OCTS AND SEAWIFS BIO-OPTICAL ALGORITHM AND PRODUCT VALIDATION AND INTERCOMPARISON IN U.S. COASTAL WATERS

Christopher Brown
NOAA/NESDIS, Camp Springs, Maryland

Ajit Subramaniam
University of Maryland, College Park, Maryland

Mary Culver
NOAA Coastal Services Center, Charleston, South Carolina

John C. Brock
USGS Center for Coastal Geology, St. Petersburg, Florida

INTRODUCTION

Monitoring the health of U.S. coastal waters is an important goal of the National Oceanic and Atmospheric Administration (NOAA). Satellite sensors are capable of providing daily synoptic data of large expanses of the U.S. coast. Ocean color sensor, in particular, can be used to monitor the water quality of coastal waters on an operational basis. To appraise the validity of satellite-derived measurements, such as chlorophyll concentration, the bio-optical algorithms used to derive them must be evaluated in coastal environments. Towards this purpose, over 21 cruises in diverse U.S. coastal waters have been conducted (Subramaniam *et al.*, 1997a, 1997b, 1997c, 1998, 1999, 2000a, 2000b; Culver *et al.* 1998; Kiambo *et al.* 1999). Of these 21 cruises, 12 have been performed in conjunction with and under the auspices of the NASA/SIMBIOS Project. The primary goal of these cruises has been to obtain *in-situ* measurements of downwelling irradiance, upwelling radiance, and chlorophyll concentrations in order to evaluate bio-optical algorithms that estimate chlorophyll concentration.

In this Technical Memorandum, we evaluate the ability of five bio-optical algorithms, including the current SeaWiFS algorithm, to estimate chlorophyll concentration in surface waters of the South Atlantic Bight (SAB). The SAB consists of a variety of environments including coastal and continental shelf regimes, Gulf Stream waters, and the Sargasso Sea. The biological and optical characteristics of the region is complicated by temporal and spatial variability in phytoplankton composition, primary productivity, and the concentrations of colored dissolved organic matter (CDOM) and suspended sediment. As such, the SAB is an ideal location to test the robustness of algorithms for coastal use.

METHODS

Sampling Location and Collection Methods

Bio-optical measurements were collected at over 100 stations during nine cruises (Table 1) conducted in the South Atlantic Bight in order to evaluate and validate the five algorithms. The cruises were conducted from early spring to late fall in optically diverse waters ranging from the extremely shallow and turbid Pamlico Sound to the deep and clear Sargasso Sea (Figure 1). Optical instruments measured surface spectral downwelling irradiance, in-water spectral downwelling irradiance, and upwelling radiance. Although sampling strategies and instrument packages varied between cruises, a Biospherical Instruments Profiling Reflectance Radiometer (PRR) cage was typically deployed off the stern of the vessel in conjunction with a reference surface unit with matching channels. Surface bucket samples were obtained for total suspended solids (TSS) concentration and for chlorophyll analysis by fluorometric and High-Pressure Liquid Chromatography (HPLC) techniques. Detailed descriptions of instruments and other ancillary measurements are presented in Subramaniam *et al.* (1997a, 1997b, 1997c, 1998, 1999, 2000a, 2000b) and Culver *et al.* (1998).

Table 1. Summary of cruise names, location, dates and sampling platforms.

Cruise	Dates	Number of Stations	Location	Vessel
FEB96LIT	22-23 Feb. 1996	7	Georgia Bight	*R/V Blue Fin*
APR96BF	3-5 Apr. 1996	18	Georgia Bight	*R/V Blue Fin*
APR96FER	22-25 Apr. 1996	16	Georgia Bight	*R/V Ferrel*
MAY97OB	5 May 1997 8 May 1997	5 4	Onslow Bay, NC, Pamlico Sound, NC	*R/V Onslow Bay,* *R/V Chipman*
SEP97SAB	5-24 Sept. 1997	11	South Atlantic Bight	*R/V Cape Hatteras*
NOV97SAR	4, 5 Nov. 1997	16	Saragasso Sea	*R/V Pametto*
APR98SAB	5-27 April 1998	23	South Atlantic Bight	*R/V Cape Hatteras*
NOV98SAB	27 Oct-23 Nov 1998	50	South Atlantic Bight	*R/V Cape Hatteras*
FEB99SAB	27 Jan–24 Feb 1999	11	South Atlantic Bight	*R/V Cape Hatteras*

