Algorithms for SeaWiFS standard products developed with the CalCOFI bio-optical data set

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Abstract

Funding from NASA's Ocean Biogeochemistry Program and the Goddard Space Flight Center SeaWiFS Project were used to implement an ocean optics program as part of the routine cruises of the California Cooperative Fisheries Investigations (CalCOFI). Since August, 1993, fifteen CalCOFI cruises and two other cruises in the region have been accomplished. Of the CalCOFI cruises, the bio-optical data set has been fully processed, merged and delivered to SeaBASS for thirteen cruises comprising a total of more than 300 stations used in analyses of bio-optical algorithms for SeaWiFS. The profiling instrument consisted of a Biospherical Instruments, Inc. MER 2040/2041 integrated with a CTD, transmissometer and fluorometer. The MER 2040 unit has 13 channels of downwelling irradiance (E_d) and upwelling radiance (L_u) in the range 340-700 nm. The system has been characterized for its spectral and cosine response, and immersion coefficients. A detailed calibration time-series has been maintained to ensure the most accurate set of data for algorithm development. The optical data is complemented by fluorometric pigment data provided by the CalCOFI program. HPLC pigments are available for approximately half of the MER stations. Good correlation has been found between chl-a estimated by the HPLC and the fluorometric methods. The fluorometric data is used for the algorithm analysis presented here. The data have been used to develop algorithms for SeaWiFS standard products including chl-a, "CZCS pigments" (fluorometric chl-a + phaeo) and for K(490). Simple two band ratio empirical algorithms provided the best retrieval of chl-a and K. Multi-band empirical algorithms also perform well but are less robust. Different functional fits, including linear, quadratic or cubic regressions in the log-log space have been investigated in an attempt to best fit the relationships over the dynamic range of the CalCOFI data set (0.05-22.3 mg m^{-3} chl-a). Relationships between spectral K and chl-a suggest that previous K algorithms may have issues related to new estimates of pure water absorption that are lower than previously used values.

Introduction

The Southern California Bight (SCB) region, from San Diego to just north of Point Conception, is a region with one of the longest, most comprehensive time-series of marine observations - the California Cooperative Oceanic Fisheries Investigation (CalCOFI) - which has been jointly sponsored by NOAA, the University of California, and California Fish and Game Department for more than 40 years. SCB is part of the California Current system, a region which has been well studied with respect to its regional optical properties in an effort to develop regional ocean color algorithms (Smith and Baker 1978a, 1978b, Gordon et al. 1983, Mitchell and Kiefer 1988, Sosik and Mitchell 1995). The CalCOFI region encompasses a large dynamic range of coastal and open ocean trophic structure. The optics data have been collected for chl-a concentrations at the surface ranging four orders of magnitude, from 0.05 mg m^{-3} for off-shore stations to 500 mg m^{-3} during a massive red tide bloom at Scripps Pier. The taxonomic composition across the onshore-offshore gradient ranges from a dinoflagellate/diatom dominated coastal community to a pico-plankton dominated community offshore. The offshore region of CalCOFI is typical of the open ocean oligotrophic subtropical gyres with low surface chl-a, a deep chl-a maximum between 100-130 m, and a nutricline between 120-150 m. The current CalCOFI station grid (Fig. 1) has 66 stations. Each cruise approximately 25 of the CalCOFI stations, on average, are suitable for remote sensing reflectance measurements during daylight hours.

Methods

Instruments

An integrated underwater profiling system was used to collect optical data and to characterize the water column. The system includes the following instruments:

- an underwater MER-2040 radiometer (Biospherical Instruments Inc., S/N 8738) measuring depth, downwelling spectral irradiance (E_d) and upwelling radiance (L_u) at the following nominal wavelengths: 340, 380, 395, 412, 443, 455, 490, 510, 532, 555, 570, 665 nm. The E_d block also includes PAR; the L_u block includes natural fluorescence;
    - a 25 cm transmissometer (SeaTech Inc.);
    - a fluorometer (Wetlabs Inc.);
    - a conductivity and temperature probe (Sea-Bird Electronics Inc.);
- a deck radiometer MER2041 (Biospherical Instruments Inc., S/N 8739) measuring downwelling irradiance at the following nominal wavelengths: 340, 380, 395, 412, 443, 490, 510, 555, 570, 665, 780, 875 nm, PAR.

The underwater instrumentation was integrated onto a stainless steel frame. Power was provided to all systems via the MER 2040, and data from all instruments was multiplexed through the MER 2040 for transmission to the surface using submarine 3-conductor cable on an oceanographic winch equipped with a slip ring. Data from the underwater unit and the deck MER 2041 were merged using Biospherical Instruments software.

Instrument characterization and radiometric calibrations

The MER 2040/2041 system used in this study has had detailed system characterization and radiometric calibration performed by the manufacturer, Biospherical Instruments Inc. (BSI), and the Center for Hydro-Optics and Remote Sensing (CHORS) of the San Diego State University according to procedures specified by the SeaWiFS Protocols (Mueller and Austin 1995). The unit was characterized by CHORS for spectral band pass, and the immersion coefficient and cosine response of the cosine collector (Mueller 1995). A calibration and spectral band characterization was obtained from the University of

California, Santa Barbara, Institute for Computational Earth System Science (UCSB ICESS). The instrument specifications called for band centers within 1 nm of the nominal BSI band center. The reported spectral band centers measured by CHORS differ by more than 1 nm from the BSI nominal band centers for 5 out of 12 channels but 2 of those are SeaWiFS bands. UCSB ICESS found all SeaWiFS bands to be within 1 nm of the BSI nominal band center. The maximum difference found by UCSB is 3.1 nm for the "380" nm channel (Table 1). All data are reported in terms of the "BSI nominal" band centers; the full spectral table from CHORS is available at http://spg.ucsd.edu/~lab/mer. Experimental determinations by BSI and CHORS were in good agreement for cosine response and immersion coefficient for the cosine collector.

