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Developing Ocean Color Algorithm using Moderate Resolution Imaging Spectroradiometer (MODIS) Sensor for Shallow Coastal Water Bodies

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FLORIDA INTERNATIONAL UNIVERSITY

Miami, Florida

DEVELOPING OCEAN COLOR ALGORITHM USING MODERATE RESOLUTION
IMAGING SPECTRORADIOMETER (MODIS) SENSOR FOR SHALLOW
COASTAL WATER BODIES

A thesis submitted in partial fulfillment of the

requirements for the degree of

MASTER OF SCIENCE

in

ENVIRONMENTAL STUDIES

by

Mohd Manzar Abbas

2018

To: Dean Michael R. Heithaus
College of Arts, Sciences and Education

This thesis, written by Mohd Manzar Abbas, and entitled Developing Ocean Color Algorithm Using Moderate Resolution Imaging Spectroradiometer (MODIS) Sensor for Shallow Coastal Water Bodies, having been approved in respect to style and intellectual content, is referred to you for judgment.

We have read this thesis and recommend that it be approved.

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Dean Michael R. Heithaus
College of Arts, Sciences and Education

Andrés G. Gil
Vice President for Research and Economic Development
and Dean of the University Graduate School

Florida International University, 2018

DEDICATION

I would like to dedicate this thesis to my family. I am thankful for their love and support.

ACKNOWLEDGMENTS

I would also like to thank the members of my committee Leonard J. Scinto, Jennifer S. Rehage and especially my major advisor Assefa M. Melesse for all their guidance and support. I would like to acknowledge my family and colleagues that provided encouragement and support throughout the duration of the program. Finally, I am thankful to the Department of Earth and Environment, Florida International University for funding my education.

ABSTRACT OF THE THESIS
DEVELOPING OCEAN COLOR ALGORITHM USING MODERATE RESOLUTION
IMAGING SPECTRORADIOMETER (MODIS) SENSOR FOR SHALLOW
COASTAL WATER BODIES

by

Mohd Manzar Abbas

Florida International University, 2018

Miami, Florida

Professor Assefa M. Melesse, Major Professor

This study analyses the spatial and temporal variability of chlorophyll-a in Chesapeake Bay; assesses the performance of Ocean Color 3M (OC3M) algorithm; and develops a novel algorithm to estimate chlorophyll-a for coastal shallow water. The OC3M algorithm yields an accurate estimate of chlorophyll-a concentration for deep ocean water (RMSE=0.016), but it failed to perform well in the coastal water system (RMSE=23.17) of Chesapeake Bay. A novel algorithm was developed which utilizes green and red bands of the Moderate Resolution Imaging Spectroradiometer (MODIS) sensor. The novel algorithm derived the chlorophyll-a concentration more accurately in Chesapeake Bay (RMSE=4.20) than the OC3M algorithm. The study indicated that the algorithm that uses red bands could improve the satellite estimation of chlorophyll-a in the coastal water system by reducing the noise associated with bottom reflectance and colored dissolved organic matter (CDOM)

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Chapter 1

1 Introduction

1.1 Background

Phytoplankton are micro autotrophs that play a major role in food production and oxygen generation for aquatic organisms. However, a disproportional increase in phytoplankton biomass may result in algal blooms. There are certain species of phytoplankton that produce bio-toxins (Van Dolah, 2000). Proliferation of these species, also called harmful algal bloom (HAB), causes serious impact on marine and human health (Van Dolah, 2000). Understanding the phytoplankton population and its distribution enables researchers to draw conclusions about the health, composition, and ecological status of a body of water. Since chlorophyll-a exists in every species of phytoplankton (Mélin and Hoepffner, 2011), its concentration is estimated as a proxy for distribution of phytoplankton biomass (Cullen, 1982, Dore et al., 2008). The conventional method of chlorophyll-a estimation requires water sample collection and laboratory analysis (Joint and Groom, 2000b). This method, tedious and time consuming, is unsuitable for large spatial and temporal scales. Satellite-based sensors are used for the synoptic assessment of chlorophyll-a at large temporal and spatial scales.

After the launch of the first satellite borne ocean color sensor, the Coastal Zone Color Scanner (CZCS), improved sensors with higher precision, and an increased number of

bands have been launched (O'Reilly et al., 1998). Currently, one operational ocean color sensor, Moderate Resolution Imaging Spectroradiometer (MODIS) aqua, collects data in 36 spectral bands with 1-2 days of temporal resolution. The default chlorophyll-a retrieving algorithm for MODIS aqua, the Ocean Color 3M (OC3M) algorithm, is a blue-green band ratio algorithm (Blondeau-Patissier et al., 2014).

1.2 Statement of the problem

In spite of the development of advanced and precise sensors, the error in the satellite estimation of chlorophyll-a concentration in coastal waters is sufficiently high (Darecki and Stramski, 2004). Researchers have classified the ocean water area as case 1 and case 2 water. The optical property of the surface of deep ocean water is dominated by phytoplankton and is termed as case 1 water (Morel and Prieur, 1977). In coastal regions, the optical property of water is influenced by colored dissolved organic matter (CDOM), bottom reflectance, and total suspended matter (TSM), and is referred as case 2 water. The blue-green band ratio strongly correlates to chlorophyll-a concentration in case 1 water, however, in case 2 waters, the correlation becomes weak (Schalles, 2006). Furthermore, owing to its low attenuating tendency, the green band is heavily influenced by bottom reflectance in shallow coastal water (Carder et al., 2005a). The OC3M algorithm that uses the blue-green band ratio has been shown to yield accurate results in case 1 waters (Moses et al., 2009). However, the band ratio overestimates the chlorophyll-a in case 2 waters (Darecki and Stramski, 2004).

1.3 Justification of the study

Over 50% of the world population lives in coastal zones (Richardson and LeDrew, 2006), and coastal water is important for human interest such as fisheries and recreation. Primary production in coastal areas influences fisheries, eutrophication, and algal blooms that affect human population. Ocean color data from a satellite-based sensor are the only practical tools for the global assessment of spatio-temporal variation in phytoplankton population. The long record of MODIS ocean color data of coastal regions could not be utilized due to lack of a precise algorithm for the chlorophyll-a estimation. A robust algorithm would make use of all available data and will have a significant effect on the understanding of various factors that regulate primary productions in the ocean water. Furthermore, precise assessment of phytoplankton biomass would help researchers to understand models of flux of atmospheric carbon dioxide to the ocean, and the influence of anthropogenic contaminants on the marine ecosystem (Joint and Groom, 2000a).

In the past, several algorithms have been developed for case 2 waters using the optical property of chlorophyll-a in red and near infra-red (NIR) bands. Gons et al. (2002) used an algorithm based on backscattering coefficients at NIR bands to retrieve the chlorophyll-a concentration. Gilerson et al. (2010) used an algorithm based on the ratio of a red to NIR band. Blakey et al. (2016) developed the Benthic Class Specific algorithm to reduce the noise due to bottom reflectance. However, these algorithms have a limited application. Applicability of the Benthic class specific algorithm is contingent on the availability of Sea

Grass Density data at the location. To utilize the treasure of MODIS ocean color data of coastal regions, a precise algorithm is required that will use the wave bands for which MODIS reflectance data are available.

1.4 Research questions

Considering the available problem in the satellite estimation of chlorophyll-a in the coastal water, this study addressed the following research questions.

- 1 How does the chlorophyll-a concentration changes spatially and temporally in Chesapeake Bay?
- 2 How does the ocean color 3M (OC3M) algorithm perform in shallow coastal water and deep ocean water? and,
- 3 What other band combinations estimate chlorophyll-a concentration more precisely than the existing algorithm?

1.5 Objectives

To develop a robust ocean color algorithm for shallow coastal water, and to address the above research questions, the following specific objectives were proposed:

- 1 To analyze the spatial and temporal variation in the chlorophyll-a concentration of Chesapeake Bay,

- 2 To assess the performance of the MODIS Aqua OC3M algorithm in estimating chlorophyll-a concentration in the coastal water system of Chesapeake Bay, and
- 3 To develop an improved chlorophyll-a retrieving algorithm for the coastal water system of Chesapeake Bay.

Chapter 2

2 Literature Review

2.1 Principle of chlorophyll-a estimation using remote sensing

It has been established that chlorophyll-a absorbs more radiations in blue and red bands than in green bands. As a result, the color of ocean water shifts from blue to green while the concentration of chlorophyll-a increases (Yentsch, 1960). Similarly, other constituents in ocean water have different absorbance tendencies to the light of different wavelengths. Satellite-based sensors measure upwelling radiance in different wavebands that are selected to discriminate chlorophyll-a from other compounds. On the basis of field observation of chlorophyll-a and observed radiance at different wavebands, empirical ocean color algorithms are developed that can derive chlorophyll-a concentration of the ocean at a global scale (Dierssen, 2010).

2.2 Ocean color sensors and their features

The first ocean color sensor, the Coastal Zone Color Scanner (CZCS), launched by NASA on October 23, 1978 (Mitchell, 1994), was designed to capture data in 6 spectral bands: 433-453, 510-530, 540-560, 660-680, 700-800 and 10500-12500nm (Hovis et al., 1980). Considering the strong absorbing property of chlorophyll-a at 443nm and very weak absorptions at 520nm and 550nm (Gordon et al., 1980), the four bands centered at 443,

520, 550 and 670nm were mainly selected with the purpose to study ocean color. The feasibility of satellite based monitoring concept was verified with the launch of CZCS. Additionally, spatially and temporally cohesive data of chlorophyll-a were obtained around the globe from October 1978 to June 1986 (O'Reilly et al., 1998).

Gordon et al. (1980) noted that phaeopigment could not be distinguished from chlorophyll-a with the bands available on the CZCS, as both of them possess the same backscattering property at available bands (Gordon et al., 1980). Because CZCS did not have a dedicated recorder, it was not able to collect global data continuously (Council, 2011). Another shortcoming of CZCS was the lack of a near-infrared (NIR) band that could be utilized for atmospheric correction (Evans and Gordon, 1994). All these shortcomings were considered while deciding on wave bands for future sensors. After the CZCS, sensors with advanced precision and increased wavebands were designed and launched with the aim of reducing errors in satellite estimation of chlorophyll-a. Table 2.1. presents a summary of various sensors.