Water Sample Analyses

Discrete water samples were collected following the PRR cast from the sea surface using a bucket or a Niskin bottle and filtered through glass fiber (GF/F) filters. The chlorophyll samples were cold extracted in 10 ml of 90% acetone (10% water) for 24 hours in the dark and the biomass was determined fluorometrically with a Turner Designs fluorometer as described in Subramaniam *et al.* (1998). The TSS concentration was measured as described by Parsons *et al.*, (1984). For cruises FEB96LIT, APR96BF, APR96FER, and NOV97SAR, chlorophyll *a* and other pigments were determined as described in Subramaniam *et al.* (1997). For the MAY97OB, SEP97SAB, APR98SAB and NOV98SAB cruises, chlorophyll *a* and other pigments were determined as described in Tester *et al.* (1995).

Quality Control

The PRR optical data were processed using the Bermuda Bio-Optics Project (BBOP) processing software (Siegel *et al.*, 1995). All optical profiles were graphed and examined. Profiles that exhibited evidence of surface perturbations, such as ship shadow, and the effects of passing clouds were excluded from further analysis. The *in-situ* downwelling irradiance (Ed-) was propagated through the water-air interface to Ed+ using a transmission loss of 4% (O'Reilly *et al.*, 1998). The *in-situ* upwelling radiance (Lu-) was propagated through water-air interface to water-leaving radiance (Lu+ or Lw) using a factor of 0.544 (O'Reilly *et al.*, 1998). The coefficient of variation (EsλErr) of the above-water downwelling irradiance (Esλ) measured by the reference sensor mounted on the ship was calculated as the ratio of the standard deviation to the mean of the Es(λ) measurements for the duration of the PRR600 profile. Es from profiles where EsλErr was greater than 10% (indicating either passing clouds or large ship roll) was not used in calculating remote sensing reflectance. The difference (dsλ) between the measured downwelling irradiance (Es) and the calculated downwelling irradiance (Ed+) was calculated and profiles with dsλ greater than 50% were excluded from analysis. Several other stations that possessed peculiar spectra were also eliminated. The remote sensing reflectance ($R_{rs}\lambda$) and normalized water-leaving radiances (nLwλ) were calculated as

$$R_{rs}(\lambda) = 0.544 * \frac{Lu(0,^{-}\lambda)}{Es(\lambda)};$$

and

$$nLw(\lambda) = F_0(\lambda) * R_{rs}(\lambda).$$

Algorithm Evaluation

Optical profiles from a total of 88 stations were used to evaluate the five bio-optical algorithms developed to estimate surface chlorophyll concentration from satellite ocean color observations. These algorithms included the current SeaWiFS algorithm (OC4v4; O'Reilly *et al.*, 2000), the previous SeaWiFS algorithm and its improvement (OC2v4 and OC2v2; O'Reilly *et al.*, 1998), an algorithm proposed for the Southeastern United States (OCse; Stumpf *et al.*, 2000), and a semi-analytical algorithm based on Garver and Siegel's inverse model (UCSB; Garver and Siegel, 1997; Maritorena *et al.*, 2000). OCse is an empirical algorithm developed using data collected from highly absorbing waters of the Gulf of Mexico. The semi-analytical algorithm (UCSB) was selected because it explicitly estimates backscatter and CDOM absorption, in addition to chlorophyll concentration, and had the potential of reducing the error attributed to high concentrations of suspended sediments and riverine contribution of CDOM found in the South Atlantic Bight. The formulations used for each algorithm to calculate chlorophyll concentration were as follows:

$$(OC4v4)Chl = 10^{\left(0.336-3.067X+1.930X^2+0.649X^3-1.532X^4\right)},$$

$$\text{where } X = \log\left(\frac{R_{rs}(443)}{R_{rs}(555)} > \frac{R_{rs}(490)}{R_{rs}(555)} > \frac{R_{rs}(510)}{R_{rs}(555)}\right).$$

$$\text{OC2v2Chl} = -0.0929 + 10^{\left(0.2974-2.2429X+0.8358X^2-0.0077X^3\right)},$$

$$\text{where } X = \log\left(\frac{R_{rs}(490)}{R_{rs}(555)}\right).$$

$$\text{OC2v4Chl} = -0.071 + 10^{\left(0.319-2.336X+0.879X^2-0.135X^3\right)},$$

$$\text{where } X = \log\left(\frac{R_{rs}(490)}{R_{rs}(555)}\right).$$

$$OCseChl = 10^{\left(-2.5\log(\frac{R_{rs}(490)}{R_{rs}(555)}\right)}.$$

OCse is valid only in (coastal) regions of high chlorophyll concentration (Stumpf *et al.*, 2000). For regions possessing low chlorophyll concentrations, the OC4v4 algorithm was applied. For regions containing moderate chlorophyll concentrations, a log-transformed weighting was used to shift from OC4v4 (low chlorophyll waters) to OCse (high chlorophyll concentrations). The transform was applied based on the following criteria:

- OCseChl < 0.1 mg/m^3, chlorophyll = OC4v4Chl (OC4v4Chl ~ 0.2 mg/m^3)
- 0.1 mg/m^3 < OCseChl < 0.5 mg/m^3,
  chlorophyll $= OCseChl = 10^{\left(\log(OCse)*\frac{\log(OCse)-\log(0.1)}{\log(0.5)-\log(0.1)}+\log(OC4v4)*\frac{\log(0.5)-\log(OCse)}{\log(0.5)-\log(0.1)}\right)}$
- OCseChl > 0.5 mg/m^3, chlorophyll = OCseChl

The logarithmic weighting was used as the OC4v4 and OCse algorithms are both in terms of log(Chl). The results remove the bias found between OC4v4 and the measured chlorophyll.

A simple linear regression analysis between measured chlorophyll and algorithm chlorophyll in log space was performed to evaluate the algorithms. Only fluorometrically determined chlorophyll concentrations (ChlF) were employed in this evaluation. Typical measures of goodness-of-fit between *in-situ* chlorophyll concentrations and modeled retrievals, such as the coefficient of determiniation, r^2, were calculated and examined. In addition, an Algorithm Performance Index (API) was calculated as the log of the ratio of algorithm derived chlorophyll to measured chlorophyll. Consequently, an API value of 0 indicates that the algorithm predicted the measured chlorophyll concentration, a negative value indicates the algorithm underestimated chlorophyll, and a positive indicates the algorithm overestimated chlorophyll.

Results

Bottle Samples

In-situ chlorophyll (ChlF) values ranged from 0.16 to 5.20 μg/L with mean value of 1.51 μg/L and a median value of 1.03 μg/L. While many of the high chlorophyll stations lay along the coast and the low chlorophyll (0-1 μg/L) stations were situated along the outer shelf, no distinct spatial pattern was discernible in the *in-situ* chlorophyll concentrations (Figs. 2). The absence of any obvious pattern in chlorophyll concentration is likely due to the temporal span over which the data were collected and the dynamic nature of phytoplankton biomass in the SAB. For example, surface chlorophyll concentration at a station located at the shelf break in September 1997 was 0.33 μg/L while a station occupied at the same position in November 1998 was 1.11

μg/L. This large variation could be attributable to interactions of the Gulf Stream with the shelf waters (McClain *et al.* 1984).

Algorithm Validation and Evaluation

Comparisons of measured and algorithm-derived estimates of chlorophyll concentration are illustrated in Figures 3 and 4. Figure 3 illustrates the frequency distribution of both measured and algorithm-derived values of chlorophyll concentration (ChlF) observed during our cruises in the South Atlantic Bight. In general, OC2v2 performed well at lower chlorophyll concentrations (up to 0.3 mg m^{-3}). As expected, OCse performed well in the high chlorophyll range (> 0.5 mg chl m^{-3}), with the shape of its cumulative frequency similar to that of in-situ chlorophyll concentration at values of 1 mg chl m^{-3} and greater. The overestimation in the 0.3 to 0.5 mg m^{-3} range is potentially due to the logarithmic weighting over this concentration interval. UCSB also exhibits roughly the same cumulative frequency shape as *in-situ* chlorophyll at higher chlorophyll concentrations, though it is less sigmoidal. Analysis of OC2v4, the "improved" version of OC2v2, performed substantially worse than its predecessor and was not presented.

Results of least-squares regression analysis are presented in Table 2. Of the five algorithms evaluated for the SAB, UCSB possessed the slope closest to 1.00 (slope = 1.036). All algorithms except OC4v4 displayed similar intercepts with a mean of 0.27 (n=4). The intercept of OC4v4 was almost twice as great (0.5). OC4v4, however, received the highest coefficient of determination ($r^2 = 0.72$), while UCSB received the lowest ($r^2 = 0.52$). The overall performance of UCSB was degraded by a few model retrievals that severely underestimated actual chlorophyll concentration (Fig. 4).

