Estimation of colored dissolved organic matter and salinity fields in case 2 waters using SeaWiFS: Examples from Florida Bay and Florida Shelf

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Estimates of water quality variables such as chlorophyll *a* concentration (Chl), colored dissolved organic matter (CDOM), or salinity from satellite sensors are of great interest to resource managers monitoring coastal regions such as the Florida Bay and the Florida Shelf. However, accurate estimates of these variables using standard ocean color algorithms have been difficult due to the complex nature of the light field in these environments. In this study, we process SeaWiFS satellite data using two recently developed algorithms; one for atmospheric correction and the other a semi-analytic bio-optical algorithm and compare the results with standard SeaWiFS algorithms. Overall, the two algorithms produced more realistic estimates of Chl and CDOM distributions in Florida Shelf and Bay waters. Estimates of surface salinity were obtained from the CDOM absorption field assuming a conservative mixing behavior of these waters. A comparison of SeaWiFS-derived Chl and CDOM absorption with field measurements in the Florida Bay indicated that although well correlated, CDOM was underestimated, while Chl was overestimated. Bottom reflectance appeared to affect these estimates at the shallow central Bay stations during the winter. These results demonstrate the need for new bio-optical algorithms or tuning of the parameters used in the bio-optical algorithm for local conditions encountered in the Bay.

1. Introduction

Florida Shelf and Florida Bay are important coastal regions where water quality monitoring is of interest due to a variety of factors such as algal die-offs, increased phytoplankton abundance, harmful algal blooms and a perceived decline in fisheries (Tilmant 1989; Philips and Badylak 1996; Boyer *et al* 1999; Fourqurean and Robblee 1999). Spatial and temporal variability in the bio-optical constituents (e.g., Chl) affecting water quality necessitates regular and synoptic monitoring that can be achieved only by remote sensing techniques. Ocean color data from the

Sea-viewing Wide Field-of-view Sensor (SeaWiFS, Hooker *et al* 1992) are being used to derive estimates of products such as chlorophyll in oceanic waters. The two major steps involved in processing remotely sensed ocean color satellite data are the application of atmospheric correction to remove the atmospheric contribution to the radiance measured by the satellite sensor, and the use of bio-optical algorithms that relate water-leaving radiance to the in-water constituents. Although the application of standard remote sensing algorithms have shown successes in case 1 or open ocean waters, they have not been successful in accurately estimating bio-optical variables such as

Keywords. Remote sensing; SeaWiFS; atmospheric correction; chlorophyll *a*; CDOM; salinity.

Chl in coastal or case 2 waters. The main reasons are that

- atmospheric correction is interfered by case 2 water constituents, and
- the co-varying relationship between Chl and other optical constituents for case 1 waters may not be applicable to case 2 waters (Morel and Prieur 1977; Carder *et al* 1991).

The atmosphere usually contributes more than 80% of the signal measured by an ocean color satellite sensor. The atmospheric correction procedure (Gordon and Wang 1994) seeks to remove this contribution from the sensor signal in order to retrieve the water-leaving radiance. The total radiance $L_t(\lambda)$ or reflectance $\rho_t(\lambda)$ (where $\rho_t(\lambda) = \pi L_t(\lambda)/(F_0(\lambda)\mu_0)$, and $F_0(\lambda)$ is the extraterrestrial solar irradiance and μ_0 is the cosine of the solar zenith angle) observed by the sensor at wavelength λ , is the sum due to Rayleigh scattering $\rho_r(\lambda)$, the aerosol scattering $\rho_a(\lambda)$ (includes the aerosol-Rayleigh interaction term) and $\rho_w(\lambda)$, the reflectance from the water column. This can be written as

$$\rho_t(\lambda) = \rho_r(\lambda) + \rho_a(\lambda) + t(\lambda)\rho_w(\lambda). \quad (1)$$