Radiometric calibrations of the instrument were performed relative to NIST standard FEL lamps. BSI performed 10 calibrations during the period corresponding to this data set, and CHORS performed 3. The unit was calibrated at BSI, CHORS and ICESS between 5/95 and 11/95. The differences in calibration between BSI and UCSB were within about 1% for E_d and within 2% for L_u whereas slightly higher differences were observed between BSI and CHORS (Figs. 2, 3). Some of the differences in the UV bands may be attributable to the differences in the spectral bandpass characterization (Table 1). Also, lamp energy in the UV is low which causes greater calibration error. Involvement in the SIRREX activities and the multiple calibrations of MER 8738/8739 at different laboratories leads to the conclusion that the overall inter-lab calibrations approach the minimum requirement set by the SeaWiFS protocols (Mueller and Austin 1995) which call for calibration reproducibility of better than 5%. However, the goal of absolute calibration within 1% has not been attained.

Reasonable agreement between BSI calibrations and those of independent laboratories and the fact that most frequent calibrations were from BSI, justified using the BSI calibrations exclusively for determining the calibration time-series for processing CalCOFI data. The experimental immersion coefficients for E_d were provided by CHORS (Mueller 1995). The immersion coefficients for the L_u window were based on the window material refractive index and were changed after cruise CAL9308 when the original window composed of Schott glass UBK7 cracked due to mishandling and was replaced with a quartz glass window which has been used on all subsequent cruises. The radiometric calibration coefficients for each channel of each cruise were found as linear interpolations to the mid-day of each cruise using all calibrations performed at BSI since the instrument was manufactured. Even for channels that are stable over time this procedure of interpolating the time-series is a superior approach to using the most recent calibration since each calibration has analytical error of several percent and some of this is compensated by taking a longer-term statistical fit to the data. For channels with significant trends, a time series fit of the data is essential. An example of the scatter of individual calibration results and the resulting linear interpolation used in the processing of the MER data is shown in Fig. 4. Several channels show significant trends, most notably the L_u (555 nm) channel example shown in Fig. 4, but also the 340 nm channel. Since the E_d (340 nm) channel filter/detector assembly was replaced in June of 1995, a dual linear interpolation was used for this channel.

Profiling procedure

The MER 2040 unit and associated underwater instrumentation were deployed using the ship's stern A-frame on each station in accordance with SeaWiFS bio-optical protocols (Mueller and Austin 1995). When skies were clear, partly cloudy or thinly overcast, the ship was typically oriented with the stern toward the sun to minimize ship shadow. This was not always possible because of winds or sea state, so some casts have significant contamination from ship shadow. The instrumentation was held near the surface for 5-10 minutes prior to starting the down cast to allow for temperature equilibration and to prime the pump for the Sea-bird conductivity and temperature system. Winch speed during the cast was kept between 20-30 m per minute for most profiles, and the nominal sampling speed of the MER was approximately 2-4 Hz. This achieved a typical sampling density of more than 4 samples per meter. The MER unit was generally deployed immediately before or immediately after the CalCOFI water bottle cast to ensure minimal offset in time/space for the optics and the pigment data set. Immediately following each cast a dark scan of the MER radiometer was run by attaching opaque PVC caps on the radiometer heads and recording the data for several minutes. Dark scan records were evaluated and the mean dark scan for each channel provided the basis for setting lower radiometric thresholds (nominally 10 times the dark voltage) for data processing (see below).

Processing of MER vertical profiles

Processing of the CalCOFI bio-optical profiles was done with a modified version of the BBOP data processing system (Siegel et al. 1995). The BBOP system was found most suitable due to its modularity and ease of adding new filters. The BBOP filters operate on the so-called LCD file format that is a self-contained ASCII file with the pertinent header, calibration and processing history included. The implementation of the BBOP processing scheme was adapted and modified in order to increase processing speed, reduce disk access, remove unnecessary complexity, and add a few new filters. The large set of UNIX shell scripts was completely replaced with a single Perl script and the proliferating “list” files were replaced with two control files. Minor modifications were done to the suite of C and C++ programs with the purpose of streamlining the whole process. Some new filters (in C++ and Perl) were added, including one for adjusting the depth of the different variables according to the position of the particular sensor in relation to the depth sensor and another for thresholding low radiance and irradiance values in comparison to the dark values. Some filters were made more versatile, for example the binning filter can now produce vertical bins in any float interval starting from 10 cm instead of integer meters. Vertical bins smaller than 1 m were essential for processing profiles with very high attenuation (e.g. the red tide cruise RED9503) and/or for very shallow water (e.g. off Scripps Pier). The new processing scheme resulted in almost 10 times faster execution speed compared to the original implementation. The speed increase was mostly due to dramatically reduced disk access. Because of the increased speed it was found more convenient to do a full reprocessing starting with the raw data whenever a new calibration was implemented rather than recalculating the LCD files. All source files of the modified BBOP code as well as the executables for IRIX 5.3 are available from ftp://spg.ucsd.edu/pub/bbop.

In order to ensure compatible depth values with the MLRG rosette-CTD system a calibration of the MER depth sensor was performed using linear regression on the depths of a large number of distinct features (e.g. fluorescence maximum, transmission minimum or bottom of the mixed layer) in profiles measured with both systems.

A typical sequence of operations performed with a set of data files collected with the MER 2040/2041 system consisted of three steps: pre-processing, MER data file processing and LCD file post-processing. The preprocessing step creates the necessary control files and is the most time consuming.

Pre-processing

- Preliminary processing either during a cruise or immediately after the cruise with the purpose of creating hard-copy plots of the vertical profiles. The at-sea procedure is run on a PC under Microsoft DOS/Windows and includes transforming the MER binary file into a preliminary LCD file, breaking the LCD file into separate downcast and upcast files and making hard-copy plots of the selected variables.
- Visual inspection of the down- and up-cast profiles, selection of the depth interval for the surface extrapolation, the depth of the surface mixed layer and the best cast (up or down).
- Creation or updating of the general control files (two per cruise) that list the files to be processed, the filters to be run and the information needed in the processing. The auxiliary information includes the corresponding calibration and dark files, date, coordinates, vertical binning interval, depth range for surface extrapolation, mixed layer depth range, interval for calculating K and a quality flag.
- Creation of the calibration files based on the middle date of the cruise and the calibration history of the MER (see section *Instrument Characterization and Radiometric Calibrations*). The calibration files are updated regularly as new calibration data become available.
- Creation of the dark-scan time series for each cruise. The median dark voltages for each channel for each cruise are used to flag the data smaller than 10 times the corresponding dark voltage.