Table 2.1 Specification of satellite borne ocean color sensors

| Sensor | Satellite | No. of bands | Launch Date | Spatial Resolution (m) | Temporal Resolution (Day) | References |
|---------|------------|--------------|-------------|------------------------|---------------------------|---------------------------|
| CZCS | Nimbus 7 | 6 | 10/24/1978 | 825 | 6 | (Gholizadeh et al., 2016) |
| OCTS | ADIOS1 | 12 | 08/17/1996 | 700 | 3 | (Kawamura et al., 1998) |
| SeaWiFS | OrbView-2 | 8 | 08/01/1997 | 1100 | 1 | (Babin et al., 2008) |
| OCM 1 | OCEANSAT-1 | 8 | 05/26/1999 | 350 | 2 | (Dash et al., 2012) |
| MODIS | Terra | 36 | 12/18/1999 | 250-1000 | 1-2 | (Streets et al., 2013) |
| MERIS | Envisat-1 | 15 | 03/01/2002 | 1200 | 1 | (Gholizadeh et al., 2016) |
| MODIS | Aqua | 36 | 05/04/2002 | 250-1000 | 1-2 | (Streets et al., 2013) |
| OCM-2 | OCEANSAT-2 | 8 | 09/23/2009 | 1000-4000 | 1-2 | (Chauhan et al., 2009) |
| VIIRS | NPP-Suomi | 22 | 10/28/2011 | 375-750 | 0.5-1 | (Gholizadeh et al., 2016) |

SeaWiFS was the follow up sensor to CZCS. It was equipped with two bands in near-infrared region with the purpose of atmospheric correction. The signal to noise ratio (SNR) was high for visible bands which were able to detect small changes in ocean color due to chlorophyll (Council, 2011). Features that made SeaWiFS a robust piece of equipment includes real-time sensor performance evaluation, the sensor tilt capability, and lunar calibration capabilities (Eplee Jr et al., 2007). It was designed to gather data for five years but it continued to operate for 13 years (Hooker and McClain, 2000). The SeaWiFS sensor

was able to estimate global ‘water leaving reflectance’ and chlorophyll-a concentration with about 5 and 35 percent uncertainty, respectively in case 1 water (Chen et al., 2013). The overall system calibration uncertainty for SeaWiFS was as low as 0.3 percent (Council, 2011).

After the success of SeaWiFS, the MODIS sensors were launched onboard spacecraft Terra in 1999 and spacecraft Aqua in 2002. Owing to inefficient radiometric stability, MODIS Terra has limited utilization for the ocean color purpose (Gordon and Franz, 2008). MODIS Aqua has similar ocean color capabilities as SeaWiFS (Esaias et al., 1998). In addition, few wavebands are included in MODIS that could measure chlorophyll fluorescence (Behrenfeld et al., 2009). With improvement in solar diffuser and spectro-radiometric calibration assembly, instrument calibration for MODIS is far better than SeaWiFS. Unlike SeaWiFS, MODIS does not have the ability to evade sun glint by tilting. The problem of sun glint was supposed to be solved by two MODIS sensors orbiting complementary to each other, one in the morning and another in the evening. However, with problems in the performance of MODIS Terra, the plan was unsuccessful (Council, 2011). According to Esaias et al. (1998), notable improvement was made in radiometric capabilities. Overall, sensitivity of MODIS sensor is 2 to 3-fold more than that of SeaWiFS, making it possible to estimate chlorophyll-a concentration with uncertainty of approximately 20 percent in case 1 water.

In March 2002, the European Space Agency launched Medium Resolution Imaging Spectrometer (MERIS), with the primary goal of ocean color mapping. The MERIS has a unique feature: the width and position of wavebands at which it acquires data could be adjusted and controlled from the ground while the sensor is in orbit (Bezy et al., 2000). The MERIS uses dual solar diffusers to keep track of sensors stability. Between 2002 and 2010, a degradation of 1.5 percent has been reported in the 443nm band. The success of the MERIS mission is mainly attributed to effective pre-launch characterization and calibration (Council, 2011).

2.3 Ocean color algorithms

Ocean Color algorithms derive chlorophyll-a concentration of near surface ocean water from remotely sensed ocean color data. Several algorithms have been developed for the satellite estimation of chlorophyll-a. Most algorithms use the absorbance of sunlight by chlorophyll and other constituents present in the water (Schalles, 2006).

2.3.1 Classification of ocean color algorithms

Ocean color algorithms could be broadly classified as semi-analytical algorithms and empirical algorithms.

2.3.1.1 Semi-analytical algorithms

In the semi-analytical model, the combination of analytical and reflectance models is used to estimate the concentration of chlorophyll-a in the water (O'Reilly et al., 1998). The semi-analytical models are potentially more useful because they allow for the derivation of other optically active substances that are present in the water, including CDOM and total suspended materials (O'Reilly et al., 1998). Major disadvantages of these models include: they are complex in their design, employ four or more radiance bands, and require accurate information about inherent optical properties (which require high spectral fidelity) in order to accomplish a target of accurate estimation of chlorophyll-a (O'Reilly et al., 1998, Chen et al., 2013).

2.3.1.2 Empirical algorithms

For the development of empirical algorithms, a statistical regression analysis of in-situ chlorophyll-a concentration data is performed with observed radiance data of that location (O'Reilly et al., 1998). The model is simple and its implementation is comparatively easy (Chen et al., 2013). However, if the relationship between optical property and chlorophyll-a concentration is geographically specific, and empirical algorithm developed using optical data of one location could not be used for another location (Chen et al., 2013). Empirical algorithms have been shown to estimate chlorophyll-a concentration more precisely than the semi-analytical algorithms (O'Reilly et al., 1998). Depending on the sensor and

available bands, empirical algorithm use two, three or four bands to retrieve chlorophyll-a concentration from the reflectance data (Dierssen, 2010).

2.3.2 Default algorithm used with major ocean color sensors

The ocean color 4 (OC4) algorithm was developed by O'Reilly for the SeaWiFS sensor, using the blue-green band ratio (O'Reilly et al., 1998). Radiance-chlorophyll data from 919 stations were collected with chlorophyll concentration ranging from 0.019 mg m⁻³ to 32.79 mg m⁻³ (O'Reilly et al., 1998). The algorithm is a maximum band ratio formulation. The maximum band ratio approach has the advantage of maintaining the highest signal to noise ratio (SNR) for a wide range of chlorophyll concentration (O'Reilly et al., 1998).

The ocean color algorithms that are currently operational for MODIS (i.e. OC3M) and CZCS (i.e. OC3C) are the extension of the OC4 algorithm that has been modified according to bands available for these sensors (Blondeau-Patissier et al., 2014). The same form of equation is used in the OC4, OC3C and OC3M algorithms. The difference lies in coefficients of equations and bands being used as the blue and green band (Table 2.2).

$$\text{Chlorophyll-a} = 10^{a_0 + a_1 * X + a_2 * X^2 + a_3 * X^3 + a_4 * X^4} \quad (2.1)$$

Where,
$$X = \log_{10} \frac{\lambda_b}{\lambda_g}$$

Table 2.2 Coefficients and bands used with ocean color algorithms

| Algorithm | Blue | Green | a0 | a1 | a2 | a3 | a4 |
|-----------|-------------|-------|--------|---------|--------|---------|---------|
| OC4 | 443>490>510 | 555 | 0.3272 | -2.9940 | 2.7218 | -1.2259 | -0.5683 |
| OC3M | 443>488 | 547 | 0.2424 | -2.7423 | 1.8017 | 0.0015 | -1.2280 |
| OC3C | 443>520 | 550 | 0.3330 | -4.3770 | 7.6267 | -7.1457 | 1.6673 |

2.4 Major challenges in satellite estimation of chlorophyll-a in coastal water

Much research is ongoing to improve the satellite estimation of chlorophyll-a in coastal water. Three major factors that are affecting the remote estimation of chlorophyll-a include atmospheric correction, chlorophyll-a modelling, and scale effects.

2.4.1 Atmospheric correction

Ninety percent of the signals received by a satellite borne ocean color sensors are from atmospheric sources (Siegel et al., 2000). Atmospheric signals come from the atmospheric scattering of light, diffused and direct transmittance of the atmospheric column, and the contribution of ocean white cap. The atmospheric correction procedure is applied to eliminate signals from atmospheric sources and obtain water-leaving radiance data that are used for chlorophyll-a estimation (Siegel et al., 2000). Precise estimation of chlorophyll-a is highly dependent on the accuracy of the atmospheric correction procedure used to

acquire water leaving radiance. An error of 0.5 percent in the atmospheric correction magnifies to about 5 percent error in the processing of the water leaving radiance, and 5 percent error in water leaving radiance would lead to 35 percent error in chlorophyll-a estimation (Zeng et al., 2016).

The ‘clear water’ method used for the atmospheric correction utilizes the fact that no light will exit the water in NIR bands. Therefore, radiance obtained in NIR bands is assumed to be from atmospheric sources. The calculated signal in the NIR band is extrapolated to estimate the atmospheric signal in other bands. However, in coastal turbid water, the ‘clear water’ assumption is not valid (Zeng et al., 2016). The scattering of radiation from the total suspended materials present in coastal water overcomes the absorption of light in the NIR signals. Therefore, the ‘clearwater’ atmospheric correction method is not applicable for coastal turbid water, and its use is a major source of error in the calculation of water leaving radiance (Zeng et al., 2016) and therefore the chlorophyll-a estimation.

2.4.2 Chlorophyll-a concentration modelling

Chlorophyll-a concentration modelling is the basic problem in the satellite estimation of chlorophyll-a that needs to be addressed. The chlorophyll-a concentration around the globe varies from 0.01 to 1000 mg m⁻³ which makes the optical property of water globally variable, thereby resulting in inefficiency of a single algorithm (Schalles, 2006). Currently,

operational algorithms use the ratio of reflectance in the blue to green bands to derive chlorophyll-a concentration. However, the algorithm that uses the blue-green band ratio fails to accurately estimate chlorophyll-a in the turbid coastal water. Chlorophyll-a estimation using a waveband from red and NIR bands will be less biased than using a waveband from blue and green bands. This happens because light from a higher wave band is attenuated early, reducing noise due to bottom reflectance (Schalles, 2006). On the other hand, when chlorophyll-a concentration is less than 1 mg m^{-3} , it is difficult to discriminate water from chlorophyll-a using spectral reflectance of wavelength above 500nm. Therefore, algorithms that use absorption peak in red band is not suitable for low concentrations of chlorophyll-a (Schalles, 2006). These factors limit the development of a unified model for deep ocean and coastal water system.

2.4.3 Scale effect

Most of the algorithm are developed using a small study area. The chlorophyll-a concentration is homogeneous at the experimental scale; however, at the remote sensing scale the chlorophyll-a distribution becomes non-homogeneous. Li et al (1999) suggested that principles that are valid in small homogeneous system might not be valid at large non-homogeneous scale. It implies that chlorophyll-a concentration estimated using MODIS ocean color imagery at 1km pixel size may not be equal to the actual average concentration of chlorophyll-a in that location. Chen et al. (2013) noted that the scale effect leads to 1.29 percent under estimation of chlorophyll-a concentration using the OC3M algorithm.

Chapter 3

3 Materials and Methods

3.1 Description of the Study Area

The shallow water system of Chesapeake Bay (Figure 3.1) was chosen as the study area. The accuracy of satellite estimation of chlorophyll-a in the coastal region is associated with depth of the water (Ha et al., 2013), correlated with the distance from the shore. Therefore, the availability of long term in-situ chlorophyll-a concentration data at spatially varied distances from the coast with diverse bathymetry makes Chesapeake Bay a special study area for the development of an ocean color algorithm. The bay is a vast, shallow water system, up to 20 to 30 m deep at its central channel (Kemp et al., 2005). The complex bio-optical property of Chesapeake Bay's water is dominated by colored dissolved organic matter (CDOM), total suspended sediments and phytoplankton (Son and Wang, 2012).