Table 2 Results of regression analysis for each algorithm.

Algorithm	**OC2v2**	**OC2v4**	**OC4v4**	**OCse**	**UCSB**
Slope	1.361	2.660	0.931	0.699	1.036
Intercept	0.288	0.299	0.503	0.236	0.269
r^2	0.693	0.644	0.721	0.695	0.523

Examining the Algorithm Performance Index (API) of the algorithms for all data indicated that OC2v2, OC2v4, and OC4v4 overestimated actual chlorophyll concentrations to varying degrees, while OCse and UCSB underestimated them (Table 3). Average API values for UCSB suggest it performed very well. This result, however, was fortuitous. Close examination revealed that the "mean" value was achieved by averaging the overestimates and underestimates of individual measurements.

Dividing the data collected in "spring" (February-May) and "non-spring" (June-January) months indicated a seasonal component to algorithm performance (Table 3). Algorithms generally performed better, i.e. API approached 0, during the non-spring months. During the spring, all algorithms overestimated measured chlorophyll concentrations (Table 3). This overestimation is likely to result from increases in CDOM concentration (and absorption) caused by elevated river discharge into the SAB during the spring. The spatial distribution and number of stations in the spring and non-spring periods were similar, eliminating geographic bias.

Table 3 Mean chlorophyll concentration (ChlF) and Algorithm Performance Index (API) for each algorithm by cruise and season.

Cruise	**ChlF**	**API OC2v2**	**API OC2v4**	**API OC4v4**	**API OCse**	**API UCSB**
SEP97SAB	2.048	0.028	0.108	0.022	-0.176	0.039
MAY97OB	1.977	0.133	0.219	0.091	-0.049	-0.043
NOV97SAR	0.227	0.113	0.054	0.165	0.084	-0.040
NOV98SAB	1.042	-0.090	-0.097	-0.041	-0.227	-0.134
Non-Spring	**1.314**	**-0.002**	**0.019**	**0.020**	**-0.129**	**-0.077**
APR98SAB	1.619	0.348	0.507	0.278	0.077	0.041
APR96FER	1.943	0.218	0.349	0.151	-0.049	-0.008
FEB96LIT	1.134	0.531	0.622	0.527	0.249	0.552
FEB99SAB	0.784	0.129	0.162	0.073	-0.016	0.103
Spring	**1.533**	**0.276**	**0.397**	**0.214**	**0.034**	**0.079**
Total	**1.421**	**0.132**	**0.202**	**0.114**	**-0.062**	**-0.003**

Summary

We evaluated the performance of five chlorophyll *a* algorithm in the South Atlantic Bight by comparing radiometrically-derived chlorophyll concentrations and *in-situ* chlorophyll concentrations. The results indicate that biogeographical provinces alone do not improve algorithm performance in the SAB. Seasonal variation must be taken into account. The high variability observed in spring is likely due to the presence of high concentrations of CDOM in shelf waters. Consequently, we expected that an algorithm that accounts for CDOM is necessary to accurately estimate chlorophyll concentration in the South Atlantic Bight. It is therefore surprising that UCSB, the algorithm that explicitly solves for CDOM absorption, does not perform well in the SAB. It's poor performance may be due to several reasons. One, it requires accurate measurements from 412 to 555 nm. In waters containing high concentrations of CDOM, in which the signal at 412 and 443 nm are very low, small errors in the propagation of Lu through the surface may generate large errors in the estimated chlorophyll concentration. Two, the algorithm is driven by a statistical tuning that is based on a large number of pixels that may not be appropriately analyzed by individual measurements. OCse, the regional algorithm, worked reasonably well in the SAB and may be improved by changing the structure of its log-transformed weighting function over the chlorophyll concentration range of 0.3 - 0.5 mg m^{-3}.

ACKNOWLEDGEMENTS

In addition to funding provided by the NASA/SIMBIOS Project, this work was accomplished in partnership with many agencies and institutions, including the National Marine Fisheries Service Southeast Fisheries Science Center, Grice Marine Laboratory of the College of Charleston, Skidaway Institute of Oceanography. We sincerely thank Dr. P. Tester for the use of her data and her invaluable participation in all aspects of this project.

