Development of Algorithms and Strategies for Monitoring Chlorophyll and Primary Productivity in Coastal Ocean, Estuarine and Inland Water Ecosystems

Quarterly Technical Report
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Summary

This is the first quarterly progress report for a contract that began in May, 1996, for the Definition Phase of a MODIS Instrument Team investigator project. The Definition Phase contrast covers the period from May 13, 1996, through June 30, 1997. The central objective of the Definition Phase contract is:

> To establish a protocol for developing and validating regional or site-specific algorithms for estimating surface chlorophyll-a concentration and primary productivity while accounting for optical variability of other water constituents.

This report describes progress in four areas: (1) project "spin-up" activities, (2) chlorophyll algorithm protocol development, (3) primary productivity algorithm protocol development, and (4) participation in MODIS Science Team meetings and related activities. A timeline for accomplishing each of these activities and associated tasks is attached.

Spin-up Activities

This contract provided funds for hiring an assistant research scientist, for purchasing a computer workstation, and for supporting a graduate-student research assistant. The research scientist position was first advertised on July 20, 1996. Review of applications began on July 29, 1996. There were 13 applicants in all, some received late in August Following a thorough review of the applications received, Timothy S. Moore was selected. Timothy Moore has a Master of Science degree in biological oceanography from the University of Rhode Island, where he has had experience working with CZCS and AVHRR satellite imagery. His master's thesis, entitled "Along-shore carbon exchange around Cape Hatteras as estimated from satellite imagery" was directed by Dr. James Yoder. The official offer was made September 18, and Tim began work on September 30, 1996. Hui Feng was offered the graduate student research assistantship. Hui received a Master of Science degree in physical oceanography from the University of New Hampshire in August of this year, and has now been accepted into the Ph.D. program in oceanography under my direction.

A Silicon Graphics INDIGO2 Solid IMPACT graphics, 250 MHz workstation was purchased with 128 MB memory, 4GB system disk, a 20" monitor, and an extra external 9 GB disk. The workstation was received in mid September and was setup and operational by October 4, 1996.

Chlorophyll Algorithm Protcol Development

This objective is largely theoretical in nature. The end result will be a paper that describes the general approach to parameterizing and validating the chlorophyll algorithm while accounting for optical variability of other water constituents found in coastal, estuarine and inland waters. There are 5 tasks involved in accomplishing this objective (see Timeline).

The basis for the chlorophyll algorithm will be a radiance model relating upwelling spectral radiance above the water surface, $L_w(\lambda_i)$, to the inherent optical properties of the water, specifically to the backscattering coefficient $b_b(\lambda_i)$, and the absorption coefficient, $a(\lambda_i)$. The inherent optical properties (IOPs) are then related to constituents in the water. Constituents of interest include phytoplankton chlorophyll (CHL), chromophoric dissolved organic matter (CDOM), and total suspended sediments (TSS).

A radiance model, run in the forward direction, predicts spectral radiances given constituent concentrations and other properties of the in-water constituents. The bio-optical algorithm is the inverse of the radiance model. That is, it predicts constituency concentrations and their optical properties given spectral radiances derived from atmospherically corrected satellite observations. Radiance models involving inherent optical properties generally involve their ratio:

$$\frac{b_b(\lambda_i)}{a(\lambda_i) + b_b(\lambda_i)} = \frac{b_b(\lambda_i)/a(\lambda_i)}{1 + b_b(\lambda_i)/a(\lambda_i)} \approx \frac{b_b(\lambda_i)}{a(\lambda_i)}$$

Progress/discussion to date on each of the tasks is as follows:

1. Evaluation of several candidate algorithms based on radiance models

We have chose the "semi-analytic" radiance model of Gordon et al., (1988) to evaluate fret. This model had been evaluated using Airborne Oceanic Lidar (AOL) measurements and found to be accurate in predicting the AOL's passive upwelled radiance measurements (Hoge et al., 1995). It is straight-forward to convert normalized water-leaving radiance to the ratio $b_b(\lambda_i)/a(\lambda_i)$ (see Table 1), but solving for the constituent properties given this ratio is difficult.