MER processing using BBOP

- Read the raw data and create LCD files (*mer2lcdn*).
- Insert cruise and cast information (*insertcastid*).
- Bin the data to a regularly spaced vertical grid (*mkbin*). For a typical CalCOFI station 1 m binning is used, for shallow profiles and/or surface blooms the interval is reduced to 10, 25, 50 or

75 cm depending on the profiling speed and sampling rate. Break the profile LCD file into separate downcast and upcast files.

- Delete variables with no apparent use (*mkfutil*).
- Calculate salinity and sigma-*t* (*mkh2o*).
- Shift the E_d samples up the number of bins closest to 75 cm (*mkshift*), i.e. 1 bin for 1 m binning interval because depth is measured at the L_u.plane on the MER 2040.
- Delete bins with no samples (*bbopdeflag*).
- Extrapolate some fields to just below the surface, e.g. to the 0^- depth (*mkscalc*). The depth range used for the extrapolation was determined by visual inspection (see Pre-processing) and was recorded in one of the control files. The depth range was the same for all the radiometric channels. The slope of the extrapolation in the log scale is the attenuation coefficient (K) for E_d or L_u.
- Flag values below the corresponding threshold value for each channel (*thresh*).
- Calculate the diffuse attenuation coefficients K for E_d (*mkkc*).
- Extract the surface diffuse attenuation coefficient K from results of *mkscalc* and insert into the surface (0^-) extrapolated record (*ksurf*).

Post-processing

- Import selected depths corresponding to water sample depths and the surface values (at 0^-) into a relational database program (Microsoft Access).
- Run queries within the database, select variables, merge with other cruise data, e.g. the hydrography data from the CalCOFI IEH files, pigment data, absorption spectra of particulate, detrital and soluble material of water samples, produce combined tables for export.

Quality control

- Usually done in IDL (or a spreadsheet) using data exported from the database by plotting various X-Y scatter plots, searching for potential outliers, looking for differences between a particular cruise and previously accumulated data.

For calculating the remote sensing reflectance just above the sea surface $R_{rs}(0^+,\lambda)$ the following equation was used

$$R_{rs}(0^+,\lambda) = 0.54\, L_u(0^-,\lambda)/[1.04\, E_d(0^-,\lambda)] \qquad (1)$$

Here $L_u(0^-,\lambda)$ is the upwelling radiance extrapolated to just below the sea surface, $E_d(0^-,\lambda)$ is the downwelling irradiance extrapolated to just below the sea surface and the coefficients 0.54 and 1.04 are the transfer coefficients of the air-sea interface for, respectively, L_u and E_d (Austin 1974). Calculation of $R_{rs}(0^+,\lambda)$ from the surface irradiance measured by the MER 2041 deck unit $E_s(\lambda)$ was also evaluated:

$$R_{rs}(0^+,\lambda) = 0.54\, L_u(0^-,\lambda) / E_s(\lambda) \qquad (2)$$

While both equations 1 and 2 gave similar results, the variability of equation 2 was higher and the number of stations where equation 2 could be applied was smaller (due to missing MER 2041 data on some cruises). The greater variance when equation 2 was applied is attributed to surface phenomenon such as wave focusing which might affect both E_d and L_u on the 2040, but not E_s on the 2041, and time/space offsets when shadows from clouds or the ship's superstructure affect the above and below water sensors differently. Therefore, equation 1 was used for the analysis reported here.

The surface layer diffuse attenuation coefficients K (λ) were estimated using the depth range that was used to derive the $L_u(0^-,\lambda)$ and $E_d(0^-,\lambda)$] surface extrapolations. For comparison to previous K(490) algorithms and the relationship between K (λ) and K(490), the remote sensing reflectance was transformed to the normalized water leaving radiance as $L_{WN}(\lambda) = R_{rs}(0^+,\lambda)* F_0(\lambda)$ where $F_0(\lambda)$ is the mean extraterrestrial irradiance.

The entire MER data set of $E_d(z, \lambda)$, $L_u(z, \lambda)$, $E_s(\lambda)$ is reprocessed as updated calibration files become available or modifications are found necessary for the control parameters or other processing details.

Water sampling

The general hydrographic data including the fluorometric pigment concentrations for the CalCOFI cruises were collected by the Marine Life Research Group of SIO and were obtained from the CalCOFI data archives (available at http://nemo.ucsd.edu). For the non-CalCOFI cruises (LID9509 and RED9503) these measurements were done by the Scripps Photobiology Group. Water sampling during CalCOFI cruises was done with a CTD-rosette system separate from the MER profiler. The time delay between those two casts was sometimes more than 1 hr. The resulting errors introduced into the matching of MER data to the water samples due to the spatio temporal variability may be significant, especially for coastal stations. No adjustments were made to correct this potential error source.

Pigments

The chl-a and phaeopigment concentrations used here were determined with the fluorometric method (Holm-Hansen et al. 1965, Venrick and Hayward 1984). HPLC measurements of chl-a using the method of Goericke and Repeta (1993) showed a consistent relationship with the fluorometric results (Fig. 5) for surface chl-a in the range 0.05 - 5 mg/m^3. However, the HPLC chl-a estimate is about 82% of the fluorometric chl-a estimate. This difference is in agreement with the findings of Bricaud et al. (1995) but different from Trees et al. (1995) who report a one-to-one (±10%) relationship. HPLC estimates for chl-a are available for approximately half of the optics stations so the fluorometric data were used for algorithm development. More detailed analysis of the HPLC pigments will be presented elsewhere.

