFS and re-processing CZCS data to generate a comparable chlorophyll products.

While appealing on the basis of simplicity, it is not a prerequisite condition that identical sensor band combinations be used for CZCS and SeaWiFS chlorophyll estimates. From an empirical and statistical perspective, the only condition is that algorithms applied to the sensors yield the same accuracy and precision when compared with *in situ* measurements (the precision and sensitivity achieved may not necessarily be comparable due to sensor design differences). For example, in **figure 14** we illustrate the overall comparability of OC2 and OC2a. Chlorophyll estimated by both equations is highly correlated (R^2=0.981), the regression slope is 0.999, and there is insignificant bias (0.000). This suggests that both are well tuned to the SeaBAM dataset and that there is good internal consistency between the two models. Agreement is excellent from lowest C to about 2ug/l and good from 2-10ug/l. OC2a estimates of C above ~10ug/l are relatively greater than OC2 estimates. Therefore, a second method for generating chlorophyll products from CZCS which would be comparable to SeaWiFS chlorophyll is to apply OC2 (490/555) to SeaWiFS and OC2a (443/555) to CZCS.

The use of the simple Rrs(443)/Rrs(555) ratio has well-known limitations at high Chl a concentrations, so the above approaches are unlikely to work well in eutrophic waters. CZCS algorithms which employ radiance data from 443, 520, and 550nm bands are expected to work better, over a large range of C, than those using just the CZCS 443 and 550 bands, as the 520/555 ratio is less noisy than 443/555 at high C concentrations. It is noteworthy that the application of a maximum band ratio scheme such as OC4 to CZCS data would probably result in the appearance of a discontinuity in chlorophyll frequency distributions, because there is little overlap between dominance curves for Rrs443/Rrs555 and Rrs510/Rrs555 (Figure 11c). Other approaches incorporating the CZCS 520 band to achieve better precision at high C concentrations might involve the use of multiple band ratios or other expressions of Rrs443, Rrs520 and Rrs550 radiance data. For example, MCP formulations inspired from the Clark 3-band algorithm (Table 1) have potential merit.

With these considerations in mind, we **tentatively recommend OC2a for generating a chlorophyll product from CZCS which would be comparable to that using OC2 for SeaWiFS, at least for C less than 2-3ug/l**. **We strongly recommend that the SeaBAM data set be expanded to include more concurrent *in situ* measurements of Rrs510, and Rrs520, along with Rrs443, Rrs490, Rrs555 and Rrs565. This would permit the development and evaluation of algorithms suitable for CZCS, SeaWiFS and other sensors such as OCTS.** Data from a set of approximately 300 stations (mostly hyperspectral data), not used in the SeaBAM dataset can potentially meet these requirements and are already available in the SeaBASS archive**.**

Table 2. Statistical and Graphical Criteria for Model Evaluation

<u>Statistical</u>	
Linear Regression Slope:	1 +- 0.01
Linear Regression Intercept:	0 +- 0.01
Bias:	0 +- 0.01
Coefficient of Determination (R^2):	>0.9
RMS:	<0.185
Negative estimates of C by model:	None
<u>Graphical</u>	
Scatter:	Linear distribution
	Few outliers (model:*in situ* >5:1 or <1:5)
	No curvature in tails of distribution
Quantile-Quantile:	Linear distribution
	Data overlap the 1:1 line
	No distributional discontinuities
Histogram Log (model/*in situ*):	Mode centered around 0
	Symmetrical distribution
	Most ratios near 0 (=1:1)
	Low Standard Deviation (<0.185)
	Skewness near 0
Relative Frequency:	Congruency in overall distribution
	Coincident Modes

Table 3. Statistics for algorithms affected by wavelengths mismatches.

