SeaWiFS Bio-optical Algorithm Mini-workshop (SeaBAM) Overview

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ABSTRACT

One of the primary goals of the SeaWiFS Project is to routinely generate global chlorophyll-a and CZCS pigment concentrations with an accuracy of ±35%. Since its inception in 1991, the SeaWiFS Calibration and Validation Program has undertaken a number of initiatives to help ensure that this goal is met, e.g. measurement protocol development, calibration round robins, the bio-optical data archive and bio-optical algorithm workshops. After the seventh bio-optical algorithm workshop held in Halifax, Nova Scotia on October 21, 1996, it was clear that algorithm and data quality issues remained that could not be adequately addressed in the standard workshop format. A more interactive analysis (data sets and algorithms) oriented workshop was deemed necessary in order to focus on specific problems. As a result, the first SeaWiFS Bio-optical Algorithm Mini-workshop (SeaBAM) was hosted by D. Siegel at UC/Santa Barbara during January 21-24, 1997. This chapter provides an overview of the workshop background, organization, approach and results from the workshop and other associated activities.

INTRODUCTION

Early in the definition of the SeaWiFS program, the ocean color science community established a mission goal of estimating global surface chlorophyll-a and CZCS pigment concentrations to within ±35% (Hooker et al., 1992). The rationale behind the CZCS pigment product (chlorophyll-a plus phaeophytin) is to provide a data set that can be compared to products derived from the CZCS for studies of decadal scale variability. Early comparisons of in situ and CZCS global products (Balch et al., 1992) indicated that this goal was feasible for most of the global ocean. Subsequent studies, however, noted significant differences even in clear water environments (Arrigo et al., 1994). The CZCS algorithm was based on 55 bio-optical stations in coastal U.S. waters (Clark, 1981; usually referred to as the Nimbus Experiment Team or NET data set) and even by 1991, that data set was the only data set generally available for algorithm development. As a result, the SeaWiFS Calibration and Validation (Cal/Val) Program initiated several activities directed at improving the quality bio-optical data collected by the ocean optics community. These activities include the establishment of measurement protocols (Mueller and Austin, 1992 and 1995), a calibration round robin (e.g. Johnson et al., 1996), the SeaWiFS Bio-optical Archive and Storage System (SeaBASS; Hooker et al., 1994), the SeaWiFS Transfer Radiometer (SXR) and the SeaWiFS Quality Monitor (SQM; Shaw et al., 1996). In addition, seven bio-optical algorithm workshops have been held, brief proceedings of which are published in the SeaWiFS Technical Memorandum cumulative index issues (see Volumes 12, 18, 24 and 36).

The bio-optical algorithm workshops have been open events and have provided a forum for presentation and detailed (often quite frank) discussions on protocols, data collection and algorithm issues. Early in the deliberations on algorithm development, it was decided to avoid switching algorithms such as was used in the global CZCS reprocessing (Gordon et al., 1983) and to use a semi-analytical chlorophyll algorithm. Switching algorithms tend to produce bimodal frequency distributions as an artifact of the switching logic (Denman and Abbott, 1988; Muller-Karger et al., 1990). Semi-analytical algorithms (Carder et al., 1991; Garver and Siegel, 1995; Carder et al., 1996) would allow more physical insight into the optical processes that determine oceanic reflectance thus providing a mechanism for incorporating strategies to account for regional and temporal variability in the algorithm. The discussions at the workshops have been very constructive in highlighting differences in perceptions and approaches to algorithm development. For example, the CZCS pigment product raised several questions. Should the algorithm be chlorophyll-a or chlorophyll-a + phaeophytin as it was just as easy to develop an empirical algorithm for chlorophyll-a (Aiken et al., 1995). If just chlorophyll-a, why is a CZCS pigment product needed? Should the CZCS pigment product be based only on CZCS bands (SeaWiFS equivalents) and should be product be derived using a CZCS atmospheric correction? The issue is that if the CZCS atmospheric correction scheme (uses 670 nm) and bio-optical band limitations (443, 520 and 550 nm) introduce a systematic bias in the pigment product that is not reproduced in subsequent ocean color data sets, the interpretation of decadal scale change will be compromised.. Another question is what measurements of pigments should be used in defining the CZCS pigment product given the evolution in measurement techniques (fluorometric, HPLC, etc.) and is consistency with the original NET CZCS data set necessary? In the end, the general concensus, though not unanimous, was to continue use the original product definition, but to use the best algorithms possible, i.e. the SeaWiFS atmospheric correction and no restriction on the bands to be used for the bio-optical algorithms.