Statistical methods

Depending on the variance of a data either the Reduced Major Axis (RMA) Type II linear regression model (Ricker 1973, Laws and Archie 1981) or the "robust" least absolute deviation linear regression (IDL routine LADFIT) was used to compute the linear slope and intercept between variables. The "robust" method is preferable in case of outliers due to various measurement errors. Outliers were usually determined as the points outside 2 standard deviations of the initial "robust" regression. The remaining points were then run through either the RMA or the "robust" linear regression models. The Root Mean Square (RMS) error formula used was the same as that of O'Reilly and Maritorena (1997).

Results

The CalCOFI-2 data set

A total of thirteen CalCOFI cruises were made in the time period 1993-1996, however, only the first eleven were fully processed and included in the CalCOFI-2 data set for the SeaBAM meeting in January, 1997 (Table 2). Out of those 271 stations eleven were identified as "outliers" due to various problems so 260 stations were actually included in the preliminary analysis. Data from two more cruises (CAL9608 and CAL9610) were subsequently added to the CalCOFI-2 data set and brought the total number of coincident MER profiles and surface pigment measurements to 304 (plus the eleven outliers). At the time of the writing of this report, processing and data merger is pending availability of the CalCOFI hydrographic data for the 1997 cruises (CAL9702, CAL9704).

Two non-CalCOFI cruises within a limited subset of the CalCOFI grid area are not included in the data set submitted to SeaBASS at this time. The quality of the LID9509 data suffered from a low MER sampling frequency caused by data errors attributed to a faulty winch slip ring. The data from cruise RED9503 during a massive red tide event off Southern California (Kahru and Mitchell 1997) diverged considerably from the typical CalCOFI conditions and required special processing. The discrepancies can be due to methodological problems such as pigment procedures, instrument shadowing in the highly turbid bloom, or due to fundamentally different bio-optical relationships. Because the red tide data need further quality control they are not included in the generic algorithm development.

The frequency distribution of chl-a in the CalCOFI data set (Fig. 6) deviates from the commonly observed lognormal distribution (e.g. Campbell and O'Reilly 1988) and may be better approximated by a sum of two or more lognormal distributions corresponding to the different regimes (oligotrophic, coastal).

Surface irradiance vs. in-water irradiance

The relationship between $E_d(0^-,\lambda)$ determined by extrapolation to the surface of the MER 2040 underwater profile and $E_s(\lambda)$ measured by the MER deck unit is shown in Fig. 7. The relationships at 412-555 nm have a curvature (demonstrated by the slightly better fits of the power function compared to the linear regression). This may be due to the effect of decreasing transmittance of the air-water interface at large solar zenith angle. For the whole data set, the surface loss of $E_d(z, \lambda)$ through the air-sea interface as estimated by the slope of the linear fit is higher than the often quoted 4% value. For example, the slope coefficients range from 1.07 (at 555 nm) to 1.10 (at 412 and 443 nm). As expected, $E_d(0^-, 665$ nm) data are more noisy as a result of surface extrapolation errors (due to strong attenuation of light at this wavelength) and possible chl-a fluorescence. The slope of less than 1.0 may be partially due to natural fluorescence source terms in the underwater data.

Remote sensing reflectance vs. chl

For a large dynamic range in surface pigments (chl-a from 0.05 to 22.3 mg m^{-3}, chl-a + phaeo from 0.06 to 27.2 mg m^{-3}) the CalCOFI-2 data exhibits a relatively consistent pigment-reflectance relationship for the SeaWiFS bands (Fig. 8). Out of the 304 measurements used for Fig. 8 some were excluded from the final regressions if outside the 2 standard deviation range of the first robust least deviation regression. The number of points outside the 2 standard deviation limits of the regression ranged from 7 at 665 nm to 19 at 510 nm. The reason why relatively few were excluded for the regression at 665 nm compared to other bands was the noisier data at that wavelength resulting in a larger tolerance.

Chl algorithms

When the $R_{rs}(443)/R_{rs}(555)$ and $R_{rs}(490)/R_{rs}(555)$ ratios were plotted against chl-a eleven of the more than 300 stations were qualified as outliers due to various anomalies and are not included in the analysis data set. Some of the anomalies were explained by features like a shallow chl-a maximum at about 10 m that influenced the R_{rs} but was not represented in the surface chl-a sample, high soluble or sediment absorption at some coastal stations, high pigment packaging for some diatom blooms. Others had no obvious explanations. Of the 304 stations included in the CalCOFI-2 data set some surface extrapolated radiometric bands are still suspect, especially at 665 nm. Due to high absorption by water at 665 nm the depth range that could be used for surface extrapolation was restricted to shallower depths that were more contaminated by ship shadow and other near surface effects.

The consistency of the data set including all 304 data points is evident by the high linear correlation between log-transformed chl-a concentration and reflectance ratios (Fig. 9). In the high chl-a range the relationship has a significant curvature especially in the $R_{rs}(443)/R_{rs}(555)$ plot which is not well described by the linear regression model. The relationship between chl-a and $R_{rs}(490)/R_{rs}(555)$ is closer to linear in the log-log space, has less variability, and in general has proven to be one of the most useful ratios in chl-a prediction. This is attributed to three main causes: both detrital and soluble absorption are lower at 490 nm compared to 443 nm, and pigment package effects are less at 490 nm due to weaker total absorption by the phytoplankton. Linear models of both the log-log transformed chl-a or chl-a + phaeo concentrations vs. $R_{rs}(490)/R_{rs}(555)$ (Table 1, equations 3) achieve r^2 of about 0.955 (Fig. 10, upper panel). Although the linear fit in log-log space for the entire data set is practically unbiased (intercept of 0.0 and slope of 1.0), there is systematic underestimation at higher chl-a. A quadratic fit was evaluated but did not bend toward the pure water value at low chl-a (data not presented). A cubic polynomial fit has more parameters to force it to bend towards the pure water value at low chl-a. However, due to the absence of chl-a concentrations less than 0.05 mg m^{-3} the downward bend in the CalCOFI data was insignificant (Fig. 9) and the least squares fit of a cubic polynomial (Table 2, equations 4) curved in the opposite direction. In order to force the model in the correct direction at low chl-a another empirical coefficient was added to the cubic polynomial (Table 2, equations 5), following the Ocean Chlorophyll 2 model (O'Reilly and Maritorena 1997). The resulting model ("CalCOFI Cubic A4") (Fig. 10, lower panel) improves the estimates at both high and low chl-a ranges and reduces the overall RMS error. The sigmoid curvature of the OC2 model of O'Reilly and Maritorena tuned to the global data set seemed to be too strong for the CalCOFI data set and resulted in higher RMS error, 0.129 of the OC2 model vs. 0.101 of the CalCOFI Cubic A4 model. The better fit to the CalCOFI data set of the Cubic A4 model is evident especially in the middle chl-a range of 0.2-3.0 mg m^{-3} (Fig. 9, lower panel). While the exact coefficients of the Cubic A4 model may undergo small changes, as more data becomes available in the high and low chl-a ends, models of the OC2 and CalCOFI Cubic A4 type are preferable to other empirical models that have been tested.