References

Culver, M.E., A. Subramaniam, J.C. Brock, M.E. Geesey, G.R. DiTullio, D. Jones (1998). NOAA CSC/CRS Cruise NOV97SAR: Sargasso Sea Cruise. CSC Technical Report CSC/9-98/002. U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Coastal Services Center, Charleston, SC.

Garver, S. A. and D. A. Siegel (1997) Inherent optical property in version of ocean color spectra and its biogeochemical interpretation. 1. Time series from the Sargasso Sea. *Journal of Geophysical Research* **102**(C8): 18,607-18,625.

Kiambo, R. W., M. E. Culver, P. A. Tester, R.P.Stumpf, A. Subramaniam, J. C. Brock and D. Eslinger (1999) NOAA Cruise APR98SAB: South Atlantic Bight Cruise. CSC Technical Report. CSC/1-99/001. U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Coastal Services Center, Charleston, SC.

McClain, C.R., L.J. Pietrafesa, and J.A. Yoder (1984). Observations of Gulf Stream-induced and wind-driven upwelling in the Georgia Bight using ocean color and infrared imagery. *Journal of Geophysical Research* **89**: 3705-3723.

Maritorena, S., Siegel, D.A., Peterson, A.R. & Lorenzi-Kayser, M. 2000: Tuning of a pseudo-analytical ocean color algorithm for studies at global scales. Presented at the 2000 AGU Ocean Sciences Meeting (OS12M-05), San Antonio TX, 2000

O'Reilly, J. E., S. Maritorena, B. G. Mitchell, D. A. Siegel, K. L. Carder, S. A. Garver, M. Kahru and C. McClain (1998). "Ocean color chlorophyll algorithms for SeaWiFS." *Journal of Geophysical Research* **103**(C11): 24937-24953.

O'Reilly, J. E., and 21 others (2000). Ocean color chlorophyll *a* algorithms for SeaWiFS, OC2 and OC4: Version 4. SeaWiFS Postlaunch Calibration and Validation Analyses, part 3. NASA SeaWiFS technical report series. pp. 8 – 22.

Parsons, T. R., Y. Maita and C. M. Lalli (1984). *A Manual For Chemical And Biological Methods For Seawater Analysis*, Pergamon Press.

Siegel, D.A., M.C. O'Brien, J.C. Sorensen, D.A. Konnoff and E. Fields (1995). BBOP Data Processing and Sampling Procedures. Vol: 19, Institute for Computational Earth System Science, UC Santa Barbara, Santa Barbara, CA, 23pp.

Stumpf, R. P., R. A. Arnone, R. W. Gould, P. Martinolich, V. Ransibrahmanakul, P. A. Tester, R. G. Steward, A. Subramaniam, M. E. Culver and J. R. Pennock (2000). SeaWiFS Ocean Color Data For U.S. Southeast Coastal Waters. Sixth International Conference on Remote Sensing for Marine and Coastal Environments, Charleston, SC, Veridian ERIM International.

Subramaniam, A., E.M. Armstrong, K.J. Waters, J.C. Brock, P.A. Tester, E.Haugen. 1997a. NOAA CSC/CRS Cruise MAR97OCC: OCTS Calibration Cruise. CSC Technical Report CSC/5-97/001. U.S. Department of Commerce, National Oceanic and Atmospheric

Administration, Coastal Services Center, Charleston, SC.

Subramaniam, A., E.M. Armstrong, K.J. Waters, J.C. Brock, A.W. Meredith, R.O. Ranheim. 1997b. NOAA CSC/CRS Cruise MAY96NY: New Bight Apex Cruise. CSC Technical Report CSC/6-97/001. U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Coastal Services Center, Charleston, SC.

Subramaniam, A., K.J. Waters, A.W. Meredith, E.M. Armstrong, R.M Bohne, W.G. Keull, J.R. Nelson, G.R. DiTullio, J.C. Brock. 1997c. NOAA CSC/CRS Cruise APR96FER: Gray's Reef Cruise. CSC Technical Report CSC/7-97/001. U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Coastal Services Center, Charleston, SC.

Subramaniam, A., J.C. Brock, P.A. Tester, E. Haugen, R.P. Stumpf. 1998. NOAA NMFS Cruise MAY97OB: Onslow Bay and Pamlico Sound Cruise. CSC Technical Report CSC/2-98/001. U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Coastal Services Center, Charleston, SC.