Using the same "semi-analytic" radiance model, Hoge and Lyon (1996) present an analysis in which IOPs were retrieved by linear matrix inversion. In their analysis, the spectral shape of the IOPs was independent of the constituent concentrations. In our parameter-ization, the spectral shape of the IOPs depends on the constituent concentrations. This results in a nerd.inear inversion problem which is more difficult to solve. Both the spectral absorption and backscattering coefficients of phytoplankton are nonlinear functions of the chlorophyll concentration (Bricaud et al., 1995; Carder et al., 1995, Gordon et al., 1988). Our challenge is to invert the radiance model to derive the constituent concentrations given the vector of normalized water-leaving radiances at any pixel in a satellite image.

In evaluating this model, we have obtained the following results:

- There are spectral radiances that do not yield any feasible inverse solution. The inversion of the radiance model yields constituent concentrations that are negative.

- Given water-leaving radiances at CZCS wavelengths, inverse solutions for CHL, CDOM, and a particle brightness parameter, b^0, are not unique (see Fig. 1). More than one set of constituent concentrations will yield the same radiances in the three CZCS bands. The addition of the SeaWiFS and MODIS bands at 412 nm and 490 nm will probably make the solution possible, but we are still investigating this.

Because of these results, we are in the process of considering other radiance models or modifications to the model as currently parametrized.

Other tasks that remain to be accomplished are:

2. Final selection of a radiance model and algorithm

3. *Parametrizing the model so as to minimize squared error*

4. Demonstrating and testing the algorithm using actual satellite and in-situ data

5. *Completion of a journal article or NASA technical report*

Primary Productivity Algorithm Protocol Development

This objective, which is also theoretical in nature, will result in a second paper that describes the general approach to parametrizing and validating a primary productivity algorithm for coastal, estuarine and inland waters. This objective entails 5 tasks (see Timeline).

1. Evaluation of several candidate algorithms

This task is being accomplished as an activity of NASA's Ocean Primary Productivity Working Group. We are conducting a Primary Productivity Algorithm Round Robin (PPARR) which is now in the second round of tests. From the frost round, we concluded that algorithm performance was regionally variable. Assuming that this is not fortuitous, but rather the result of parametrization at the regional scale, it is possible to obtain a composite algorithm made up of algorithms which performed best in each region (Fig. 2).

In the second round of the PPARR, we have learned that algorithms are highly correlated. Results from the more elaborate algorithms tend to be highly correlated with results from simpler formulations. This has led to the selection of the simplest algorithm as a candidate for testing during the SeaWiFS era beginning next year.

Plans call for a third round of the PPARR. In this round, algorithm developers will be asked to apply their algorithms to the same set of globally gridded forcing variables (surface chlorophyll, surface irradiance, etc.) resolved at monthly intervals.

A password-protected homepage has been developed for participants of the round robins (http://rossby.unh.edu/pparr/PPARR1 .html). For access to the report of the first round robin:

Username: PPARR3
Password: psi=0.5

2. *Selection of an analytical model and algorithm for demonstration purposes*

3. *Parameterizing the algorithm so as to minimize squared error*

4. *Demonstrating and testing the algorithm using actual satellite and in-situ data*

5. *Publication of a journal article or NASA technical report*

Participation in MODIS Science Team meetings and related activities

I have attended and participated in two MODIS Science Team meetings: May 1-3, 1996, and October 9-11, 1996, and a meeting of the MODIS Oceans Discipline Group (MOCEAN) on July 15-17, 1996. Related activities include partication in the NASA Ocean Primary Productivity Working Group which met at Goddard on June 11-13, 1996. As part of this working group, I have been acting as “referee” for the round robins to evaluate primary productivity algorithms.