The term $t(\lambda)$ is for the diffuse transmittance from the target to the sensor. While $\rho_r(\lambda)$ can be accurately calculated (Gordon *et al* 1988), $\rho_a(\lambda)$, $t(\lambda)$, and $\rho_w(\lambda)$ are unknowns to be determined. The SeaWiFS algorithm makes an assumption of zero $\rho_w(\lambda)$ in the near-infrared part of the spectrum enabling $\rho_a(765)$ and $\rho_a(865)$ to be computed. Ratios of these two values are used to select an aerosol type and an aerosol optical depth in the near-infrared. Based on the aerosol model selected, the optical depth is extrapolated to the visible wavebands. In case 2 waters however, high concentrations of organic and inorganic suspended matter may cause the water-leaving signal in the near infrared to be significantly greater than zero (Arnone *et al* 1998; D'Sa *et al* 2000; Ruddick *et al* 2000; Hu *et al* 2000, 2001). As a result, the aerosol optical thickness that is derived from this signal in the near infrared, may be over-estimated and further propagated to an "over-correction" in the visible part of the spectrum. The problem of zero water-leaving radiance in the near-infrared or the black pixel assumption has been addressed through iterative approaches for SeaWiFS data processing (Arnone *et al* 1998; Siegel *et al* 2000) and have shown improvements in obtaining more realistic estimates of Chl in turbid coastal waters. The iterative approach of Siegel *et al* 2000 (now included in the SeaWiFS processing software—SeaDAS V4.1) assumes some fixed

relationship between Chl and water-leaving radiance in Bands 6, 7, and 8. This assumption may not be applicable for turbid coastal waters where the optical properties may be dominated by other constituents or the shallow bottom, not by Chl. In contrast, another approach to correct for the effect of the near-infrared contribution of water-leaving radiance to the atmospheric correction is to transfer an aerosol type of the nearest less turbid waters to the turbid water pixels (Hu *et al* 2000). In this study we apply the turbid water correction (Hu *et al* 2000) to SeaWiFS data of the Florida Shelf and the Florida Bay and compare the results to the atmospheric correction schemes used in the standard SeaWiFS data processing.

Ocean color bio-algorithms used in processing SeaWiFS data use empirical relationships between band ratios of remote sensing reflectances and Chl to obtain estimates of Chl (O'Reilly *et al* 1998). These empirical relationships are based on the assumption that variations in ocean color optical signal is determined mainly by phytoplankton pigments. However, in coastal waters other oceanic constituents that include suspended matter and CDOM can also contribute significantly to the optical signal (Tassan 1994). The semianalytic algorithms (Garver and Siegel 1997; Carder *et al* 1999) have been developed mainly through improved knowledge of the in-water bio-optical properties and the relationships between remote sensing reflectance and backscattering to absorption ratios (O'Reilly *et al* 1998). In this study we use the Carder semianalytic algorithm (Carder *et al* 1999) to derive Chl and CDOM absorption at 400 nm (a_g400), for a coastal region.

The two recently developed atmospheric correction (Hu *et al* 2000) and bio-optical algorithms (Carder *et al* 1999) have shown promising results with retrieval of oceanic constituents from SeaWiFS. In this work, we further test and present results using these algorithms to estimate Chl and CDOM, two water quality parameters of interest in the Florida Bay and the Florida Shelf. These results are then compared with those from the standard algorithms that have been used for SeaWiFS data processing. Using measured CDOM absorption-salinity relationship we then generate sea surface salinity images from CDOM absorption estimates derived from the remote sensing data.

2. Methods

The standard atmospheric correction scheme used in this study combines the Gordon and Wang (1994) and Ding and Gordon (1995) algorithms that are incorporated in the NASA standard

processing software (SeaDAS V4.1). Further, we also process the SeaWiFS data over Florida Bay using the Siegel iterative approach to deal with the non-black pixel problem. The atmospheric correction procedure of Hu *et al* (2000) used in this study provides a practical method to separate the water-column reflectance from the total reflectance at 765 and 865 nm over turbid coastal waters. Based on an initial identification of turbid pixels, the aerosol type defined over a nearby, non-turbid region is transferred to the turbid area by using a “nearest neighbor” method. It is based on the assumption that the type of aerosol does not vary much over relatively small spatial scales (~ 50 – 100 km). The selection of an appropriate aerosol type for the turbid pixel from a neighboring non-turbid pixel, enables the aerosol reflectance and the water-column reflectance at 765 and 865 nm to be derived. Subsequently, the default NASA atmospheric correction scheme is used to obtain aerosol scattering components at visible wavelengths.