Even with the coefficient of determination between the measured and predicted chl-a above 0.95 there is still a fair degree of variability around the regression line which is even more accentuated in the linear scale instead of the logarithmic scale. If part of the variability is due to accessory pigments, CDOM or other spectrally dependent phenomena, then appropriate additional bands could explain some of the variability and reduce the RMS error of the prediction. To test this hypothesis, multiple linear regressions between two log-transformed R_{rs} ratios and chl-a were evaluated. All possible combinations of the two R_{rs} ratio combinations were run and the combinations with highest r^2 and lowest RMS error were selected. The best combination using three bands is given by equations 6 and the best 4-band combination is given by equations 7 in Table 2. In essence, very little (if any) additional information was gained by including other band ratios besides Rrs490/Rrs555 to estimate chl-a or chl-a + phaeo. Although the 3 and 4 band combinations resulted in a slightly lower RMS error compared to the single linear Rrs490/Rrs555 ratio model, they were inferior to the quadratic and cubic fits of the Rrs490/Rrs555 ratio. Using more than one band ratio may be advantageous in cases of high variability due to instrumental and environmental noise or for quality control. The multi-band empirical algorithms resulted in better predictions for the much noisier CalCOFI-1 data set. However, it appears that the 3- and 4-band models tend to be specific to the particular data set and not robustly applicable to other data sets. As a result, the best combinations of bands changed when more data points were added to the CalCOFI data set. For actual satellite applications, algorithms using more bands will be complicated by the need to know the on-orbit calibration time series of all the bands used. Clearly, simple 2-band algorithms will pose a simpler challenge for maintaining robust algorithms during a satellite mission life. However, the sensitivity of multi-band multiple regression models may be used for screening the data set for possible inconsistencies. In conclusion, it appears that the residual noise is in most part due to methodological errors and environmental variability and not due to other optically significant components that should co-vary with band ratios other than Rrs490/Rrs555 (e.g. accessory pigments, CDOM). Bio-optical measurements at sea have significant variability due to variable illumination conditions, ship shadow, instrument tilt and other methodological effects that cannot be completely eliminated and contribute to the residual RMS error.

With the coefficient of determination (r^2) between the log-transformed variables of a simple R_{rs} ratio model about 0.96 it is unlikely that more advanced bio-optical models can produce a significant improvement. The analyses of O'Reilly and Maritorena (1997) using the global data set containing this conclusion were based on application of semi analytical models to the CalCOFI data set to test chl-a and chl-a + phaeo algorithms. However, advanced models may extend the chl-a range and/or provide additional variables besides chl-a, e.g. CDOM, $a_{ph}(\lambda)$, coccoliths, backscattering coefficient, etc.

K(490) algorithm

Since the work of Jerlov (1976) it has been assumed that the diffuse attenuation coefficient for downwelling irradiance $K_d(\lambda)$ at any wavelength can be expressed as a linear combination of K_d at a reference wavelength (e.g. 490 nm). At low K_d values this is a good approximation. Austin and Petzold (1986) have tabulated the slopes M (λ) from the equation:

$$[K_d(\lambda) - K_w(\lambda)] = M(\lambda)\,[K_d(490) - K_w(490)]. \qquad (8)$$

They used values of K_w that were very close to those of Smith and Baker (1981) or Morel and Prieur (1977). Recently new values of pure water absorption have been determined using an integrating cavity absorption meter (Pope and Fry 1997), and there are some concerns within the ocean optics community that the values of K_w or a_w used in previous literature may be too high, especially between 400-500 nm. For the analysis presented here, values of K_w from Morel (1988) for data between 400-700 nm and from Smith and Baker (1981) for wavelengths below 400 nm were used. A comparison between the CalCOFI-2 data set and the results of Austin and Petzold (1986) are shown in Fig. 11 for the coefficient M indicating good agreement between the CalCOFI data set and theirs, when similar methods were used.

The relationship between chl-a and $K_d(\lambda)$ - $K_w(\lambda)$ has been studied by many investigators (e.g. Baker and Smith 1982, Morel 1988, Mitchell 1992). In Fig. 12 it appears that this relationship is not well described by a linear fit in the log-log space for SeaWiFS wavelengths 412, 443 and 455 nm. Baker and Smith (1982) fit their data with a non-linear function in log space, while Morel (1988) used a power law model (equivalent to linear in the log-log space). Some of the curvature observed between 400-460 nm at low chl-a, which is also observable in the Baker and Smith fit, could be caused by subtraction of K_w that is larger than the true value of K_w. The K vs chl-a and K (λ) vs K(490) relationships should be re-evaluated using modern estimates of the absorption and K for pure water, if the unpublished pure water absorption values proposed by Pope and Fry become generally accepted.