With regard to the SeaWiFS Science Working Group bio-optics subgroup's recommendation to pursue semi-analytical algorithms for operational use, it has become clear that the existing semi-analytical algorithms are limited to Case I, relatively low pigment waters. The main issues are a paucity of data on scattering and the variability in spectral absorption. While new methods and instrumentation for measuring the backscattering coefficient hold promise, little is currently available. Also, the measurement of spectral absorption, let alone a way of parameterizing its variability, remains an issue. In response to this problem, the SeaWiFS Cal/Val program funded a workshop at Scripps Institute of Oceanography, hosted by G. Mitchell and A. Bricaud, in December 1996 to compare and evaluate different methods. The results of the workshop are not available as yet. Thus, at the present time, the semi-analytical algorithms are inherently empirical, at a different level, and some resort to strictly empirical relationships at high concentrations (Carder et al., 1996). The limitations, at the present time, reside in the determination of the various absorption and backscattering coefficients, i.e., measurement methodologies, parameterizations, etc. Despite these limitations, semi-analytical algorithms do generate reasonable chlorophyll-a values for most of the global ocean as well as a number of other quantities that could be routinely produced by the SeaWiFS Project, if required by the science community. Also, they can be easily adapted to any combination of wavelengths commensurate with any satellite sensor. Therefore, whether or not the initial SeaWiFS algorithms are semi-analytical, their development should continue because the original rationale remains valid and justified.

Finally, another issue which complicates the algorithm evaluation process stems from differences in reflectance measurement methodologies, i.e. above-surface vs. below-surface. Both methods have limitations. Above-surface measurements are contaminated by sky-light, glint, polarization and plaque bidirectional reflectance effects. Below-surface measurments require absolute radiance calibrations, an extrapolation through the air-sea interface and a correction for instrument self shading in turbid water. The Carder et al. (1996) algorithm utilizes above-surface measurements, but the bulk of the data available for independent algorithm verification are below-surface observations. No systematic comparison of the two methods has been conducted and published and the protocol for making above-surface reflectance measurements (Mueller and Austin, 1995) is considered by many to be inadequate. The SeaWiFS Project sponsored a workshop on Case II measurement protocols in the spring of 1996 (see Vol. 36) with the objective of refining the existing protocols, but the workshop coordinators have not completed the document that was outlined at the meeting. The SIMBIOS Project plans to sponsor focused field experiments designed to clarify, and hopefully, resolve this issue.

After the seventh bio-optical algorithm meeting in October 1996, it was clear that convergence on the operational algorithms was not happening in a satisfactory manner. Indeed, the primary candidate algorithms for chlorophyll-a (Carder et al., 1996) and CZCS pigment (Aiken et al., 1995) were seriously inconsistent at moderate and high concentrations, i.e. chlorophyll-a >> CZCS pigment. It is with all the above-mentioned considerations in mind that SeaBAM was initiated. The consensus was that further progress would result only if the participants work collectively with open access to data and code (data processing and algorithm) in a similar fashion to the data analysis round robin held at UC/SB in 1994 (Siegel et al., 1995). The following sections outline the workshop strategy including pre- and post-workshop activities and a summary of the findings derived as a result of the SeaBAM process. It is the philosophy of the SeaWiFS Project not to develop the operational algorithms, but to expedite algorithm development via whatever mechanisms are possible and to provide an independent and objective evaluation. From the SeaWiFS Project's perspective, SeaBAM has achieved more than was initially hoped for because of the enthusiasm and openness of all the participants. Data and software were freely exchanged, errors were revealed and corrected (without angst), and substantial improvements in almost all the evaluated algorithms have been made. Last, but not least, a consistent set of chlorophyll-a and CZCS pigment algorithms have been identified using a large bio-optical data set representing a diversity of bio-optical provinces.