The Chesapeake Bay is the largest estuary in North America and is located along the United States east coast, lying inland from the Atlantic Ocean. The Chesapeake Bay Watershed extends to an area of more than 64,000 miles that covers parts of Delaware, Maryland, New York, Pennsylvania, Virginia and West Virginia. The bay is classified as a highly productive water system (Boesch et al., 2001). The high productivity is associated with the excessive nutrient carried into the bay water by the rivers emptying into it (Ryberg et al., 2018).

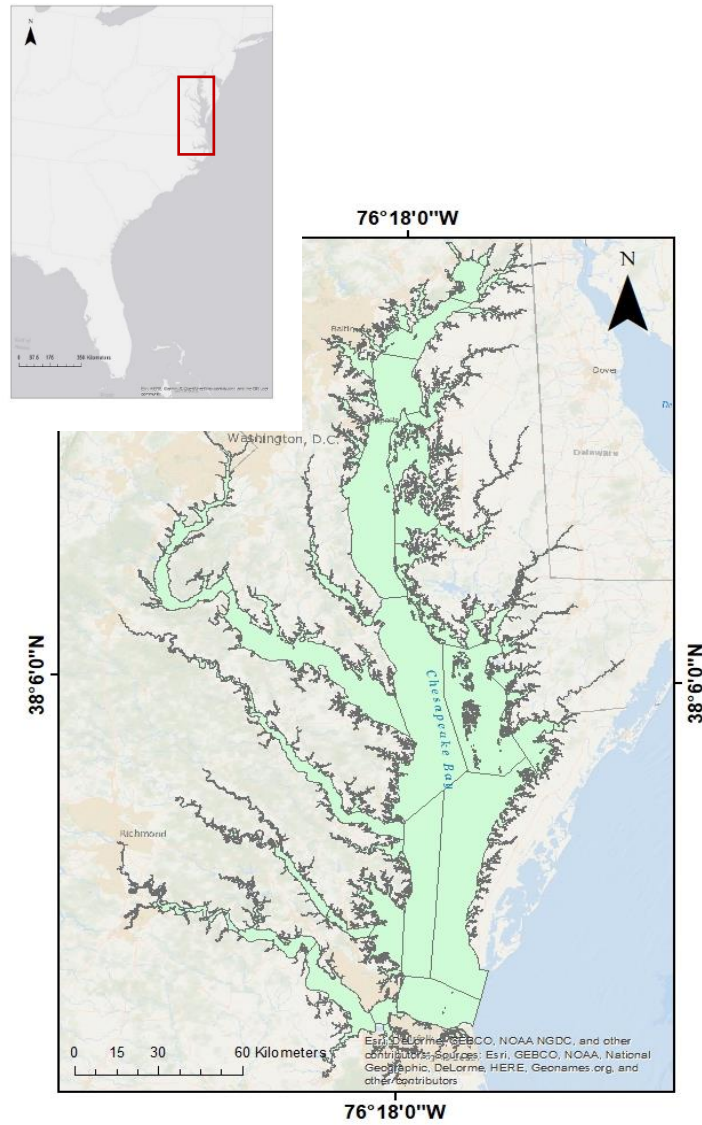


Figure 3.1 Map showing the location of Chesapeake Bay (Generated on ArcGIS 10.4 using Chesapeake Bay shape file)

The Chesapeake Bay Watershed is in the temperate geographical belt. The climatic conditions in the area vary from season to season. Mean monthly air temperature within the watershed varies from 0°C in January to 24°C in July (Mikhailov et al., 2009). Chesapeake Bay watershed receives a high volume of precipitation (1250mm annually) that generates an annual run-off equivalent to 400 mm. Most precipitation occurs from January to March consequently, 60% of the annual runoff is generated in March, April, and May (Mikhailov et al., 2009).

More than 150 streams and rivers flow into the Chesapeake Bay watershed. Major rivers that drains into the bay include the Susquehanna, James, York, Rappahannock, Potomac from the west, and the Wicomico, Nanticoke and Choptank from the east. The main source of fresh water inflow in Chesapeake Bay is the Susquehanna River, responsible for about 50% of the total inflow. The Susquehanna and Potomac Rivers carry 62 percent of the nitrogen and 44 percent of the phosphorus flux to the bay water (Ator et al., 2011).

Agricultural activities are quite common in the Chesapeake Bay watershed. More than 25 percent of watershed area is utilized for agricultural activities. Run-off from agricultural lands is the major source of nitrogen (54%) and phosphorus (43%) loading in the Bay (Ator et al., 2011). The eastern shore of the bay inputs disproportionately a high amount of nutrients from agricultural fertilizers. In 2001, 49% of land area in this region was used for agriculture (Ator and Denver, 2015). Soils and sediments in the region are sandy and

permeable which promotes the movement of nutrients from source to streams and tidal waters (Ator and Denver, 2015).

The Chesapeake Bay witnesses frequent algal blooms and hypoxic conditions (Ryberg et al., 2018). The bay is a major economic resource for the neighboring states, and associated economic activities (fishing, tourism etc.) are highly dependent on the water quality. Considering the economic importance of the bay and its deteriorating condition, a major restoration project is underway (Powledge, 2005).

3.2 Data

3.2.1 In-situ chlorophyll-a data

The Chesapeake Bay Program (CBP) provides a long record of chlorophyll-a concentration data of the bay water at spatially diverse locations. The field-measured chlorophyll-a data, along with sampling dates and co-ordinates of the sampling locations, were downloaded from the CBP website (<http://data.chesapeakebay.net/WaterQuality>). Data from 285 monitoring stations (Figure 3.2a) were used for this study. In-situ observations from 52 sampling stations (Figure 3.2b) were used to obtain field-observed and remote sensing matchup pairs.

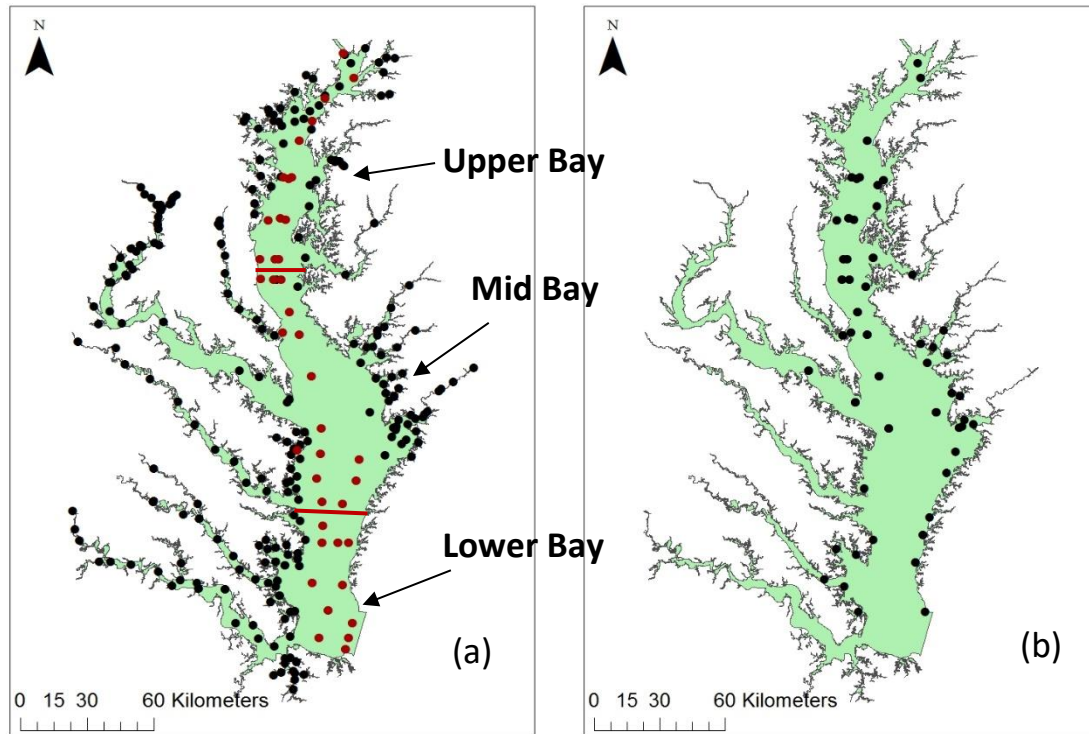


Figure 3.2 Map showing the locations of monitoring stations (a) Black and red dots denote stations used for the spatial and temporal analysis of chlorophyll-a. Red dots represent the locations of Central Bay (CB) Monitoring Stations as per the definition of the Chesapeake Bay Program. Red lines divide the main stream into three sections namely Upper Bay, Mid Bay and Lower Bay, according to the sectioning of Magnuson et al. (2004) (b) Monitoring stations used for the validation of the OC3M algorithm and development of a novel algorithm.

In-situ chlorophyll-a data for Sargasso Sea was obtained from the National Centre for Environmental Information (NCEI) database (<https://www.nodc.noaa.gov>). Chlorophyll-a samples were collected by the National Science Foundation (NSF) owned research vessel, *Oceanus*, in 2004 and 2005. The link to the data archive is: (<https://www.nodc.noaa.gov/archive/arc0030/0067471/1.1/data/>)

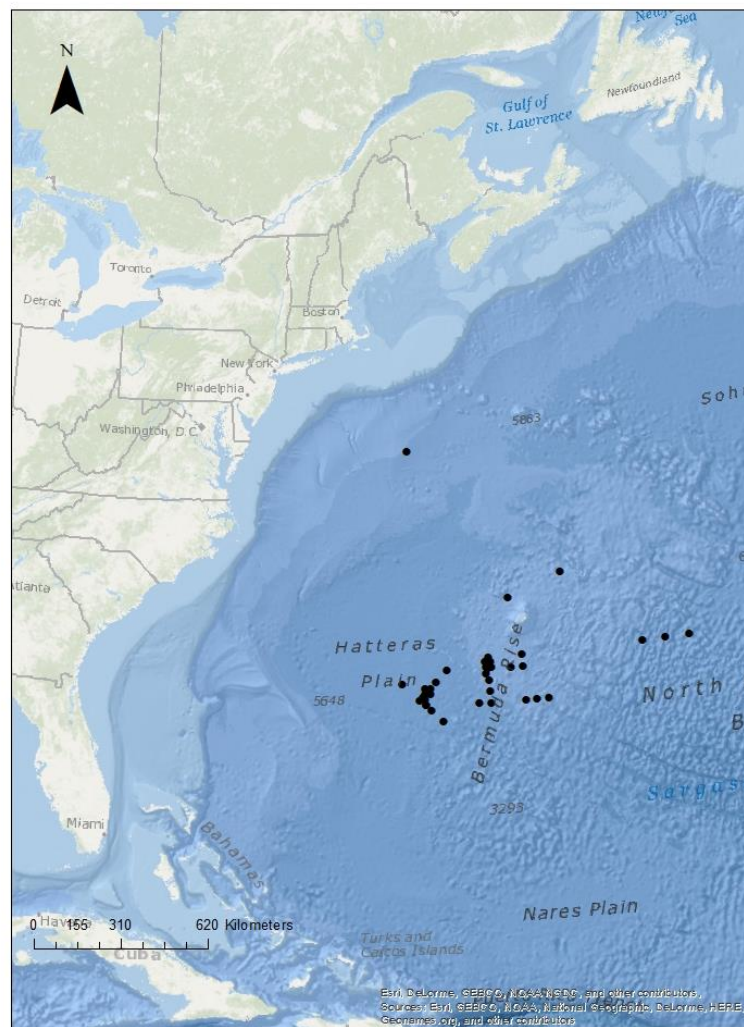


Figure 3.3 Map showing in-situ sampling locations (black dots) in the Sargasso Sea, Atlantic Ocean