Activity Name	Start Date	Finish Date
Spin-up Activities	5/13/96	7/28/96
Chlorophyll Algorithm Protocol Development		
Evaluation of candidate algorithms	5/13/96	12/1/96
Selection of radiance model and algorithm	12/1/96	
Parameterizing algorithm to minimize errors	12/1/96	1/1/97
Demonstrating and testing algorithm	1/1/97	2/1/97
Completion of journal article or NASA technical report	2/1/97	3/1/97
Primary Productivity Algorithm Protocol Development		
Evaluation of candidate algorithms	5/13/96	3/1/97
Selection of analytical model and algorithm	3/1/97	
Parameterizing algorithm to minimize errors	3/1/97	4/30/97
Demonstrating and testing algorithm	5/1/97	6/30/97
Completion of journal article or NASA technical report	6/30/97	
Participation in MODIS Science Team meetings and related activities	5/1/96	6/30/97

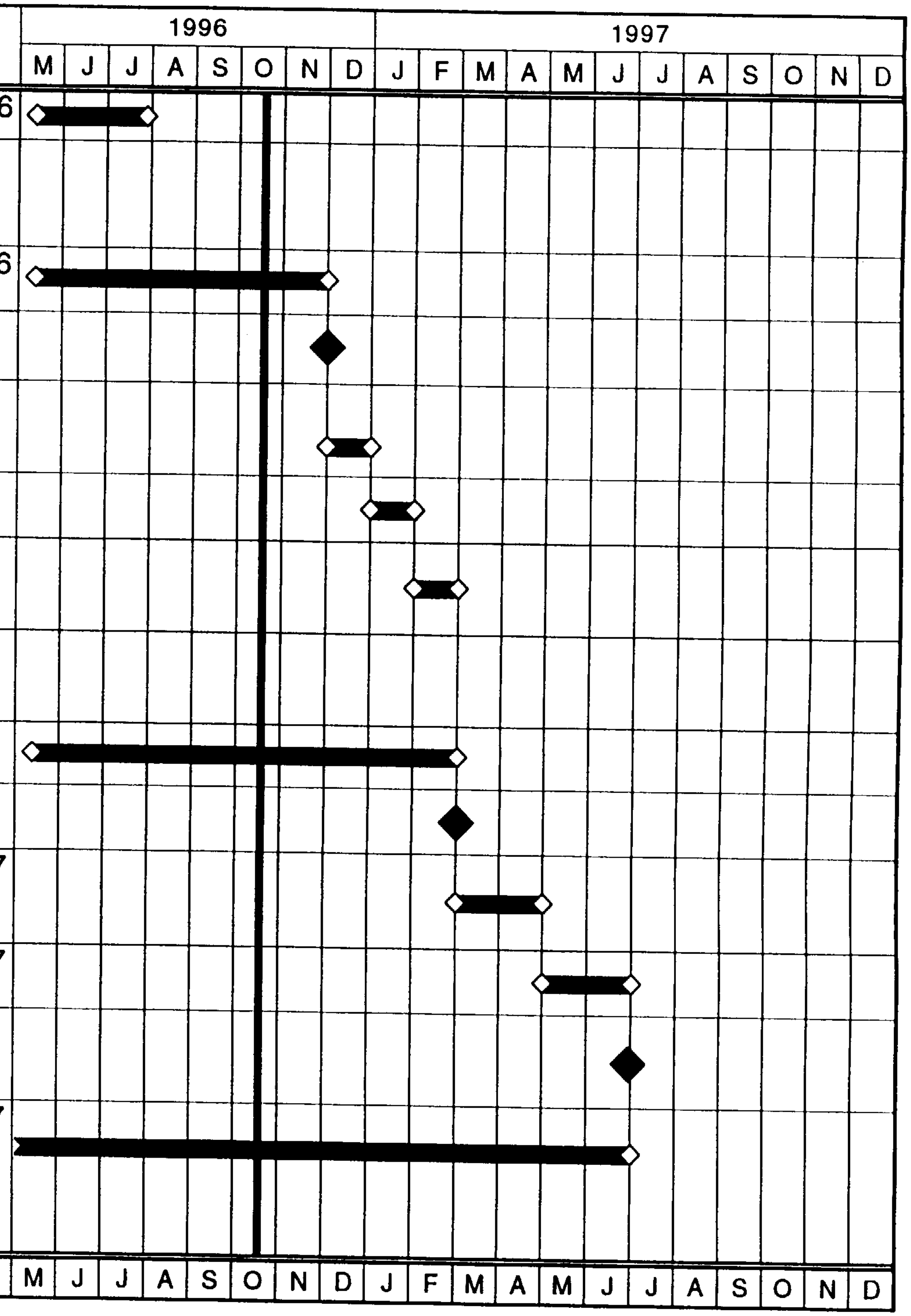

Table 1. Equations used to derive L_{WN} from b_b and a (left column) and the inversion equations used to derive b_b/a from L_{WN} (right column). Eqs. 1.1 to 1.3 predict the normalized water-leaving radiance given a and b_b, whereas eqns. 1.4 to 1.6 are the basis for analytical algorithms used to derive in-water optical properties given water-leaving spectral radiance measurements.

Given the inherent optical properties, a and b_b, we define X' as follows:

$$X' \equiv \frac{b_b}{a+b_b} \qquad (1.1)$$

where a and b_b are the effective absorption and back-scatter coefficients within the upper optical depth.

Based on results of Gordon (1986), the remote-sensing reflectance is accurately represented as:

$$\frac{R}{Q} = 0.0949\,X' + 0.0794\,X'^2 \qquad (1.2)$$