OBJECTIVES AND APPROACH

Given that the primary objective was to finalize and deliver the operational SeaWiFS chlorophyll-a and CZCS pigment algorithms in a relatively short time, it was agreed by the participants (listed below) that a successful workshop would require a substantial amount of pre-workshop preparation and the free and rapid dissemination of data, code and results. It also required that all involved be willing to assist one another, work out problems and differences of opinion internally and that recognize that all options were open with regard to the final algorithm selections. The strategy was to have a balanced, but small, group of participants including representatives from the SeaWiFS Project and others who had been active in the bio-optics subgroup as algorithm developers (empirical and semi-analytic) and bio-optical data providers (Table 1). It was also agreed that D. Siegel would host the workshop at UC/SB and that he would assume responsibility for providing a workshop environment that efficiently accommodated both group discussion and presentation sessions and a heterogenous computing and data storage environment. GSFC would coordinate pre- and post-workshop activities including maintenance of an access-restricted SeaBAM web page where data, results and email would be posted and archived. Both S. Maritorena (GSFC) and S. Garver (UC/SB) had been developing data sets of water-leaving radiances (and other related quantities) with associated pigment data for the purposes of independent evaluation and algorithm development, respectively (Maritorena et al., and Garver and Siegel, this volume). They would continue the refinement and expansion of these data sets, coordinate their activities, e.g., exchange data, in preparation for the miniworkshop and provide the data sets to the other participants. The initial version of the Maritorena et al. data set which was presented at the Halifax workshop consisted of approximately 90-100 clear-sky stations. It was agreed that this condition was too restrictive and that other data should be incorporated. Finally, it was agreed that all groups would provide documentation on their evaluations and results to be combined into a SeaWiFS TM.

Table 1. SeaBAM Participants

Individuals	Institution
Dave Siegel & Sara Garver	University of California/Santa Barbara
Greg Mitchell & Mati Kahru	Scripps Institute of Oceanography
Gerald Moore	Plymouth Marine Laboratory
Jim Mueller	San Diego State University
John O'Reilly	National Marine Fisheries Service
Ken Carder & Steve Hawes	University of South Florida
Chuck McClain, Stephane Maritorena & Brian Schieber	SeaWiFS Project, NASA Goddard Space Flight Center

To establish a framework for SeaBAM, an initial set of issues, tasks and goals were outlined which included the following:

(a) Settle on the definition of "CZCS pigments". This question is the result of the differences in measurement methodologies.

(b) Establish a clear definition of accuracy and identify the appropriate statistical parameter(s) for quantification of accuracy as it applies to algorithms.

(c) Establish criteria for final selection of the "best" algorithm for both pigment parameters.

(d) Identify the algorithms to be compared and identify probable reasons for differences.

Ultimately, the algorithms included the following:

- Aiken et al. (1995)
- Carder et al. (1996)
- Clark (1996)
- Garver & Siegel (1995)
- Mitchell & Kahru (CalCOFI; unpublished)
- Morel (1996)
- New empirical (e.g. one based on the evaluation data set)
- Gordon et al. (1983)
- OCTS operational chlorophyll-a
- POLDER operational algorithm

(e) Establish data set selection guidelines. Considerations included:

- Blending of HPLC pigments with fluorometric pigments
- SeaWiFS measurement protocols compliance
- Blending of in-water and above-water estimates of R_{rs} or L_{WN}
- Consistency in analyses used to derive L_W from in-water measurements

(f) Select the data sets to be used for the comparisons. The individual data sets were:

- Carder et al. (above-water observations)
- Garver & Siegel (in-water observations)
- Maritorena et al. evaluation data set (in-water observations)
- Mitchell & Kahru (CalCOFI, in-water observations)

All issues were eventually addressed. Several items are discussed in detail in other chapters of this TM.