Subramaniam, A., M. Culver, D. Phinney, D. Phinney, J. Brown, B. Schieber, J. Brock, D. Eslinger, and C. Brown. (1999). NOAA Cruise JUL98NAN: Nantucket Shoals Cruise. NOAA CSC Technical Report, 99043-PUB. U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Coastal Services Center, Charleston, SC.

Subramaniam, A., N. Blough, L. Harding, M. E. Geesey, C. W. Brown and M. E. Culver (2000) NOAA Cruise OCT99MAB: Mid Atlantic Bight Cruise. Technical Report. CSC/20016-PUB. U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Coastal Services Center, Charleston, SC.

Subramaniam, A., M. E. Culver and M. E. Geesey (2000) NOAA Cruise APR00FWS: West Florida Shelf Cruise. CSC Technical Report. CSC/20018-PUB. U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Coastal Services Center, Charleston, SC.

Tester, P.A., M.E. Geesey, C. Guo. H.W. Paerl and D.F. Millie (1995) Evaluating phytoplankton dynamics in the Newport River estuary (North Carolina, USA) by HPLC-derived pigment profiles. *Mar. Ecol. Prog. Ser.* **124**:237-245.

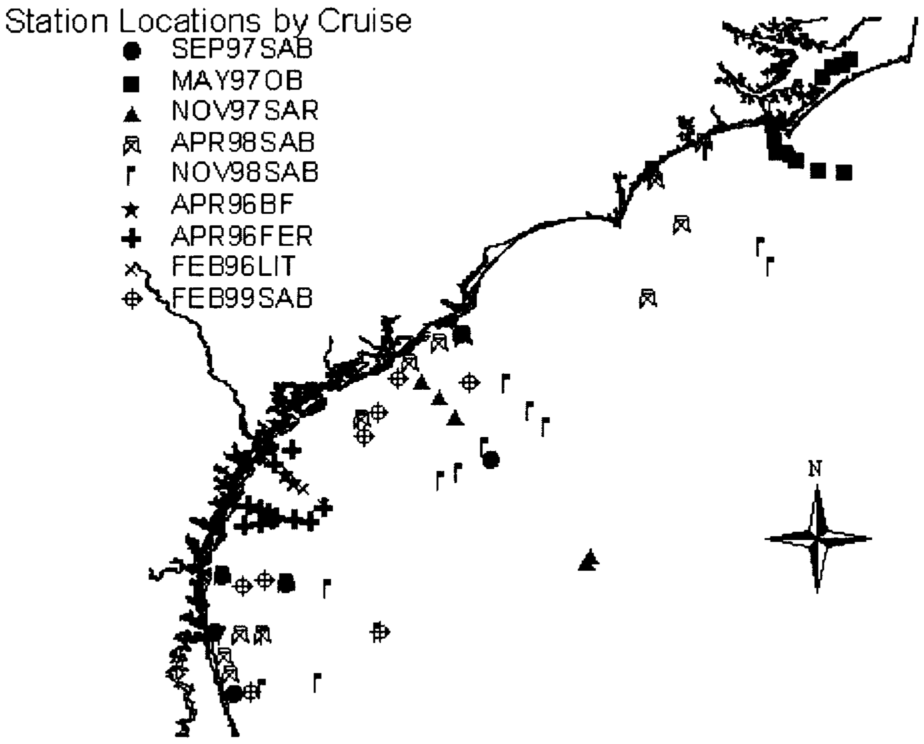

Figure 1. Location of stations.