Without radiometric correction

Algorithm	N	Intercept	Slope	Rsq	RMS1	Bias
Polder	919	0.249	1.116	0.911	0.266	0.157
OCTS_C	919	0.117	1.065	0.895	0.220	0.080
OCTS_CP	919	-0.225	1.605	0.817	0.691	-0.495
Calcofi_3b	919	0.080	0.917	0.878	0.244	0.127
Calcofi_4	919	0.094	0.913	0.861	0.264	0.144
Gordon_Sw	919	-0.228	1.021	0.927	0.287	-0.237
Clark_3	919	-0.316	0.942	0.907	0.341	-0.290

With radiometric correction

Algorithm	N	Intercept	Slope	Rsq	RMS1	Bias
Polder	919	0.215	1.19	0.921	0.241	0.107
OCTS_C	919	0.054	1.148	0.933	0.190	-0.03
OCTS_CP	919	-0.345	1.750	0.913	0.842	-0.68
Calcofi_3b	919	0.062	0.939	0.908	0.205	0.097
Calcofi_4	919	0.073	0.934	0.900	0.218	0.110
Gordon_Sw	919	-0.239	1.004	0.923	0.292	-0.241
Clark_3	919	-0.306	0.913	0.905	0.323	-0.267

FIGURES

1. Comparisons between model and *in situ* data for Carder, Garver/Siegel, Gordon GPSw, and Clark 3-Band algorithms. Upper row: Scatter plots; Second Row from top: Quantile-Quantile plots; Third row from top: Relative Frequency of Model (thin black line) and *in situ* (thick grey line); Bottom row: Band ratio vs *in situ* C for single band ratio algorithms (plus symbols) and band ratio vs. model (curve). Note, the axes for each row of figures are shown in the first column.
2. Comparisons between model and *in situ* data for Aiken 21+23, OCTS-C, OCTS-P, and POLDER algorithms.
3. Comparisons between model and *in situ* data for CalCOFI 2-band, CalCOFI Cubic, CalCOFI 3-band and CalCOFI 4-band algorithms.
4. Comparisons between *in situ* and model C for Morel 1, Morel 2, Morel 3, and Morel 4 algorithms.
5. Ratios of Rrs510/Rrs520 and Rrs555/Rrs565 predicted from semi-analytical models of Morel (1988) and Gordon *et al.* (1988).
6. Comparisons between *in situ* and model C for Gordon GPSw, Clark 3-Band, OCTS-C, and POLDER algorithms after adjusting some of the radiance data to match the bands expected by the algorithm.
7. Comparisons between *in situ* and model C for CalCOFI 3-band, and CalCOFI 4-band algorithms after adjusting some of the radiance data to match the bands expected by the algorithm.
8. Comparisons between model and *in situ* data for Ocean Chlorophyll 1a (power), Ocean Chlorophyll 1b (geometric), Ocean Chlorophyll 1c (quadratic polynomial) and Ocean Chlorophyll 1d (cubic polynomial) algorithms tuned to the SeaBAM dataset.
9. Comparisons between model and *in situ* data for Ocean Chlorophyll 2 (modified cubic polynomial), Ocean Chlorophyll 2a (modified cubic polynomial), Ocean Chlorophyll 4 (maximum band ratio) , and Ocean Chlorophyll 4 (using actual Rrs510 data; N=854) algorithms tuned to the SeaBAM dataset.
10. Relationship between chlorophyll and Rrs490/Rrs555 for Ocean Chlorophyll 2 empirical (solid curve), and Gordon `88 (dashed curve) and Morel `88 (dotted curve) semi-analytical models. *In situ* Rrs490/Rrs555 vs. *in situ* C (plus symbols). (The aw coefficients used in semi-analytical models are from Pope & Fry (submitted, 1997); bb coefficients are from Baker and Smith 1981).
11. Ocean Chlorophyll 4 algorithm. a) Maximum band ratio vs. *in situ* C; b) Relative frequency of maximum band ratios; c) Cumulative frequency distribution of maximum band ratios Model showing regions of overlap between adjacent maximum band ratios (dotted vertical lines at 0.3 and 1.5 ug/l).
12. Comparisons between model and *in situ* data for Ocean Pigment 2a (modified cubic polynomial) algorithm tuned to the SeaBAM dataset.
13. Comparisons between *in situ* C and *in situ* pigment; Comparisons between model and *in situ* data for algorithms OP2a and OP2 tuned to the SeaBAM dataset; Comparisons between pigment predicted by OP2a and OP2 with chlorophyll estimated using OC2 model.

14. Comparisons between chlorophyll estimated using OC2 vs. OC2a and OC2 vs. OC4.

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