A simple band ratio approach was used to estimate $K_d(490)$ from the normalized water leaving radiance data following the original approach for CZCS (Austin and Petzold 1981). In spite of the high variability at low $K_d(490)$ (Fig. 13), the equation that was obtained by using the "robust" least absolute deviation linear regression

$$K_d(490) – K_W(490) = 0.22 + 10^\wedge(-0.964 – 1.301\ L_{WN}(443)/L_{WN}(555)) \quad (9)$$

is in excellent agreement with the recent estimate of Mueller and Trees (1996). Mueller and Trees concluded that the data set they had compiled (including some CalCOFI data) led to a regression that was significantly different, in a statistical sense, from the regression used for CZCS. This may in part be attributed to the difference between the 550 nm band in CZCS and the 555 nm band used in the this data set and that of Mueller and Trees. The good agreement between Mueller and Trees (1996) and the results presented here indicates that the simple method used here to estimate surface layer K is consistent with the integral least-squares method of Mueller (1991).

The ratio of $L_{WN}(490)/L_{WN}(555)$ instead of $L_{WN}(443)/L_{WN}(555)$ gives a slightly higher r^2 and lower RMS error (Fig. 13, lower panel) and proved more reliable for ocean color applications in cases of very high 443 nm absorption (e.g. in red tide or other blooms or when CDOM in coastal waters is very large). The equation using the $L_{wn}(490)/L_{wn}(555)$ ratio, including data from the RED9503 cruise is given by:

$$K_d(490) = 0.22 + 10^\wedge(-0.813 – 1.636\ L_{WN}(490)/L_{WN}(555)) \quad (10)$$

The improvement using the 490/555 ratio compared to 443/555 is also found for empirical chl-a algorithms (see previous discussions and O’Reilly and Maritorena (this volume). It is recommended that the SeaWiFS Project consider K(490) algorithms based on the 490/555 ratio, and perhaps attempt to assemble a larger global data set for developing a K(490) algorithm. An evaluation of the issues related to the previous methods which may have assumed K_w that are too large should be carried out as well.

Conclusions

An analysis of a set of more than 300 concurrent measurements of remote sensing reflectance, chl-a, and diffuse attenuation coefficients is presented. The CalCOFI data set comprises more than 30% of the total “global” data set that was assembled by the SeaWiFS Project for this effort (Maritorena, et al. 1997). In general, the CalCOFI data set was consistent with the other global data and covered all but the lowest pigment range (chl-a < 0.05 mg m^{-3}). Evaluation of empirical algorithms and semi-analytical models show that simple empirical algorithms perform better than semi-analytical models at this time for SeaWiFS Standard Products including chl-a, chl-a + phaeo and K(490). Relatively little, if any, improvement in estimation is attained by using more complex sets of multi-band ratios for this type of empirical algorithm. Given the added complexity of accurate knowledge of the on-orbit calibration if multiple spectral bands are used, it seems advisable to use the R_{rs} (490)/R_{rs} (555) ratio as a basis for at-launch algorithms for chl-a and chl-a + phaeo. It may be advisable, as well, to consider this band ratio for the K(490) algorithm given the improvement that was found with the CalCOFI data set using L_{WN} (490)/L_{WN} (555) compared to L_{WN}(443)/L_{WN} (555). It is also important to recognize that previous K(490) algorithms depend in part on assumptions about the value of K for pure water. Those assumptions may now need to be revised since recent laboratory measurements imply that the K for pure water in the region of relevance for SeaWiFS bio-optical algorithms may be smaller than previously reported.

The "global" data set assembled by Maritorena et al. (this volume) includes only 8 data points from polar regions (less than 1% of the data). It has been shown, based on in situ bio-optical observations, that polar regions have bio-optical relationships that are significantly different from low latitude relationships (Mitchell and Holm-Hansen 1991, Mitchell 1992, Cota 1997). Unfortunately, some earlier polar data sets suffer from uncertainty in the upwelling radiance calibration accuracy, and do not include the L_u (412) channel so they are not appropriate for the quality controlled data set that has been assembled here. Few newer data sets with better specified calibration have been delivered to the SeaWiFS Project, although there are some large data sets supported by NASA that have been collected in the Southern Ocean recently. Since the Southern Ocean relationships of Mitchell (1992) have been independently supported by statistical analyses of CZCS retrievals and in situ data sets (Sullivan et al. 1993, Arrigo et al. 1994), perhaps the issues for defining a satisfactory polar algorithm should be addressed. Given the known differentiation of polar bio-optics from low latitude relationships the present global data set which is biased toward low and mid-latitudes, and agrees well with the original CZCS NET team data set, will yield an algorithm that under-predicts chl-a in polar waters north and south of 50^{o} by up to a factor of 2, as was shown originally in Mitchell and Holm-Hansen (1991). This should be of concern to the SeaWiFS Project and there should be an explicit plan developed to address this issue if the at launch algorithm is deemed unsatisfactory at high latitudes. It is recommended that the SeaWiFS Project convene a polar bio-optical algorithm working group to identify the available data and specify a plan to incorporate it into the SeaBAM "global" data set. Issues about upwelling radiance calibration for earlier data sets should be addressed, and perhaps those data which have not been included here could be included once they have been compared to data with better defined calibration.

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GLOSSARY

BBOP	Bermuda Bio-Optics Project
BSI	Biospherical Instruments, Inc.
C	A programming language
C++	A programming language
CalCOFI	California Cooperative Oceanic Fisheries Investigation
CDOM	Colored dissolved organic material
CHORS	Center for Hydro-Optics and Remote Sensing (San Diego State University)
CTD	Conductivity, Temperature, Depth
CZCS	Coastal Zone Color Scanner
FEL	NIST calibrated standard lamp
ICESS	Institute for Computational Earth System Science (University of California, Santa Barbara
IDL	Interactive Data Language of RSI, Inc.
HPLC	High Performance Liquid Chromatography
IEH	File format of the CalCOFI data archive
IRIX	A computer operating system
LCD	Least Common Denominator (data file format)
MER	Multispectral Environmental Radiometer
MLRG	Marine Life Research Group
NASA	National Aeronautics and Space Administration
NIST	National Institute of Standards and Technology
NOAA	National Oceanic and Atmospheric Administration
PAR	Photosynthetically Available Radiation
Perl	A programming language
RMA	Reduced Major Axis (regression)
RMS	Root Mean Square (error)
SeaBAM	SeaWiFS Bio-optical Algorithms Mini-workshop
SeaBASS	SeaWiFS Bio-optical Archive and Storage System
SIO	Scripps Institution of Oceanography
SIRREX	SeaWiFS Intercalibration Round-Robin Experiment
SCB	The Southern California Bight
UCSB	University of California, Santa Barbara
UCSD	University of California, San Diego
UNIX	A computer operating system