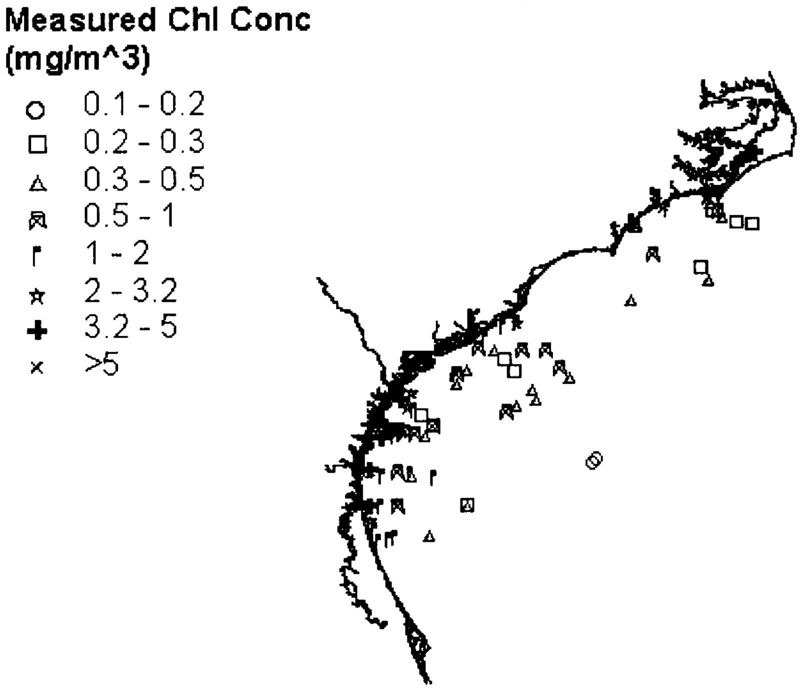

Figure 2. Spatial pattern of measured chlorophyll concentration in the South Atlantic Bight in this study.