Table 3.1. Summary of field observed chlorophyll-a data used in the study

| Purpose | Total Stations | Total samples | Period | Chlorophyll-a (mg m ⁻³) | | |
|---|----------------|---------------|---------|-------------------------------------|------|-------|
| | | | | Max | Min | Mean |
| Annual trend | 40 | 9601 | 2003-17 | 160.73 | 0.29 | 10.49 |
| Seasonal variability | 40 | 1383 | 2012-16 | 151.30 | 0.85 | 11.42 |
| Spatial Analysis | 285 | 10227 | 2012-16 | 1100.04 | 0.01 | 16.96 |
| Algorithm validation (Coastal Water) | 52 | 74 | 2012-16 | 63.36 | 1.78 | 9.26 |
| Algorithm Validation (Deep Water) | 25 | 25 | 2004-05 | 0.061 | 0.03 | 0.05 |
| Algorithm Development | 52 | 74 | 2012-16 | 63.36 | 1.78 | 9.26 |

3.2.2 Satellite Data

Remote sensing reflectance data from the MODIS sensor has been used for the study. MODIS acquires remote sensing data in 36 spectral bands. The swath width of viewing is 2330 Km. MODIS covers the entire earth in 1-2 days. The spatial resolutions of MODIS bands are 250, 500 or 1000m. Out of 36 bands, 10 bands are useful for ocean color studies (Table 3.2). The spatial resolution in these bands are 1000m.

Table 3.2. MODIS bands useful for ocean color studies

| Serial No | Wave Length (nm) | Band |
|-----------|------------------|-------|
| 1 | 412 | Blue |
| 2 | 443 | Blue |
| 3 | 469 | Blue |
| 4 | 488 | Blue |
| 5 | 531 | Green |
| 6 | 547 | Green |
| 7 | 555 | Green |
| 8 | 645 | Red |
| 9 | 667 | Red |
| 10 | 678 | Red |

The Ocean Biology Processing Group (OBPG) located at NASA’s Goddard Space Flight Centre, manages Ocean Color Web (OCW), and collects, validates, archives and distributes ocean-related remote sensing data. The MODIS ocean color level-2 data were downloaded for Chesapeake Bay (2012-2016) and Sargasso Sea (2004-2005) from OCW (<https://oceancolor.gsfc.nasa.gov/>) using the level-2 data browser. The level-2 data come in netCDF format; this format contains atmospherically corrected raster images of reflectance values at available bands. Swaths that contain the study area (Chesapeake Bay or Sargasso Sea) and dates for which in-situ data is available were the criteria to download the data.

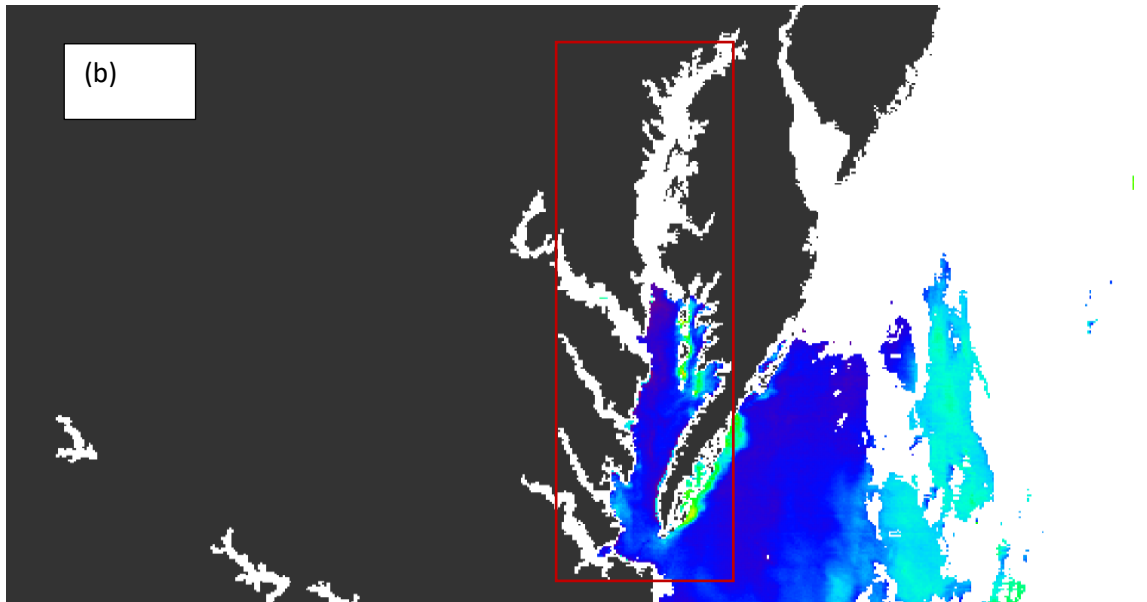
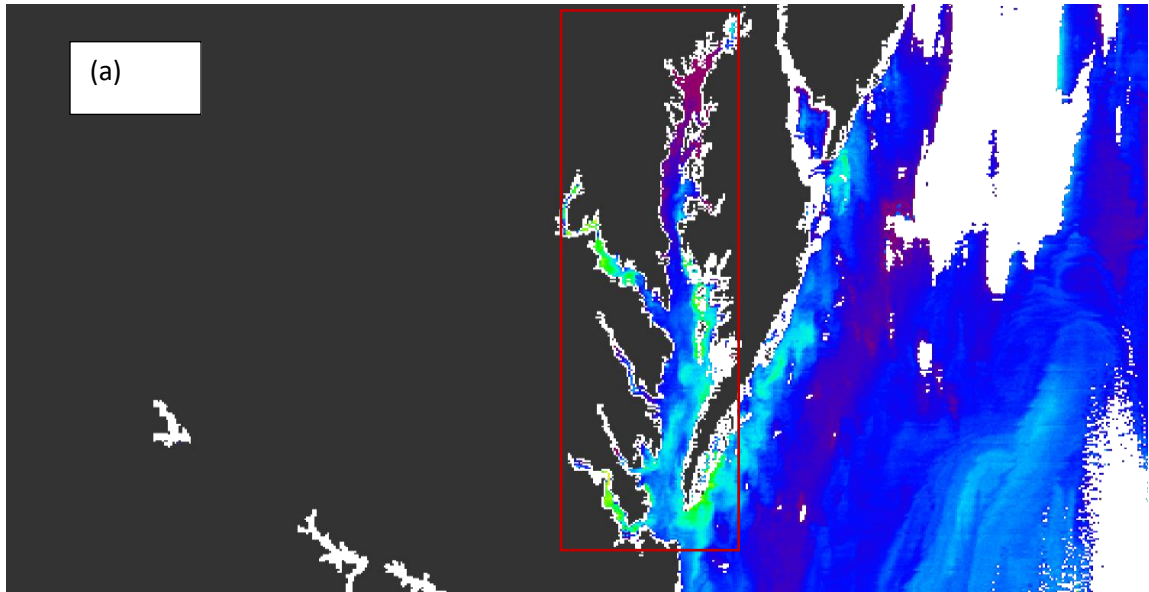


Figure 3.4 MODIS Imageries of the study area dated (a) 03.14.2014 (b) 05.10.2014, generated using SeaDAS. The red rectangle demarcates Chesapeake Bay

3.2.3 Ocean Color algorithm

Ocean color algorithm derives chlorophyll-a measure of water surface using remote sensing data. O'Reilly et al. (1998) developed an ocean color algorithm (i.e. OC4) for SeaWiFS that uses the ratio of reflectance in blue to green bands (O'Reilly et al., 1998). OC4 uses the maximum of reflectance in 443, 490 and 510 nm as blue band, and reflectance in 555nm band as the green band. The Ocean Color 3M (OC3M) algorithm currently operational for MODIS is an extension of the OC4 algorithm, that has been modified according to MODIS bands.

The OC3M algorithm is a polynomial relationship of the fourth-order between chlorophyll-a concentration and the ratio of reflectance at 443, 488 and 547 nm as input and gives chlorophyll-a concentration in mg m^{-3} as output.

$$\text{Chlorophyll-a} = 10^{a_0 + a_1 * X + a_2 * X^2 + a_3 * X^3 + a_4 * X^4} \quad (3.1)$$

$$X = \log_{10} \frac{\lambda_b}{\lambda_g} \quad (3.2)$$

Where λ_b is greater of R_{rs} at 443 and 488, and λ_g is R_{rs} at 547. The a_0 , a_1 , a_2 , a_3 and a_4 are constants whose values are 0.2424, -2.7423, 1.8017, 0.0015 and -1.2280, respectively.

3.3 Analyzing the temporal and spatial variability of chlorophyll-a

3.3.1 Annual variability of chlorophyll-a

The study area was divided into three sections; namely Upper Bay, Mid Bay and Lower Bay (Figure 3.2a). All CB monitoring stations from each section of the bay were selected as the representatives of that section. Mean annual chlorophyll-a concentrations at these monitoring stations were estimated from 2003 to 2017 to understand the inter-annual variability in chlorophyll-a in the three sections of Chesapeake Bay.

3.3.2 Seasonal and spatial variability in chlorophyll-a

The spatial and seasonal variability in chlorophyll-a was analyzed by: (1) Evaluating five-year mean concentrations (2012-2016) for spring (March, April and May) and summer (July, August and September) at CB monitoring stations and (2) Obtaining a chlorophyll-a map of Chesapeake Bay for spring and summer. Month of June was excluded from this study because it is a transition period from spring to summer and high variability in chlorophyll-a pattern is observed during this month (Buchanan et al., 2005). Observations from 285 monitoring stations were used for the development of chlorophyll-a map. Five-year mean chlorophyll-a concentration at each monitoring station were evaluated for spring and summer season. For each season, a single surface estimate of chlorophyll-a was assessed for each monitoring station. If chlorophyll-a data were collected at multiple depths, an average of all observations up to 1 meter of depth was estimated. Then, Kriging

interpolation was executed using ArcGIS 10.4 software to generate chlorophyll-a map for spring and summer. Additionally, standard deviations of observations at all monitoring stations in each season was estimated and interpolated to further understand the variance of concentrations during spring and summer in different part of Chesapeake Bay.