After applying atmospheric correction to the at-sensor measured radiances, different approaches are used to determine oceanic constituents from the resulting normalized water leaving radiances ($nL_w(\lambda)$). The two-band ratio or OC2 algorithm (O’Reilly *et al* 1998) used to estimate Chl (mg m^{-3}) is given by the relation:

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

where $X = \log(\text{Rrs}490/\text{Rrs}555)$ and Rrs (remote sensing reflectance) is defined as nL_w/F_0 (F_0 is the solar constant). For the specific case of Florida Bay, we process the SeaWiFS data using the Ocean Color OC4 bio-optical algorithm. The current version of OC4 is a four-band maximum band ratio formulation (O’Reilly *et al* 2000) and uses a fourth order polynomial (five coefficients) to estimate Chl and is given by:

$$\text{Chl} = 10.0^{(0.366 - 3.067X + 1.930X^2 + 0.649X^3 - 1.532X^4)} \quad (3)$$

where $X = \log(\text{Rrs}443/\text{Rrs}555 > \text{Rrs}490/\text{Rrs}555 > \text{Rrs}510/\text{Rrs}555)$. We compare the results of the band ratio algorithms to the Carder semianalytic algorithm (Carder *et al* 1999) that uses both analytical and empirical formulae in conjunction with the remote sensing reflectance values at five bands (412, 443, 490, 510 and 555 nm) to derive the absorption coefficient of phytoplankton at 675 nm, $a_{\text{ph}}(675)$ and the absorption coefficient of CDOM at 400 nm. An empirical relationship between Chl and $a_{\text{ph}}(675)$ is then used to estimate Chl.

We evaluate these algorithms over the coastal region of the Florida Shelf and further compare the results with *in situ* measurements in the Florida Bay. Florida Bay is located at the southern tip of the Florida Peninsula, United States and is a unique subtropical estuary that has seen many ecological changes to its ecosystem (Fourqurean and Robblee 1999). The climate in Florida Bay is characterized by a relatively warm wet season from May to October and a cooler dry season from November to April. Data from two field measurements conducted in October 1997 and January 1998 are compared to SeaWiFS derived variables using a combination of atmospheric and bio-optical algorithms. Chl and phaeopigment concentrations were determined using fluorometric method (Parsons *et al* 1984). A 0.5 m long capillary waveguide system was used to measure spectral absorption coefficient of CDOM (D’Sa *et al* 1999). Surface salinity was measured using an airborne scanning low frequency microwave radiometer (D’Sa *et al* 2000; Le Vine *et al* 2000; D’Sa *et al* 2002). A Secchi disk was used to measure water clarity. The field stations were along two transects at the western and central Bay regions (location of stations shown as triangles in figures 4a and 4b).

3. Results and discussion

In figures 1(a) and 1(b) we show results of Chl estimates from SeaWiFS data of 18th October 1999, obtained using two atmospheric correction schemes (Gordon and Wang 1994; Hu *et al* 2000) and the same bio-optical algorithm (OC2). We observe two main differences. With the default NASA algorithm (Hooker *et al* 1992; McClain *et al* 1995) a large region in the Bay that has been masked due to “atmospheric-correction failure” and “negative water-leaving radiance” flags (dark region) have been evaluated for Chl by the “nearest neighbor” correction algorithm (figure 1b). Also, generally higher Chl estimates have been obtained by the default NASA algorithm in comparison to the coastal algorithm. We then applied the Carder semianalytic algorithm to the water-leaving radiance spectra obtained with the “nearest neighbor” atmospheric correction algorithm. The SeaWiFS image (figure 1c) shows high CDOM levels in the Bay and was indicative of the flooding that occurred after Hurricane Irene (15th October 1999). Salinity field (figure 1d) derived from CDOM estimates also shows features due to coastal runoff in the Bay and West Florida Shelf.