The UC/SB MEETING

Prior to the workshop, a global evaluation data set was assembled by combining a number of data sets contributed, primarily, by the participants. J. O'Reilly and S. Maritorena used this data set to complete an initial comparison of all algorithms prior to the meeting. The first day of the meeting consisted of briefings by all groups to provide updates on all preparations and results stemming from pre-workshop activities. During the presentations, an issues and analysis action item list was developed and reviewed at the end of the session. Thereafter, the groups conducted hands-on analyses to address the action items and periodically reconvened to report progress and register any additional issues that needed to be tracked. On the last day, a plenary was held to review the final status of all action items and to outline the post-workshop activities and schedule. To provide some insight into what the action items were and how they were resolved, several are described in the appendix..

FINAL RESULTS AND CONCLUSIONS

As discussed above, all the original issues have been addressed as well as a number of others that developed during SeaBAM. Conducting algorithm development in this fashion greatly expedited resolution of many questions. Most of the algorithms and the evaluation data set have been improved as a result of SeaBAM as discussed in detail in other chapters of this TM. The most important results are the final recommendations on the operational SeaWiFS algorithms which are summarized below.

1. *Chlorophyll-a.* Because the evaluation data set has the most bio-optical diversity of the data sets listed above and was quality controlled and processed in a consistent manner (Maritorena et al., this volume), it was used to obtain the "best" algorithm possible. Therefore, it evolved from being an independent data set to one used to develop empirical algorithms as well. Not only were all final versions of the algorithms as submitted by the developers considered, but also, for the empirical algorithms, these and other algorithmic forms (band ratio combinations) were fit to the evaluation data to see what improvements were possible. The algorithm that gave the best overall result based on the selection criteria outlined in O'Reilly and Maritorena (this volume) uses only a ratio of 490 nm to 555 nm, i.e.,

$$Chla = -0.040 + 10^{(0.341 - 3.001 \cdot X + 2.811 \cdot X^2 - 2.041 \cdot X^3)}$$

where

$$X = \log_{10}\left(\frac{R_{rs}(490)}{R_{rs}(555)}\right).$$

This result is consistent with the Aiken et al. (1995) finding that a 490:555 band ratio yielded the highest correlation ($r^2 = 0.95$) for the data sets in their analysis.

2. *CZCS pigment.* As discussed in O'Reilly and Maritorena (this volume), there are a number of options for this product, not all of which follow the original guideline of using an algorithm that utilizes only the CZCS bands. Clearly, there should be reasonable consistency between the two pigment products. Also, an evaluation data set for the CZCS comparable to the one just completed for SeaWiFS needs to be generated. For the at-launch algorithm, the recommendation is the following relationship which is based on a empirical relationship chlorophyll-a and chlorophyll-a + phaeophytin concentrations derived from the SeaBASS pigment data base, i.e.,

$$CZCS\ pigment = 1.34 \cdot Chla^{0.98}$$

It is important to note that the SeaWiFS Project plans to periodically reprocess the entire SeaWiFS data set as algorithms (atmospheric, bio-optical, mask and flag), sensor calibration and product suites are updated. Thus, it is critical that the SeaBAM activity be continued.

APPENDIX: Workshop Action Items

In order to emphasize the benefits of conducting workshops that are oriented around data analysis and real time algorithm evaluation, the following list of results stemming from action items are provided below. This meeting format expedited, even forced, the resolution of questions and issues, usually at the meeting. In the typical meeting format, questions often go unresolved resulting in continued debate and misunderstanding.