for solar zenith angles $\theta_0 > 20°$.

According to the "Semi analytic Radiance Model" of Gordon et al., (1988), the normalized water-leaving radiance can be modeled as:

$$L_{wN} = \frac{(l-p)\,(1-p')F_0 R/Q}{m^2(l-rQ^*R/Q)} \qquad (1.3)$$

where the symbols are defined previously (see text). In this expression, the term (1-rR) which appears in the paper by Gordon et al., (1988), (their equation 1), is replaced by the term (1-rQ*R/Q) where Q* is an estimate of Q. Q* does not need to be particularly accurate since (1-rR) only varies from about 0.92 to 1.0, and is sometimes assumed to be 1.0.

Given normalized water-leaving radiance, L_{WN} equation (1.3) is inverted to obtain the remote-sensing reflectance:

$$\frac{R}{Q} = \frac{L_{WN}/F_O}{M + rQ^*L_{wN}/F_0} \qquad (1.4)$$

where $M = (1-p)(l-p')/m^2$. Note that both L_{WN} and F_O depend on wavelength, whereas the other terms in (1.4) do not.

Equation (1.2) is a quadratic equation with two roots. The only positive root is:

$$x' = \frac{-0.0949 + \sqrt{0.0090 + 0.3176\,R/Q}}{0.1498} \qquad (1.5)$$

Since a>> b_b in most Case 1 waters, equation (1.1) is often approximated by $X' = b_b/a$. However, this approximation is unnecessary, since the ratio of b_b to a is easily computed as:

$$\frac{b_b}{a} = \frac{x'}{1-x'} \qquad (1.6)$$

Thus, beginning with normalized water-leaving radiances in the first five spectral bands of the SeaWiFS, the variables X'_i, i = 1,...,5, can be computed, and these used to compute the ratio of backscatter, $b_b(\lambda_i)$, to absorption $a(\lambda_i)$, in the SeaWiFS bands centered at wavelengths λ_i = 412, 443, 490, 510, and 555 nm.