Various field measurements have indicated a conservative mixing or dilution behavior for the

Figure 1. (a) Chl (mg m⁻³) derived from SeaWiFS data obtained on 18th October 1999 using NASA default atmospheric correction and OC2 algorithm, (b) Chl derived from the same SeaWiFS data using the “nearest neighbor” atmospheric correction and OC2 algorithm, (c) CDOM absorption a_{g400} (m⁻¹) using the “nearest-neighbor” atmospheric correction and 1st order semianalytic algorithm, and (d) sea surface salinity image derived from (c) using measured CDOM absorption-salinity relationship.

Figure 2. (a) SeaWiFS image of Chl (mg m^{-3}) acquired on 24th February 1999 and processed using the NASA atmospheric correction and OC2 algorithm, (b) Chl derived from the same data using the “nearest neighbor” correction algorithm and Carder semianalytic algorithm, (c) CDOM image computed using Carder’s semianalytic algorithm, and (d) salinity image derived from a_{9400} .

Figure 3. SeaWiFS images of Chl (mg m^{-3}) acquired on (a) 4th October 1997 and (b) 31st January 1998 and processed using the NASA atmospheric correction, the Siegel near-infrared iterations and the OC4 bio-optical algorithms.

optical properties of the dissolved material permitting derivation of the salinity field from the optical field (Blough *et al* 1993; D’Sa *et al* 2000; Hu *et al* 2002). A relationship between sea surface salinity (SSS) and CDOM absorption at 400 nm ($\text{SSS} = 35.71 - 6.954 \times a_g 400$) was found from field measurements (Jennifer Patch, USF, personal comm.) and was used to derive SSS maps from satellite data (figure 1d). Similarly, correlation between CDOM and sea surface salinity in the continental margin of NE Gulf of Mexico was reported to be consistently high ($r^2 \sim -0.85$ or higher for >7500 data points), suggesting it can be used effectively to obtain salinity estimates from satellite data (Hu *et al* 2002). Figure 2(a) shows the Chl estimates obtained with the default NASA algorithm, while figure 2(b) shows Chl estimates obtained with the “nearest neighbor” correction and Carder semianalytic algorithm applied

to a SeaWiFS image of 24th February 1999. We again observe lower Chl estimates for both coastal and offshore regions of the Bay and Shelf. CDOM absorption at 400 nm was further determined (figure 2c) using the semianalytic algorithm and salinity field derived (figure 2d) from the absorption image. Figures 3(a) and 3(b) correspond to two SeaWiFS images of 4th October 1997 and 31st January 1998 processed with SeaWiFS processing software (SeaDAS V4.1) for the Florida Bay region. Field data obtained during the above days correspond to a generally warm wet season (May to October) and a cooler dry season (November to April). Sea surface salinity and *in situ* bio-optical variables (Chl, CDOM absorption, Secchi depth) were obtained along two transects (field stations shown as triangles in figures 4a and 4b) at the western and central regions of the Bay (D’Sa *et al*

Figure 4. CDOM absorption field at 400 nm derived for the SeaWiFS image of (a) 4th October 1997 and (b) 31st January 1998 and computed using the “nearest neighbor” correction algorithm and Carder semianalytic algorithm.

Figure 5. A comparison of Chl derived from (a) 4th October 1997 and (b) 31st January 1998 SeaWiFS data versus *in situ* measurements at stations in the Florida Bay shown in figures 4(a and b) (triangles). The SeaWiFS data were processed using the “nearest neighbor” correction algorithm and Carder semianalytic algorithm.