3.4 Validation of the OC3M algorithm

The present study analyzed the performance of currently operational OC3M algorithm in coastal water (Chesapeake Bay) and the mid ocean (Sargasso Sea). The MODIS level-2 data were matched with in-situ chlorophyll-a measurements using the sampling date and location. An in-situ observation and a single pixel of remote sensing data, covering the in-situ sampling location on the same day as the satellite flyover, were considered as a match-up pair. The OC3M algorithm was applied to the remote sensing pixels and algorithm-derived concentrations were compared with the corresponding in-situ measurements. The SeaDAS software, a software package for analysis of remote sensing ocean color data, was used for this purpose. Finally, the overall performances of the algorithm in Chesapeake Bay and Sargasso Sea were compared.

To further understand the seasonal performance of the OC3M algorithm in coastal water, Chesapeake Bay's matchup pairs were categorized according to seasons: spring, summer, autumn and winter (Table 3.3). Statistical parameters including Root Mean Square Error

(RMSE), Mean Absolute Percent Error (MAPE) and Mean absolute error (MAE) were derived to examine the accuracy of the OC3M algorithm in each season.

Table 3.3. Summary of the matchup data used for the performance evaluation of the OC3M algorithm in Chesapeake Bay, and development of the novel algorithm

| Seasons | 2012 | 2013 | 2014 | 2015 | 2016 | Total |
|---------|------|------|------|------|------|-------|
| Spring | 3 | 0 | 6 | 10 | 7 | 26 |
| Summer | 7 | 2 | 0 | 13 | 0 | 22 |
| Autumn | 7 | 1 | 0 | 9 | 0 | 17 |
| Winter | 0 | 0 | 1 | 8 | 3 | 12 |

Equations used to calculate statistical parameters

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (X-Y)^2}{n}} \quad (3.3)$$

$$MAE = \frac{\sum_{i=1}^n |X-Y|}{n} \quad (3.4)$$

$$MAPE = \frac{100}{n} \sum_{i=1}^n \left| \frac{X-Y}{X} \right| \quad (3.5)$$

where X = In-situ measurements, Y = Algorithm derived values and

n = Number of samples.

3.5 Development of a novel algorithm

Match-up pixels obtained in the previous study (Table 3.3) were used for this study. A novel algorithm was developed for coastal water (case 2) through regression analysis of the MODIS reflectance data against matching field-measured chlorophyll-a observations. In the coastal water, bottom reflectance and the presence of color dissolved organic matter (CDOM) yields an error in satellite estimation of chlorophyll-a using OC3M algorithm (Blakey et al., 2015). The OC3M algorithm uses blue-green band ratio that is susceptible to noise due to bottom reflectance and CDOM (Blondeau-Patissier et al., 2014). The red band has a tendency of attenuating early in water, and therefore it is less affected by bottom reflectance (Carder et al., 2005b). Furthermore, it is less sensitive to CDOM (Gilerson et al., 2010). An algorithm that uses the red band has been shown to yield a better estimate of chlorophyll-a concentration (Gilerson et al., 2010). Therefore, in this study the red band was included for the development of the algorithm.

The rationale behind selection of bands for the algorithm was based on the mesocosm tank experiment performed by Schalles et al. (1997). In that experiment, reflectance spectra was analyzed at different chlorophyll-a concentrations ranging from 0.4 to 62.2 mg m⁻³ (Figure 3.5). It could be observed from the plot that as the concentration increases, the peak at the green band becomes higher and depression at the red band becomes sharper. Therefore, the ratio of reflectance in green to red bands should correlate with chlorophyll-a concentration.

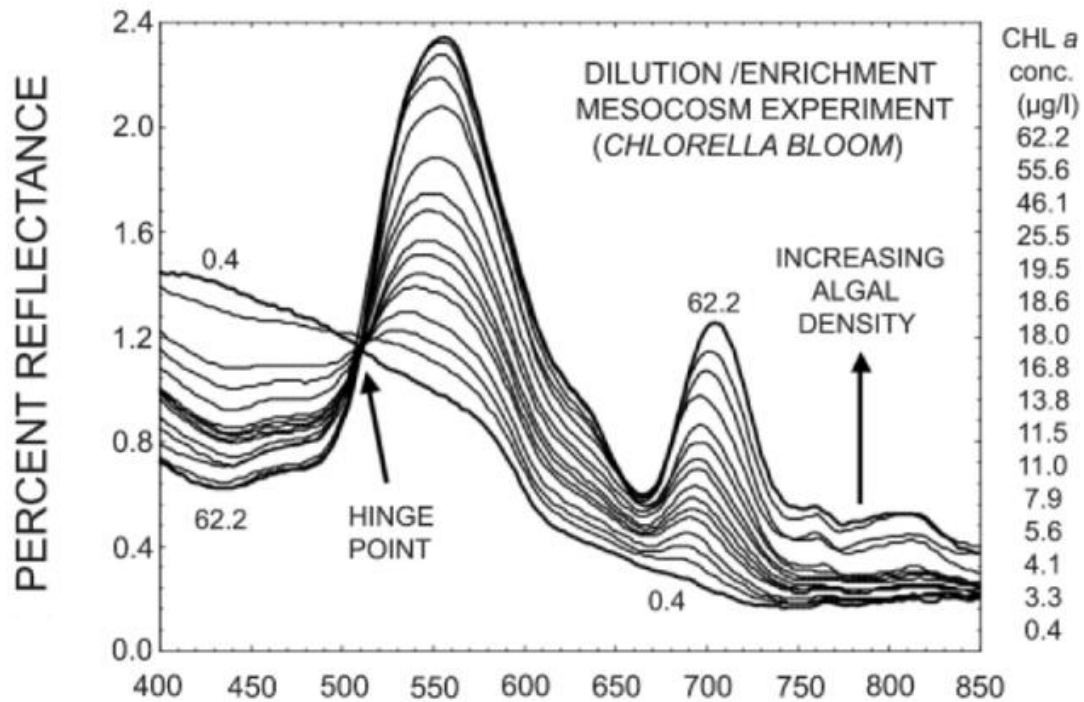


Figure 3.5 Reflectance spectra at different concentrations of chlorophyll-a obtained from mesocosm tank experiment (Schalles et al., 1997)

The peak in the green band shifts from 510nm to 560nm as the chlorophyll-a concentration increases (Figure 3.5). Similarly, trough in the red band moves between 660 to 680nm as the concentration changes. Therefore, band ratio formulation that uses maximum of reflectance at 531 and 551nm as numerator, and minimum of 667 and 678nm band as denominator, was adapted for this study. Regression analysis was performed using matchup pixels between logs of reflectance in the green/red band and In-situ chlorophyll-a concentrations to generate coefficients for a polynomial of order four used in the algorithm.

3.6 Test of the novel algorithm

The novel algorithm developed in this study was validated by using an independent test sample consisting of 42 pairs of match-up data. These match-up pairs were not used in the development of the algorithm. The algorithm-derived concentrations were compared with the corresponding in-situ measurements. Performances of the novel algorithm and OC3M algorithm were also compared using this data set.

Chapter 4

4 Result and Discussion

This section covers discussion on the results obtained by the study in three fragments. The first part discusses the temporal and spatial variability of chlorophyll-a concentration in the Chesapeake Bay. In the second part, the performances of OC3M algorithm in deriving chlorophyll-a concentration using MODIS data of deep ocean water and shallow water has been evaluated. The final part discusses the novel algorithm that has been developed in this study.

4.1 Temporal and spatial variability of chlorophyll-a in Chesapeake Bay

4.1.1 Annual variability of chlorophyll-a

The annual variation in chlorophyll-a from 2003 to 2017 was analyzed in the three sections (Upper Bay, Mid Bay and Lower Bay) of Chesapeake Bay. The time series of chlorophyll-a (Figure 4.1) exhibits that the annual concentration is variable in all three sections of Chesapeake Bay. For most of the years, concentration in the Upper Bay was highest, followed by Mid Bay and Lower Bay (except for 2003 when the highest concentration was observed in the Mid Bay). The highest mean chlorophyll-a (18.06 mg m^{-3}) was observed in the Upper Bay in 2014 whereas the lowest (4.31 mg m^{-3}) was observed in Lower Bay during 2017. The mean annual concentration in the Upper Bay varied between 12.23 to

18.06 mg m⁻³; whereas, the range of concentration in Mid Bay and Lower Bay were 8.02-16.80 mg m⁻³ and 4.31-12.41 mg m⁻³, respectively, during the study period.

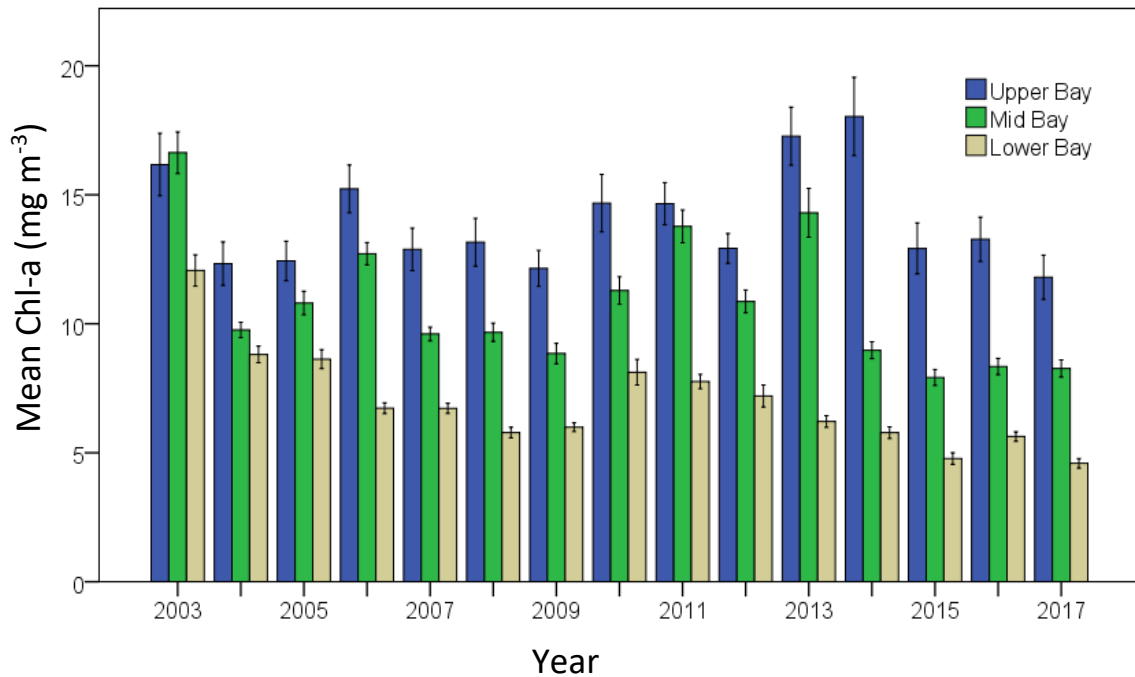


Figure 4.1 Time series of annual chlorophyll-a variability in the three sections of Chesapeake Bay. Error bars represent the standard error of mean.

The availability of nutrient is the main driving factor of phytoplankton growth in Chesapeake Bay. Nutrient loading in Chesapeake Bay is co-related with the fresh water inflow from the Susquehanna River (Harding Jr et al., 2016). The high variability in annual freshwater inflow from the Susquehanna River during the study period (Harding Jr et al., 2016) could explain the high annual variability in chlorophyll-a concentration of the Chesapeake Bay, as visible in the time-series graph (Figure 4.1).