SYMBOLS

λ	Wavelength, nm
a_{ph} (λ)	Phytoplankton pigment spectral absorption coefficient
a_w (λ)	The absorption coefficient for pure water
chl-a	Chlorophyll-a or chlorophyll-a concentration
E_d (λ)	Downwelling spectral irradiance
E_d (0^-,λ)	Downwelling spectral irradiance just below the sea surface
E_s (λ)	Surface irradiance
F_0 (λ)	Mean extraterrestrial spectral irradiance
K (λ)	Diffuse attenuation coefficient of seawater
K(490)	Diffuse attenuation coefficient of seawater measured at 490 nm
K_d (λ)	Diffuse attenuation coefficient of seawater for downwelling irradiance
K_w (λ)	Diffuse attenuation coefficient of pure seawater
ln	Natural logarithm
L_u (λ)	Upwelling spectral radiance
L_{WN} (λ)	Normalized water-leaving radiance
M (λ)	The slope coefficient between different spectral K values
N	The total number of measurements
phaeo	Fluorometric phaeopigment concentration
r^2	The coefficient of determination
R_{rs} (λ)	Remote sensing reflectance
R_{rs}(0^-,λ)	Remote sensing reflectance just below the sea surface
R_{rs}(0^+,λ)	Remote sensing reflectance just above the sea surface
sigma-*t*	Density of sea water

FIGURE CAPTIONS

Fig. 1. The current CalCOFI station grid.

Fig. 2. A comparison of MER-2040 E_d calibrations by different laboratories: ratios of UCSB calibration on 18-May-95 to BSI calibration on 2-Jun-1995 (filled circles), CHORS calibration on 2-Nov-95 to BSI calibration on 25-Nov-95 (open squares).

Fig. 3. A comparison of MER-2040 L_u calibrations by different laboratories: ratios of UCSB calibration on 18-May-95 to BSI calibration on 2-Jun-1995 (filled circles), CHORS calibration on 2-Nov-95 to BSI calibration on 25-Nov-95 (open squares).

Fig. 4. Calibration time series of the MER-2040 L_u (555 nm) channel. The filled symbols are the actual calibrations performed at BSI. The straight line with open symbols represents the interpolated wet scale factor plotted against the middle date of a CalCOFI cruise. Similar interpolations are used for all the E_d and L_u channels. Of the 13 different channels each of E_d and L_u on the MER-2040, the 555 nm channel is particularly important since this part of the spectrum often serves as the denominator of band ratio algorithms. All the calibration time-series plots are available online at http://spg.ucsd.edu/~lab/mer.

Fig. 5. Correlation between fluorometric estimate of chl-a and the HPLC estimate. The HPLC estimate is based on the sum of chlorophyll-a, chlorophyllide-a, allomerized chlorophyll-a, divinyl chlorophyll-a and chlorophyll-a'. Data presented here are only for the upper mixed layer.

Fig. 6. Relative frequency distribution (bars) of fluorometric chl-a concentration for the upper 15 m in the CalCOFI data set. In total 1910 chl-a measurements (all the CalCOFI cruises between 1993 and 1996) are used including stations with no bio-optical measurements. The mean and the median are 1.07 and 0.31 mg m^{-3}, respectively. A theoretical lognormal distribution with the same mean and standard deviation is shown for comparison (continuous line).

Fig. 7. Surface irradiance $E_s(\lambda)$ as a function of the downwelling irradiance extrapolated to just below the surface $E_d(0^-,\lambda)$ from measurements of the underwater MER at the six SeaWiFS wavelengths. All values greater than the corresponding mean extraterrestrial irradiance $F_0(\lambda)$ (caused by wave focusing) were considered errors and were excluded. The remaining M points were fit to a linear regression and all points deviating more than 2 standard deviations from the regression line (attributed to temporal/spatial offsets of cloud or ship shadow) were excluded. The remaining N points were fit with both RMA linear regression and a power function. The respective sample size ("N of M"), coefficients and RMS errors are shown.

Fig. 8. $R_{rs}(\lambda)$ at the six SeaWiFS wavelengths as a function of chl-a concentration. The points deviating more than 2 standard deviations from an initial regression were excluded from the plots and the final statistical fit. As the total data set consists of 304 observations the number excluded can be determined based on N reported for each wavelength.

Fig. 9. Near-surface chl-a concentration as a function of R_{rs} (443)/ R_{rs} (555) and R_{rs} (490)/ R_{rs} (555) with RMA linear regression (dotted straight line), CalCOFI Cubic A4 model (bold curved line, equations 5a and 5c, respectively, in Table 2) and the OC2 model (dash-dot line) proposed by O'Reilly and Maritorena (1997). The regression results are given in Table 2.

Fig. 10. Results of the CalCOFI 2-band linear algorithm (top panel, equations 3 in Table 2) and the CalCOFI Cubic A4 algorithm (bottom panel, equations 5 in Table 2). Both algorithms use the ratio $R_{rs}(490)/R_{rs}(555)$. The one-to-one lines are shown.

Fig. 11. Slope M (λ) for equation 8 from Austin and Petzold (1986) (continuous line) compared to CalCOFI data (filled symbols). Only K_d (490) less than 0.1 m^{-1} were used to estimate M (λ).

Fig. 12. $K_d(\lambda)$ **-** $K_w(\lambda)$ as a function of chl-a concentration. The $K_w(\lambda)$ values are from Morel (1988) and Smith and Baker (1981). The dotted line is the prediction of equation 9 in Morel (1988), and the solid line is the CalCOFI best estimate (RMA linear regression in the log-log space).