2002). The Gulf of Mexico influences the western region of the Bay, while the central Bay is a hydrographically isolated area influenced by terrestrial freshwater inputs (Boyer *et al* 1999). The range in Chl distributions (0.88 to 6.5 mg m⁻³)

along the western transect were similar during the two seasons and generally increased at stations to the north. However, at the central stations the range of high Chl concentrations (4.6 to 14.9 mg m⁻³) observed in October 1997 were

Figure 6. A comparison of SeaWiFS-derived CDOM absorption at 400 nm of (a) 4th October 1997 and (b) 31st January 1998 versus *in situ* measurements at stations shown in figures 4(a and b) (triangles). The SeaWiFS data were processed using the “nearest neighbor” correction algorithm and Carder semianalytic algorithm. The solid line is a linear regression fit for the estimated and measured CDOM absorption data. The coefficient of determination (r^2), intercept and slope are given.

absent in January 1998 (0.5 to 0.9 mg m^{-3}). This resulted in the Secchi disk being visible at the bottom for all the stations in the central region. Bottom reflectance would thus obviously affect the remote sensing signal in this region. CDOM absorption was generally higher at the central stations and increased to the north due to terrestrial inputs.

The SeaWiFS derived Chl images (figures 3a and 3b) were obtained using the atmospheric correction scheme (Gordon and Wang 1994), the Siegel iterative approach, and the OC4 band ratio algorithm. We observe a larger fraction of the Chl pixels being retrieved in the October (figure 3a) than the January image (figure 3b), although most pixels corresponding to the location of the field

stations were not retrieved for both the data sets. In comparison, we observe a much higher percentage of retrieval (CDOM as well as Chl) when using the “nearest neighbor” atmospheric correction scheme together with the Carder semianalytic algorithm (figures 4a and 4b). Although there was a high correlation between SeaWiFS derived and *in situ* measurements (figure 5a), SeaWiFS derived Chl was overestimated for all stations for the October 1997 image. For the 31st January 1998 SeaWiFS data, large overestimates of SeaWiFS-derived Chl were all associated with the central Bay stations (figure 5b). At all these stations, the bottom was visible, suggesting that bottom reflectance clearly contributed to the water leaving radiance that resulted in Chl overestimates. Previous studies (Stumpf *et al* 1999) have also indicated high reflectance due to bottom effects at the central region of the Bay in winter. The CDOM absorption field (a_g400) derived from SeaWiFS data for October 1997 and January 1998 (figures 4a and 4b) are compared to *in situ* CDOM absorption measurements at the same wavelengths (figures 6a and 6b). We observe that although they are well correlated, the SeaWiFS-derived estimates of CDOM absorption underestimated *in situ* measurements for both images. These results suggest that the general parameters used in the Carder semianalytic algorithm may have to be tuned locally, i.e., for bio-optical conditions encountered in Florida Bay. Besides, the seasonal effect of bottom reflectance may also have to be accounted for in future bio-optical algorithms for the region.

In summary, these and previous results (Carder *et al* 1999; Hu *et al* 2002) indicate improved performance of the turbid-water atmospheric correction algorithm and the Carder semianalytic algorithm for chlorophyll estimates for CDOM-rich waters. The application of the turbid-water atmospheric correction or the aerosol propagation scheme provides important advantages as it can be applied to unknown water types such as estuaries or shallow waters where bottom reflection contributes to the visible bands. The use of the multi-waveband semianalytic algorithm enabled differentiation between Chl and CDOM in coastal waters. In specific regions such as the Florida Bay, the need to account for bottom reflectance (Lee *et al* 1994) and tuning of parameters used in the bio-optical algorithm will be necessary in order to improve estimates of Chl and CDOM. CDOM maps provide important information on salinity field especially in coastal waters where often there is conservative mixing. In coastal estuaries, these derived phytoplankton pigment and salinity distributions can be used for coastal management to monitor and predict the health of the ecosystem.

Acknowledgements

This work has been supported by the National Aeronautics and Space Administration (NASA Grants NAG-3446, NAG5-6448, NAS5-97128 and NAG5-10738). We thank two anonymous reviewers for their comments and suggestions.

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