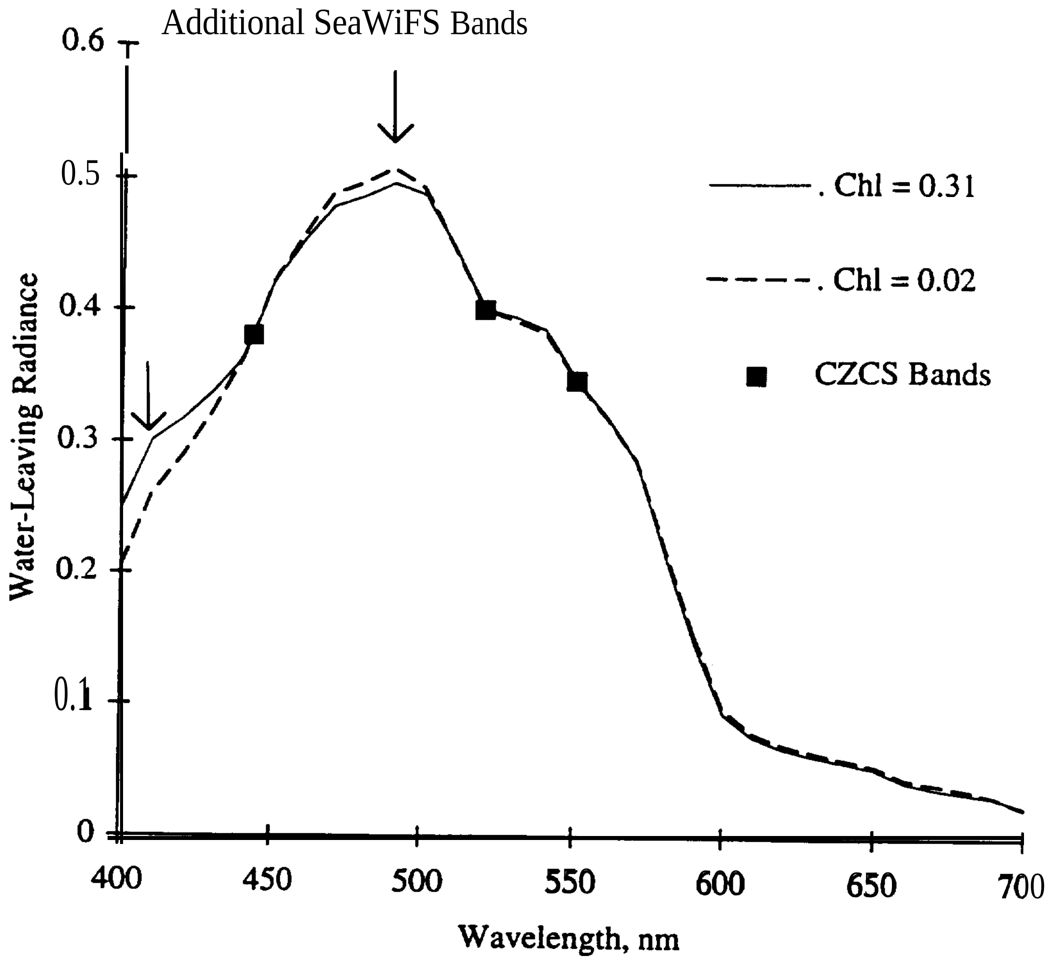

Figure 1 .- Model-generated radiance spectra derived using very different constituent concentrations as input. The red curve resulted from chlorophyll = 0.31 mg m^{-3}, b^0 = 0.3 m^{-1}, and CDOM absorption, $a_g(400)$ = 0.15 m^{-1}. The black dashed curve resulted from chlorophyll = 0.02 mg m^{-3}, b^0 = 0.9 m^{-1}, and $a_g(400)$ = 0.25 m^{-1}.

This illustrates the problem of non-uniqueness for the three CZCS bands. Two widely separated points in Constituent Space can map to the same point in the Radiance Space of CZCS bands (blue squares). Additional bands on SeaWiFS (arrows) will allow differentiation between these two cases.