Fig. 13. Upper panel, K(490) as a function of the ratio of normalized water leaving radiances $L_{wn}(443)/L_{wn}(555)$. A comparison of the CalCOFI estimate (equation 9) with the results of Mueller and Trees (1996) and Austin and Petzold (1981) is given. Lower panel, K(490) estimated from $L_{WN}(490)/L_{WN}(555)$ including data from cruises RED9503 and LID9509. The RMS error and r^2 were calculated for the log-transformed data.

Table 1. Measured E_d band centers as determined by UCSB and CHORS versus the nominal BSI centers for MER 2040-8738.

BSI nominal wavelength, nm	UCSB center - BSI nominal, nm	CHORS center - BSI center, nm
340	-1.7	-1.4
380	-3.1	-2.4
395	0.9	1.6
412	-0.6	0.0
443	0.2	0.8
455	-0.7	0.1
490	0.3	1.1
510	-1.0	-0.1
532	-0.3	0.0
555	0.3	0.0
570	-0.6	0.0
665	0.4	1.5

Table 2. Summary of the CalCOFI bio-optical data set.

Cruise	Start	End	MER stations	Processing Status
CAL9308	11-Aug-93	26-Aug-93	28	Completed
CAL9310	11-Oct-93	25-Oct-93	17	"
CAL9401	17-Jan-94	8-Feb-94	30	"
CAL9403	22-Mar-94	7-Apr-94	32	"
CAL9408	5-Aug-94	21-Aug-94	21	"
CAL9410	30-Sep-94	16-Oct-94	25	"
CAL9504	6-Apr-95	22-Apr-95	24	"
CAL9507	6-Jul-95	22-Jul-95	28	"
CAL9510	12-Oct-95	26-Oct-95	29	"
CAL9602	29-Jan-96	10-Feb-96	22	"
CAL9604	15-Apr-96	30-Apr-96	16	"
CAL9608	7-Aug-96	25-Aug-96	20	"
CAL9610	10-Oct-96	1-Nov-96	30	"
CAL9702	30-Jan-97	2-Feb-97	30	Pending
CAL9704	2-Apr-97	17-Apr-97	22	Pending
LID9509	16-Sep-95	27-Sep-95	33	Completed
RED9503	8-Mar-95	30-Mar-95	12	"

Total: 17 cruises 419 stations

Table 3. Results of estimating chl-a and pigment concentrations from remote sensing reflectance ratios. The intercept (a), slope (b), determination coefficient (r^2) and root-mean-square error (RMS) of the observed vs. modeled regressions are given. Equations 5c and 5d are the preferred models for estimating chl-a and the sum of chl-a and phaeopigment (pha), respectively, for the CalCOFI data set. The OC2 and OC4 models of O'Reilly and Maritorena (1997) were tuned to the global and not the CalCOFI data set.

Model	a	b	r^2	RMS	Eq. #
CalCOFI 2-band linear model (*CalCOFI 2-Band*)					
chl-a = 10.^(0.444 –2.431 log[R_{rs} (490)/ R_{rs} (555)])	0.000	1.000	0.955	0.108	3a
chl-a + pha = 10.^(0.557 –2.440 log[R_{rs} (490)/ R_{rs} (555)])	0.000	1.000	0.956	0.107	3b
CalCOFI 2-band cubic model (*CalCOFI Cubic*)					
chl-a = 10.^(0.450 –2.860 R + 0.996 R^2 – 0.367 R^3) where R = log[R_{rs}(490)/ R_{rs}(555)]	-0.012	0.980	0.960	0.101	4a
chl-a + pha = 10.^(0.564 –2.753 R + 0.571 R^2 – 0.002 R^3) where R = log[R_{rs}(490)/ R_{rs}(555)]	-0.010	0.980	0.959	0.102	4b
CalCOFI Cubic A4					
chl-a = 10.^(0.239 –2.224 R + 0.888 R^2 – 0.053 R^3) **-** 0.02 where R = log[R_{rs}(443)/ R_{rs}(555)]	-0.012	0.978	0.959	0.103	5a
chl-a + pha = 10.^(0.357 –2.185 R + 0.665 R^2 – 0.1018 R^3) – 0.02 where R = log[R_{rs}(443)/ R_{rs}(555)]	-0.009	0.979	0.959	0.102	5b
chl-a = 10.^(0.455 –2.842 R + 1.000 R^2 – 0.080 R^3) – 0.02 where R = log[R_{rs}(490)/ R_{rs}(555)]	-0.011	0.978	0.960	0.101	5c
chl-a + pha = 10.^(0.568 –2.740 R + 0.571 R^2 –0.2411 R^3) – 0.02 where R = log[R_{rs}(490)/ R_{rs}(555)]	-0.009	0.978	0.959	0.102	5d
CalCOFI 3-band model					
chl-a = exp(1.025 – 1.622 ln(R_{rs}(490)/ R_{rs}(555)) – 1.238 * ln(R_{rs}(510)/ R_{rs}(555)))	-0.013	0.978	0.956	0.106	6a
chl-a + pha = exp(1.265 – 1.937 ln(R_{rs}(490)/ R_{rs}(555)) – 0.737 * ln(R_{rs}(510)/ R_{rs}(555)))	-0.010	0.978	0.956	0.106	6b
CalCOFI 4-band model					
chl-a = exp(0.753 – 2.583 ln(R_{rs}(443)/ R_{rs}(555)) + 1.389 * ln(R_{rs}(412)/ R_{rs}(510)))	-0.013	0.977	0.956	0.106	7a
chl-a + pha = exp(0.995 – 2.528 ln(R_{rs}(443)/ R_{rs}(555)) + 1.285 * ln(R_{rs}(412)/ R_{rs}(510)))	-0.010	0.978	0.957	0.105	7b
***OC2* (O'Reilly and Maritorena 1997)**	-0.085	0.976	0.955	0.129	
***OC4* (O'Reilly and Maritorena 1997)**	-0.045	0.991	0.957	0.112	