4.1.2 Seasonal and spatial variability in chlorophyll-a

All CB monitoring stations located in each section of Chesapeake Bay were selected as the representatives of that section and mean chlorophyll-a concentrations at CB stations in spring and summer were estimated for the study period (2012-2016). The five-year average shows that the mean concentration of chlorophyll-a in Upper Bay and Mid Bay was higher during spring; whereas, the concentration in the Lower Bay was higher during summer (Figure 4.2).

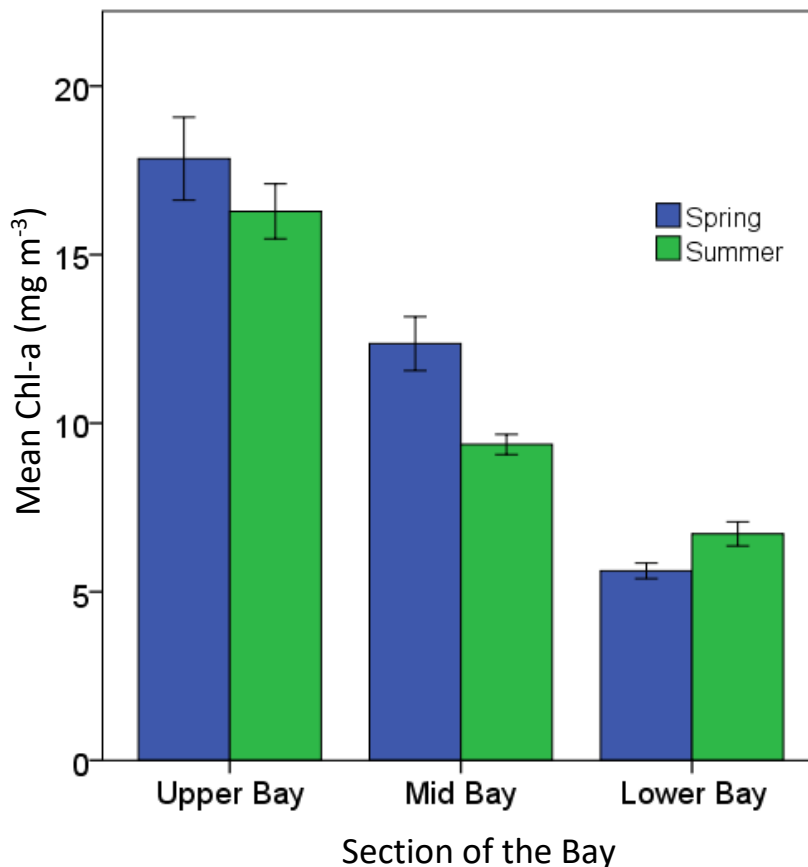


Figure 4.2 Graph showing the chlorophyll-a variability in the three sections of Chesapeake Bay during spring and summer. Error bars represent the standard error of mean.

The inter-seasonal difference was largest in the Mid Bay where concentrations during spring and summer were 12.42 mg m^{-3} and 9.21 mg m^{-3} , respectively. The difference was smallest in the Lower Bay where chlorophyll-a concentration varied from 5.58 mg m^{-3} during spring to 6.78 mg m^{-3} during summer.

The higher concentration of chlorophyll-a in the Upper Bay and Mid Bay during spring is because of a recurring phenomenon in Chesapeake Bay known as the spring phytoplankton bloom (Cercó, 2000). The spring bloom is triggered by the abundant availability of nutrients that drains into the bay with freshwater inflow from the Susquehanna River. However, the nutrient concentration in the Lower Bay might not be influenced by nutrient loading from the Susquehanna River due to long travel distance and the tidal mixing of water. The spring bloom is characterized by the growth of diatoms comprising *Skeletonema*, *Leptocylindrus*, and *Cyclotella* that begin in February and stays until May, resulting in the higher concentration of chlorophyll-a during spring (Cercó, 2000). The algal biomass produced during spring consumes the nutrient available in water. After their subsequent decay, the nutrients are released into the water that is source of nutrient availability during summer (Cercó, 2000). The reduced availability of nutrients during summer (Cercó, 2000) might explain the lower algal biomass and chlorophyll-a concentration during summer in the Upper Bay and Mid Bay.

Chlorophyll-a map of Chesapeake Bay was produced for spring and summer seasons by interpolating five-year (2012-16) mean chlorophyll-a concentrations at 285 monitoring stations in the respective seasons (Figure 4.3).

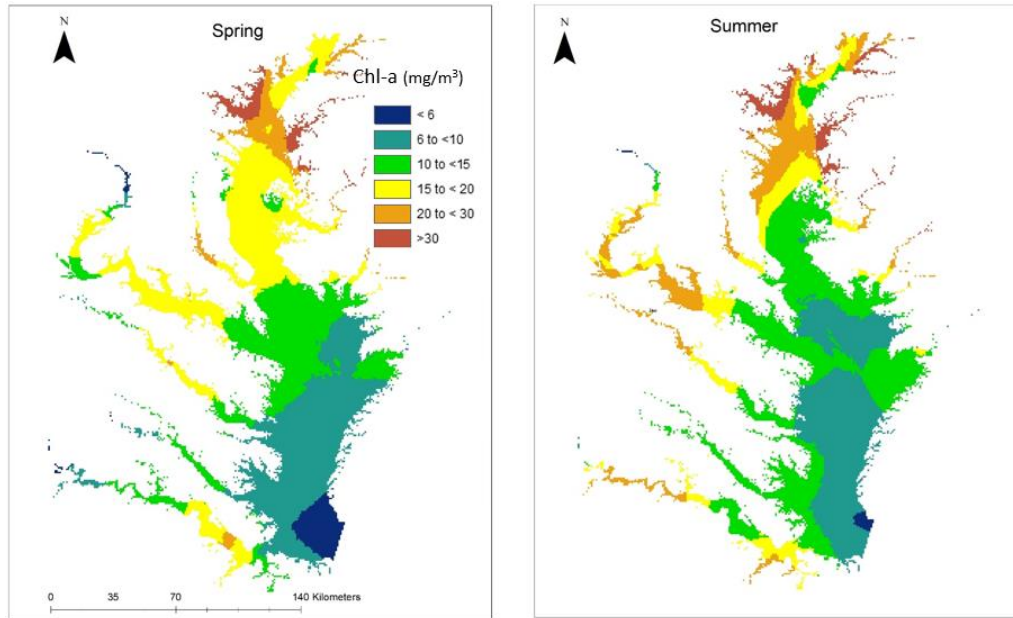


Figure 4.3 Interpolated map showing the chlorophyll-a variation in Chesapeake Bay during spring and summer. Observations from 2012 to 2016 were used for the analysis.

During spring and summer seasons, the chlorophyll-a concentration in the Upper Bay was highest followed by Mid Bay and Lower Bay. Concentrations in the Upper Bay and Mid Bay were generally higher in spring than that of summer; whereas, in Lower Bay the concentration during summer was higher than spring (Figure 4.3). At the head of Chesapeake Bay, where Patapsco River meets the Bay, the concentration was very high ($>30 \text{ mg m}^{-3}$), during both spring and summer. The chlorophyll-a level in all tributaries was higher than that of the main channel.

The elevated growth of phytoplankton leads to hypoxia condition that has detrimental effect on the marine ecosystem. The chlorophyll-a concentration is an indicator of the phytoplankton biomass (Graff et al., 2012). Based on salt regime and season, studies have defined the threshold chlorophyll-a concentrations (Table 4.1) for different parts of Chesapeake Bay (Buchanan et al., 2005, Lacouture et al., 2006, Williams et al., 2008). The water quality of a region is considered poor if the chlorophyll-a level in that region crosses the threshold concentration.

Table 4.1 Threshold chlorophyll-a concentration of Chesapeake Bay (Williams et al., 2008)

| Salinity Regime | Season | Threshold concentration (mg m ⁻³) |
|-----------------|--------|---|
| Oligohaline | Spring | ≤ 20.9 |
| Mesohaline | Spring | ≤ 6.2 |
| Polyhaline | Spring | ≤ 2.8 |
| Oligohaline | Summer | ≤ 9.5 |
| Mesohaline | Summer | ≤ 7.7 |
| Polyhaline | Summer | ≤ 4.5 |

The result reflects that during spring, the chlorophyll-a concentration in most of the regions of Chesapeake Bay was above the threshold concentrations. The chlorophyll-a concentration in part of the Upper Bay (oligohaline) was in the range of 15.0-20.0 mg m⁻³. However, the concentration in the rest of the Upper Bay was way above the threshold concentration of 20.9 mg m⁻³ for spring season. The concentration in the Mid Bay (Mesohaline) was between 10-20 mg m⁻³, about one-fold above the threshold concentration

of 6.2 mg m^{-3} . In most of the Lower Bay, chlorophyll-a concentration was above the threshold level of 2.8 mg m^{-3} . The concentration in a portion of Lower Bay was in the range of $0\text{-}6 \text{ mg m}^{-3}$, so it could not be determined whether the chlorophyll-a level was less than the threshold concentration of 2.8 mg m^{-3} or not.

The chlorophyll-a map of summer season (Figure 4.3) shows that the concentration in the entire Upper Bay was more than the threshold concentration. The chlorophyll-a concentration in the major part of the Mid Bay was in the range of $10\text{-}15 \text{ mg m}^{-3}$ whereas the threshold level in Mid Bay (Mesohaline) for summer season is 7.7 mg m^{-3} . The concentration in some parts of the Mid Bay was between $6\text{-}10 \text{ mg m}^{-3}$ class, so it could not be determined whether the chlorophyll-a level in this region was below the threshold concentration or not. Almost the entire region of the Lower Bay was above the threshold concentration of 4.5 mg m^{-3} , except for a tiny portion where the chlorophyll-a concentration could not be compared with the threshold level.

The higher concentration of chlorophyll-a in Upper Bay and Mid Bay during spring could be explained by the spring bloom that is a recurring phenomenon in Chesapeake Bay (Cercó, 2000). Very high chlorophyll-a in the region where Patapsco River meets the Bay water could be because of the excess nutrient loading from the river (Ator et al., 2011).

Standard deviations (SD) of chlorophyll-a observations during spring and summer were interpolated to obtain the concentration variance map for the two seasons. The result of the

analysis shows that the variance in chlorophyll-a concentration across different locations of Chesapeake Bay is higher during spring as compared to that during summer (figure 4.4). As observed from the variance map of summer, the SD of chlorophyll-a concentration differed at most places by a magnitude of <5 to <15 mg m^{-3} . However, the variance map of spring clearly demonstrates higher deviation in the concentration in some parts of the Upper Bay and tributaries as depicted by a SD value of >20 mg m^{-3} . The phytoplankton growth is very dynamic during spring due to the spring bloom. That might be the reason for higher variance during the spring season.