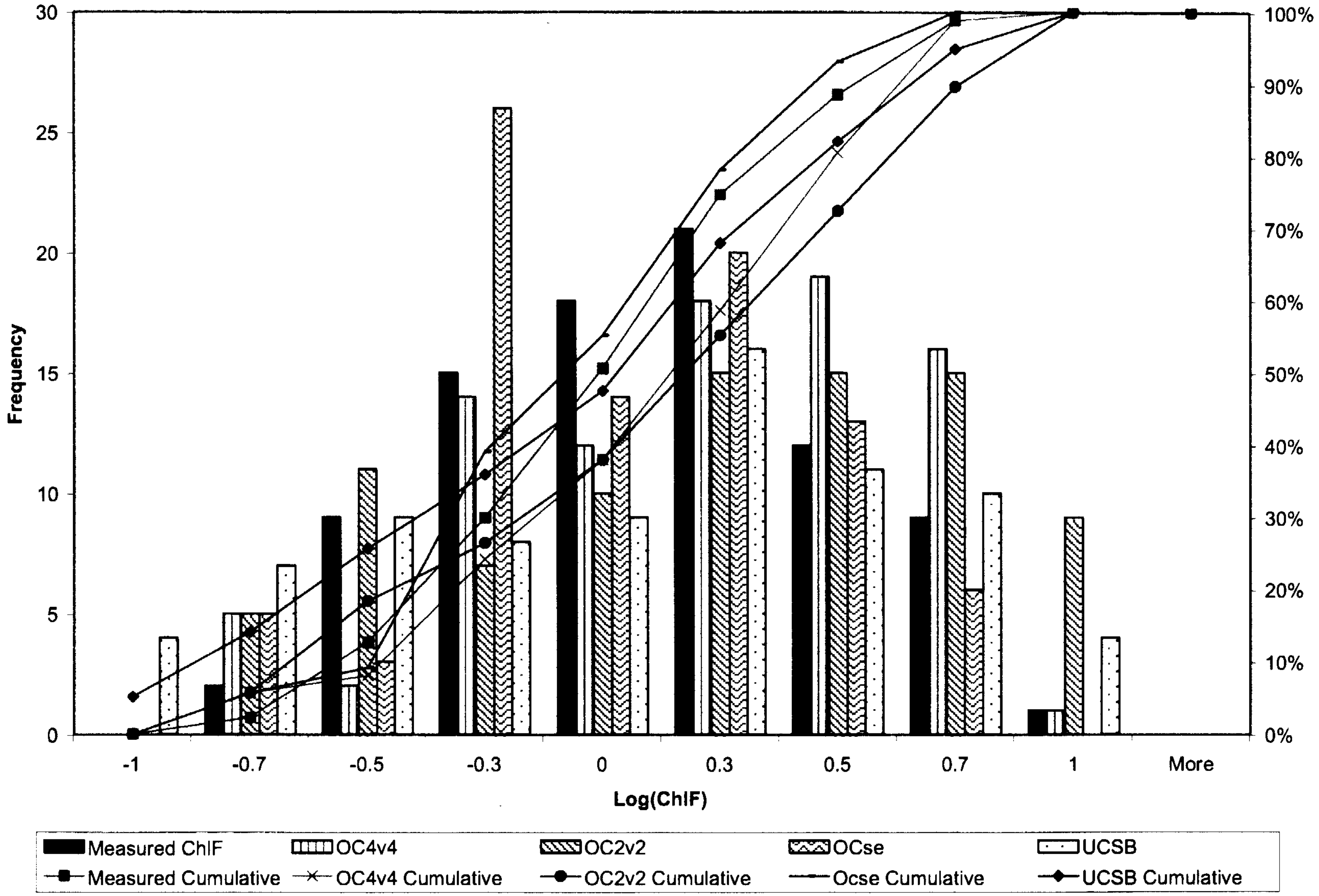

Figure 3. Histogram of measured and algorithm-derived chlorophyll concentrations.

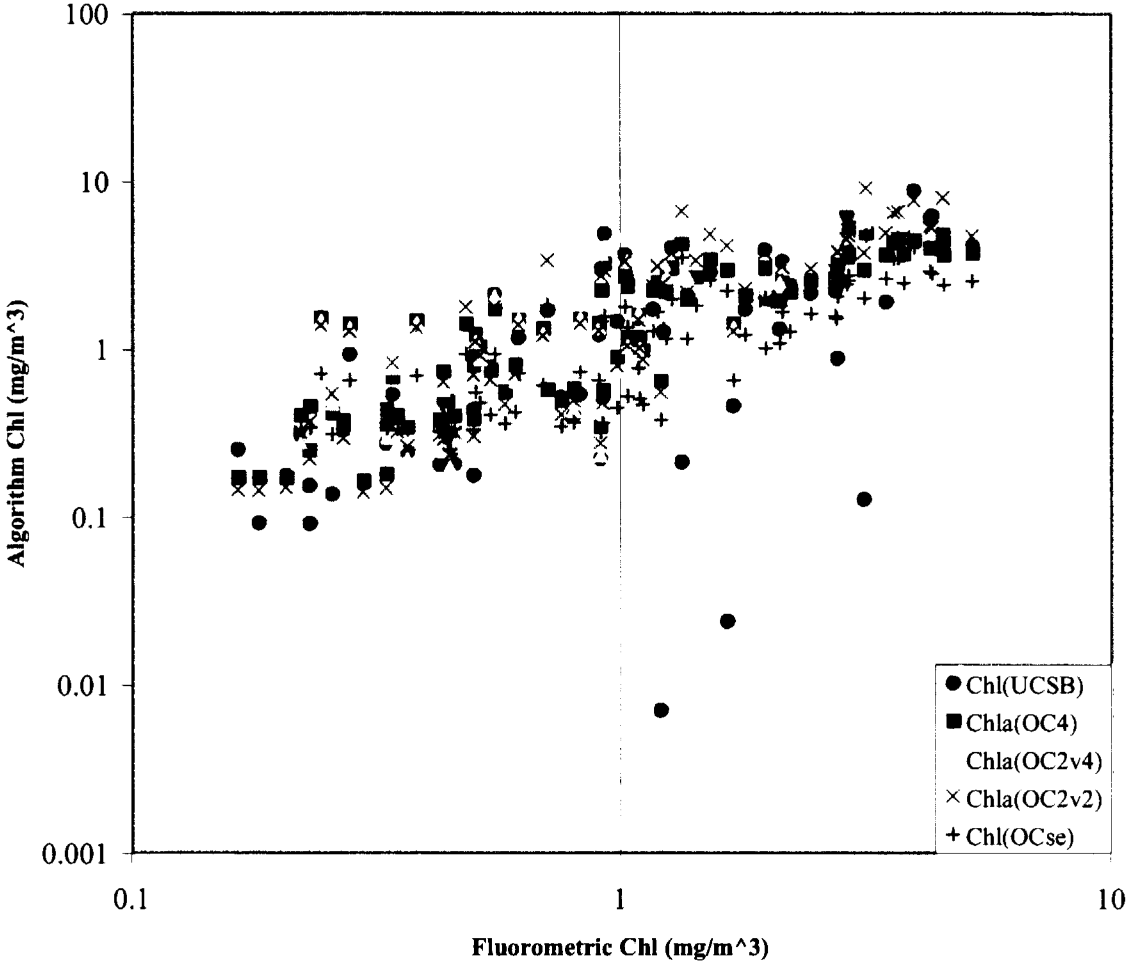

Figure 4. Scatter plot of measured and algorithm-derived chlorophyll concentration.