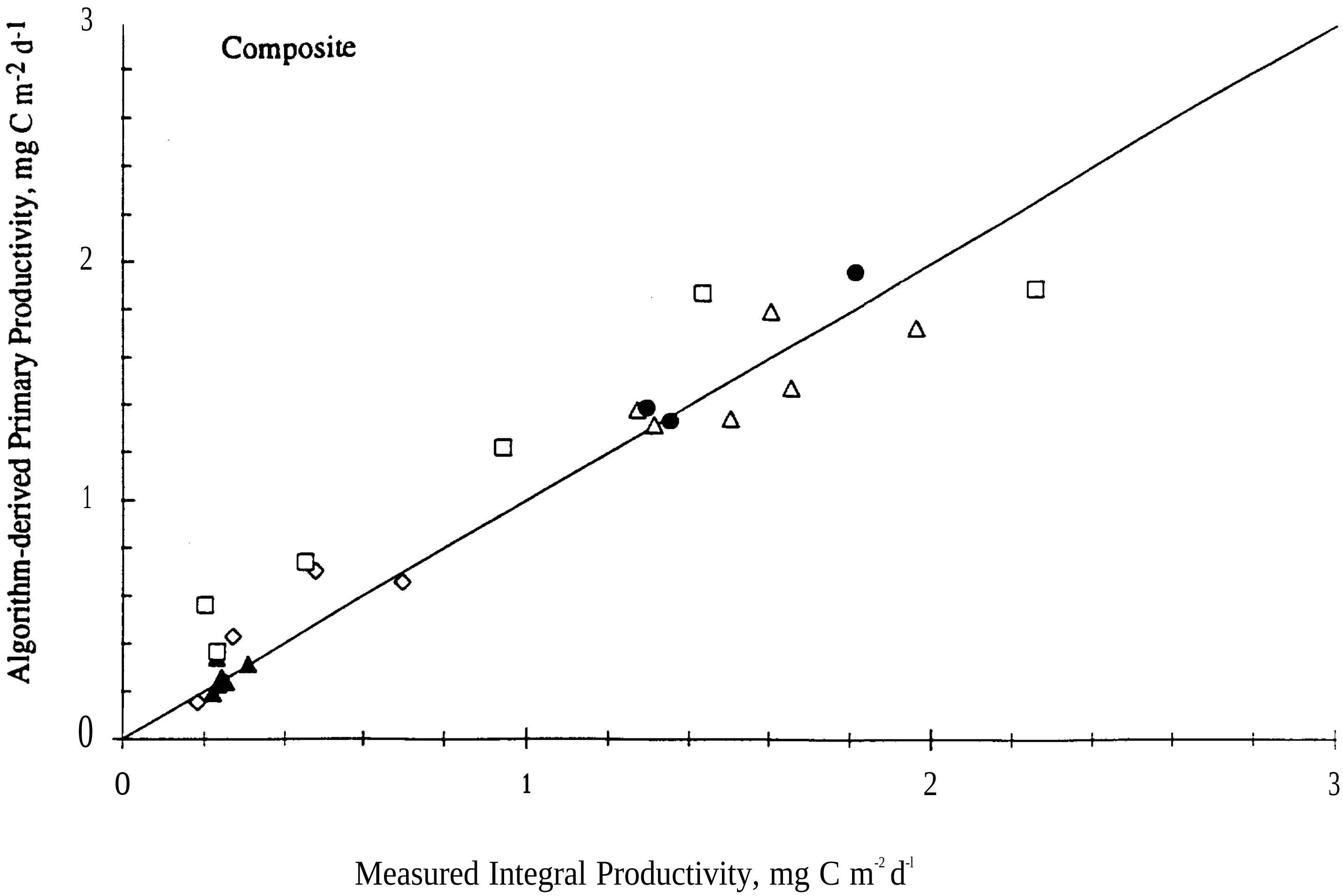

Figure 2. Results of a composite primary productivity algorithm comprised of the best-perrforming algorithms in each region of the PPARR-1 analysis.