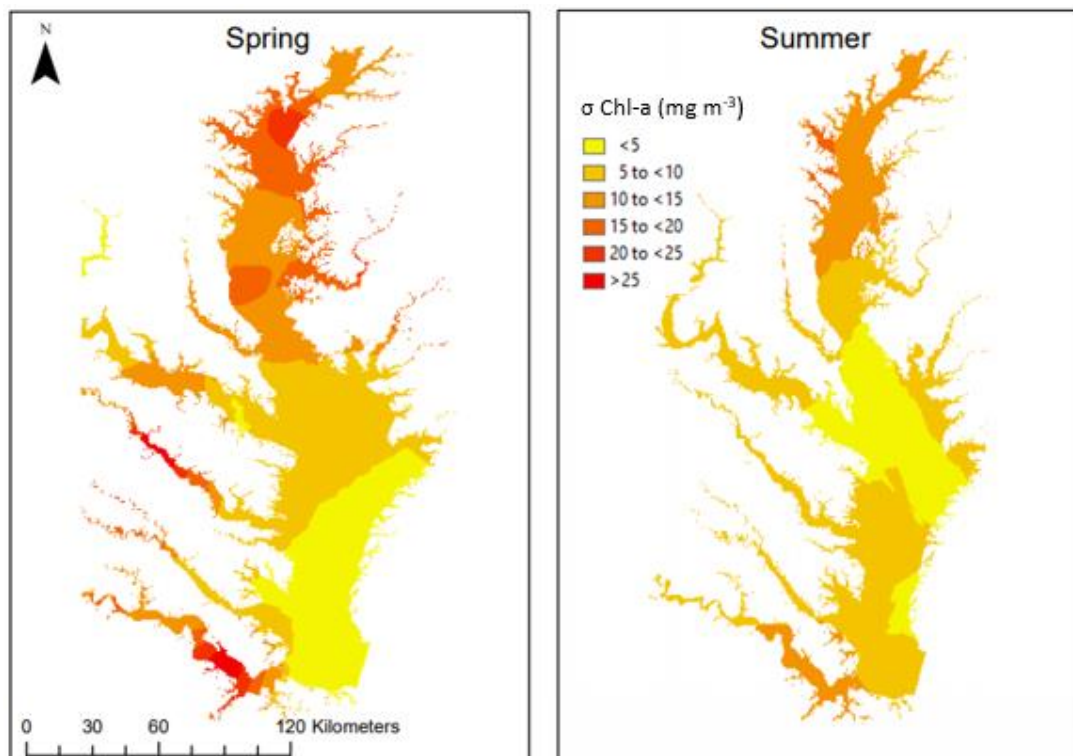


Figure 4.4 Map showing the variance of chlorophyll-a concentration during spring and summer in Chesapeake Bay.

4.2 Assessment of the satellite derived chlorophyll-a using OC3M algorithm

Field-measured chlorophyll-a data from Sargasso Sea (case 1) and Chesapeake Bay (case 2) were compared with the OC3M-derived chlorophyll-a concentrations for those regions, to evaluate the performance of OC3M algorithm in deep ocean water and shallow coastal water.

4.2.1 Deep ocean water (case 1)

In this analysis, 25 pairs of in-situ chlorophyll-a observations and co-incident MODIS reflectance data of Sargasso Sea were used. Chlorophyll-a concentrations were derived by applying OC3M algorithm on remote sensing data. The algorithm-derived concentrations were compared with matching ground truth observations. The scattered plot and clustered column shown in Figure 4.5 and 4.6, respectively, compare the algorithm derived and in-situ concentrations.

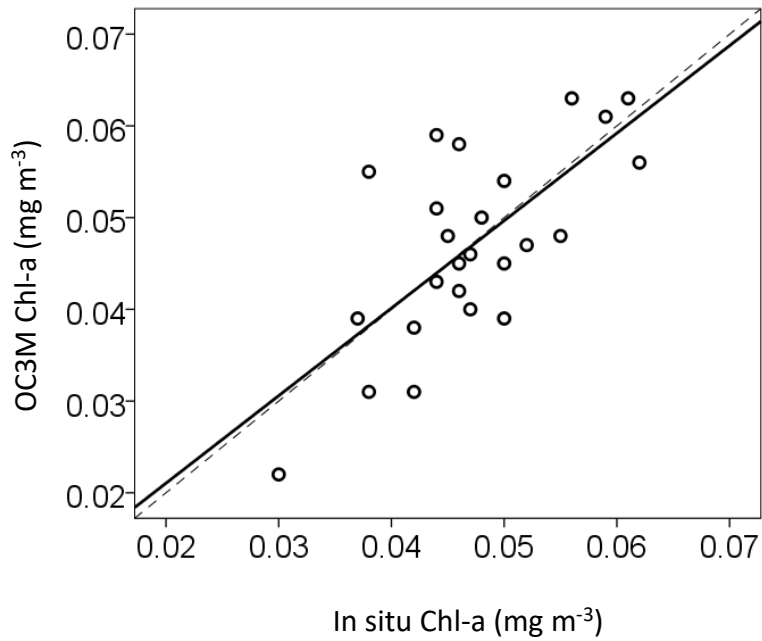


Figure 4.5 Plot compares the OC3M derived chlorophyll-a concentrations with ground truth concentrations in Sargasso Sea. The dotted line represents 1:1 line

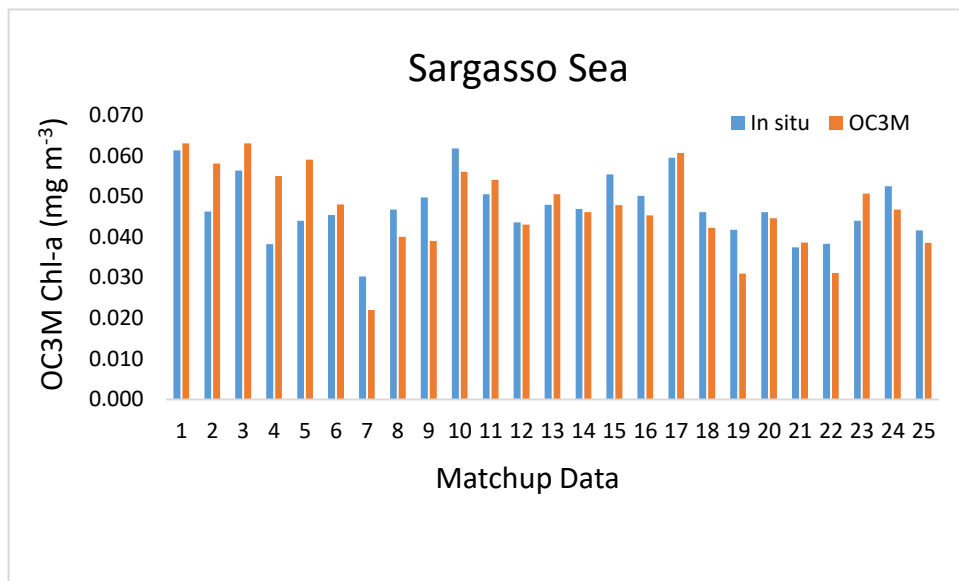


Figure 4.6 Clustered column compares the algorithm derived and in-situ chlorophyll-a concentrations in the Sargasso Sea.

The coefficient of determination obtained through this analysis is $r^2 = 0.494$ ($p < 0.001$). Bubbles in the scatter plot of the OC3M derived chlorophyll-a against in-situ observations is mostly located along 1:1 line. The cluster column shows the satellite estimated and ground truth concentrations are similar in most cases. Based on the obtained result, it could be said that the OC3M algorithm is performing well in the deep ocean water (case 1). The result supports the finding of previous studies that point towards good performance of the OC3M algorithm in deep ocean water (Moses et al., 2009).

4.2.2 Coastal Water (Case 2)

Seventy-four pairs of matchup pixels comprising of field observed chlorophyll-a data and co-incident remotely sensed reflectance data from MODIS were used to evaluate the performance of OC3M algorithm in the coastal water system of Chesapeake Bay. Algorithm derived chlorophyll-a concentrations were compared with the corresponding in-situ observations using a scatter plot (Figure 4.7) and a cluster column (Figure 4.8).

Points in the scatter plot are widespread. It is clearly visible in the cluster column that in most cases, the difference between the algorithm derived and in-situ concentrations are high (Figure 4.8). Most of the points in scatter plot are above 1:1 line which shows that the

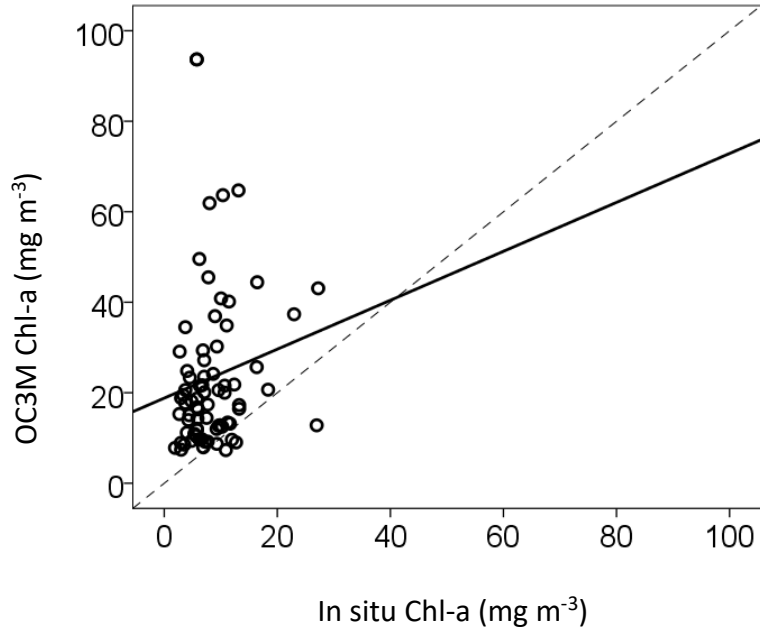


Figure 4.7 The scatter plot of OC3M derived and in-situ chlorophyll-a concentration in Chesapeake Bay. The dotted line represents 1:1 line

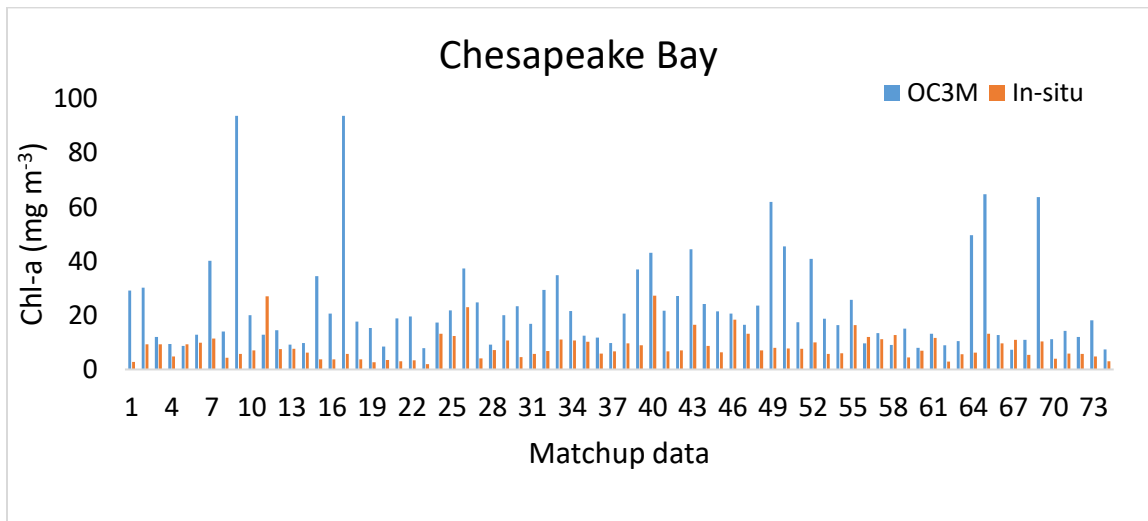


Figure 4.8 Cluster column compares the OC3M derived chlorophyll-a concentrations with corresponding ground truth concentrations

algorithm is over estimating the chlorophyll-a concentration in Chesapeake Bay. The result is in accordance with the finding of previous studies that the OC3M algorithm overestimates the chlorophyll-a concentration in Case 2 water (Gilerson et al., 2010).