1. State succinctly the practical definitions of CZCS pigments and chlorophyll-a with rationale for the choices.

> *CZCS pigment*: A fluorometric pigment concentration (chlorophyll-a + phaeopigments) that can be calculated using bands comparable to the CZCS wavelengths (443, 520, 550). Note that the SeaWiFS protocols need to be more detailed on this topic. The purpose of generating this product is to provide a means of comparing products that can be derived from the CZCS to those from later missions for examining decadal scale variability. Restricting the algorithm to the CZCS wavelengths minimizes biases introduced in the products that are artifacts of the algorithm form. It is assumed that the global CZCS data set will be reprocessed using an updated pigment algorithm that is consistent with the SeaWiFS pigment algorithm. S. Maritorena will evaluate the assumption that the differences between fluormetric and HPLC bio-optical data sets are indistinquishable using the evaluation data set.
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> The issue of how to validate the reprocessed CZCS products using simultaneous measurements was discussed. Given that algorithms being developed at this time are based on different pigment measurement methodologies which yield different values, validation using historical data will require some adjustment in the historical values.
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> Status: Post-workshop examination of the SeaBASS data sets showed that there are a very limited number of stations available having the CZCS bands and chlorophyll-a + phaeophytin concentrations on which to base a “global” algorithm (Maritorena et al., this volume) and alternative strategies are outlined in O’Reilly and Maritorena (this volume).
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> *Chlorophyll-a*: Any fluorometric or HPLC concentration identified as chlorophyll-a by the provider. While there are differences in the values obtained by the two techniques, globally the difference has been shown to be of the order of 10% (analyses by C. Trees). Also, at least for the time being, both HPLC and fluorometric data have been combined in order to have a data

set sufficiently large with enough diversity to cover the broad range of chlorophyll concentrations required for development of a general chlorophyll algorithm. Debate continues as to what pigments should or are being summed and reported as "chlorophyll" concentration in the data sets being submitted to SeaBASS.

Status: Because other sources of variability in the bio-optical data sets, e.g. data processing methods and calibration have been found to be as great, and in order to have enough data over a large dynamic range to develop and evaluate algorithms, this definition was adopted.

2. Reconcile the differences in the CalCOFI-2 L_w spectral shapes as obtained independently by S. Garver and M. Kahru. The problem is an elevated shoulder at 490nm relative to 443 nm in the Kahru analysis.

Status: The anomalous spectral shoulder was found to be a typographical error in a table used in the transformation of subsurface Lu(443) to the above-surface L_w(443).

3. Resolve a problem S. Garver and D. Siegel observe with some of C. Tree's NABE (North Atlantic Bloom Experiment) optical data.

Status: J. Mueller checked the scaling factor Garver and Siegel were using and the problem was a misinterpretation of the scaling factor format. NABE is consistent with other data sets.

4. Determine the reason by the 412 nm surface reference values in G. Cota's Resolute Bay data are inconsistent with values in the profile data (a 2-4 fold difference was found in all profiles for all three cruises, each in a different year).

Status: G. Cota was contacted and will try to develop a time series of his calibration data. The 412 nm filters were replaced in both instruments after the 1995 field campaign. As a result, the 1994 and 1995 data were excluded from the evaluation data set, but the 1996 data were retained.

5. Verify a constant offset between the evaluation data set and D. Clark's algorithm (the algorithm had the highest r^2 when compared with the evaluation data set).

Status: J. Mueller and S. Maritorena spoke with D. Clark after the workshop. The source of the offset could not be readily identified, so further evaluation of the Clark algorithm was deferred until an update is made available.

6. Examine the impact of data with 565 nm rather than 555 nm on the algorithm comparisons. The WOCE and early BATS data have 565 nm measurements rather than 555 nm. Both data sets are from low pigment waters. Given the significant slope in water absorption spectrum at these wavelengths, the data should be corrected or omitted from the SeaWiFS algorithm evaluations.

Status: S. Maritorena analyzed several data sets and derived a correction factor for transforming 565 nm to 555 nm radiances. Tthe corrected data were retained in the evaluation data set.

7. Investigate what appears to be anomalous 412 nm data in J. Marra's WOCE data set. Some 412 nm data appears to be very high even for very clear water.

Status: J. Mueller did the calibration on J. Marra's MER and followed up on this question. As a result, the 1991 data was removed from the evaluation data set because of concerns about the calibration, but the data from 1993 and 1994 were retained.

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