Table 4.2 Statistics of the accuracy of OC3M derived chlorophyll-a in case 1 and case 2 water

| Water type | Algorithm | R ² | P-value | RMSE | MAE | MAPE |
|------------|-----------|----------------|---------|--------|-------|-------|
| Case 1 | OC3M | 0.492 | < 0.001 | 0.016 | 0.012 | 23.5 |
| Case 2 | OC3M | 0.023 | 0.195 | 23.174 | 15.6 | 246.7 |

The accuracy of OC3M algorithm in case1 and case2 water using MODIS reflectance data has been compared through different statistical methods (Table 4.2). The R², p-value, RMSE, MAE and MAPE calculated for two cases clearly show that the accuracy of OC3M algorithm in case1 water is satisfactory but the performance of the algorithm is not reliable in case 2 water.

To further determine the seasonal performance of the OC3M algorithm, the match-up pairs were divided into four groups according to seasons: spring (March, April, May), summer (July, August, September), autumn (October, November), and winter (December, January, February). Figure 4.9 shows the seasonal performance of OC3M algorithm in Chesapeake Bay.

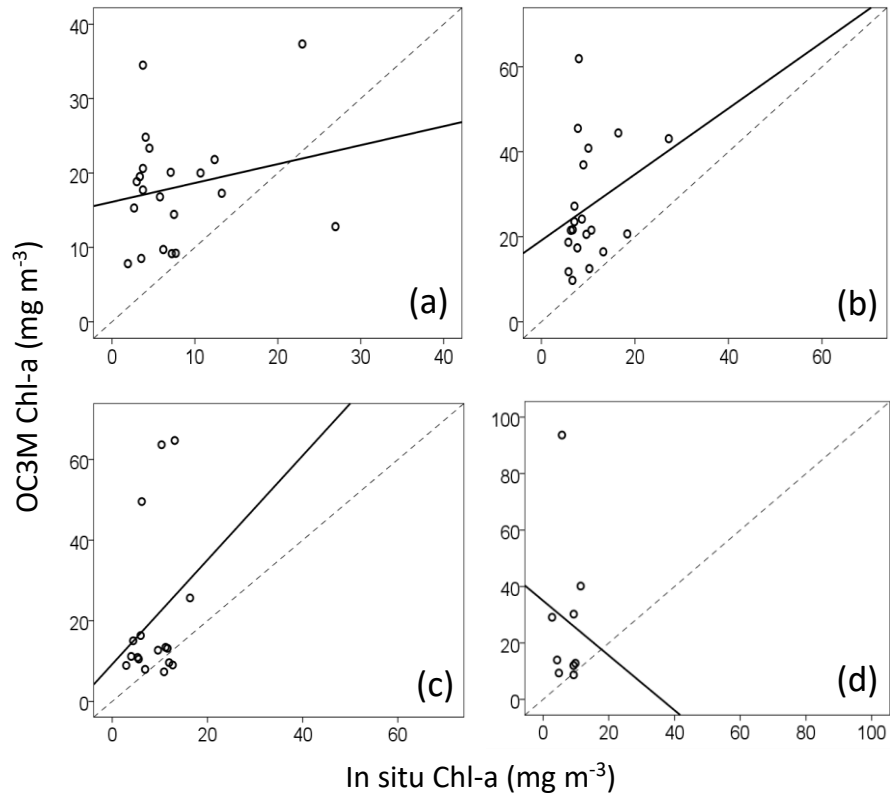


Figure 4.9 Seasonal comparison of in-situ and OC3M derived chlorophyll-a in Chesapeake Bay for (a) spring (b) summer (c) Autumn and (d) winter. Dotted lines represent 1:1 relationship.

Data displayed in Figure 4.9 shows a large biasness in satellite estimation of chlorophyll-a using OC3M algorithm in all seasons. Generally, the algorithm overestimated the chlorophyll-a concentration in all seasons, as most of the points are above 1:1 line for all cases. The statistical result of the seasonal evaluation is presented in table 4.3. It can be observed that the performance of the algorithm was especially poor in winter (RMSE = 33.03, p-value = 0.780) and comparatively superior in spring (RMSE = 13.62, p-value = 0.353). The error in satellite estimation of chlorophyll-a in coastal water is mainly due to noise from the bottom reflectance and presence of CDOM (Gilerson et al., 2010).

Table 4.3 Statistics of the seasonal evaluation of OC3M algorithm in Chesapeake Bay

| Season | R ² | P-value | RMSE | MAE | MAPE |
|--------|----------------|---------|--------|-------|-------|
| All | 0.023 | 0.195 | 23.174 | 15.6 | 246.7 |
| Spring | 0.045 | 0.353 | 13.62 | 11.71 | 256.7 |
| Summer | 0.088 | 0.204 | 21.24 | 16.88 | 196.0 |
| Autumn | 0.068 | 0.312 | 21.52 | 12.92 | 165.0 |
| Winter | 0.039 | 0.780 | 33.03 | 20.49 | 373.4 |

4.3 Novel Algorithm

4.3.1 Development of the novel algorithm

Regression analysis was performed to best fit a fourth order polynomial (Figure 4.10) between the log of field observed chlorophyll-a and log of reflectance ratio that includes red bands. The band ratio formulation which is used in OC3M algorithm was retained in this study. The best fit was obtained by using the reflectance ratio that employs the maximum of reflectance in 531 and 551 nm band as numerator and minimum of reflectance in 667 and 678 nm bands as the reference band. The coefficients of the OC3M algorithm and the novel algorithm developed in this analysis has been shown in table 4.4

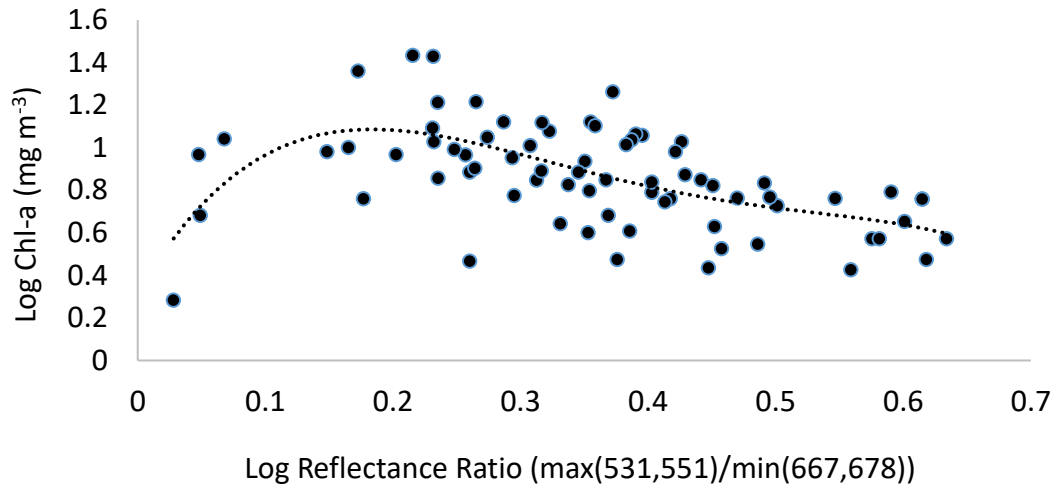


Figure 4.10 Best-fit polynomial between the green-red reflectance ratio and in-situ chlorophyll-a concentration, obtained through regression analysis

Table 4.4 Coefficients of the OC3M algorithm and the novel algorithm

| Algorithm | Band Ratio | a0 | a1 | a2 | a3 | a4 |
|-----------|------------|--------|---------|---------|--------|---------|
| OC3M | X_{bg} | 0.2424 | -2.7423 | 1.8017 | 0.0015 | -1.2280 |
| Novel | X_{gr} | 0.314 | 10.472 | -46.923 | 77.994 | -45.63 |

4.3.2 The performance of the novel algorithm

The performance of the novel algorithm was analyzed using the same data set that was used for the development of the algorithm. Bubbles in the scatter plot of in-situ against novel algorithm derived chlorophyll-a was condensed and most of the points fell along the 1:1 line (Figure 4.11). Novel algorithm derived chlorophyll-a are significantly correlated ($r^2=0.323$, $p<0.001$) with the in-situ observations, specially bellow the concentration of 15 mg m^{-3} . The RMSE obtained for this analysis is 4.20 mg m^{-3} . The cluster column shows the algorithm-derived concentrations are comparable to in-situ concentrations for most of the match-up pairs (Figure 4.12).

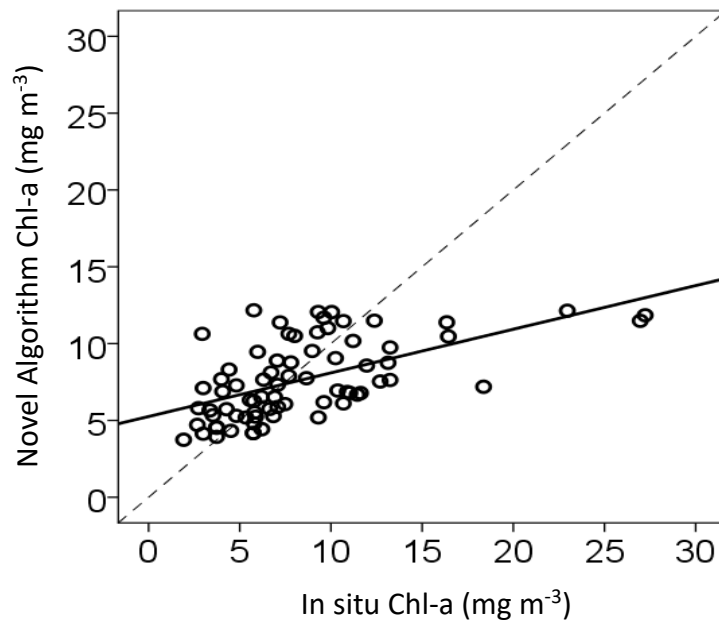


Figure 4.11 Scatter-plot of in-situ and satellite derived chlorophyll-a using the novel algorithm for Chesapeake Bay. The dotted line represents 1:1 line.

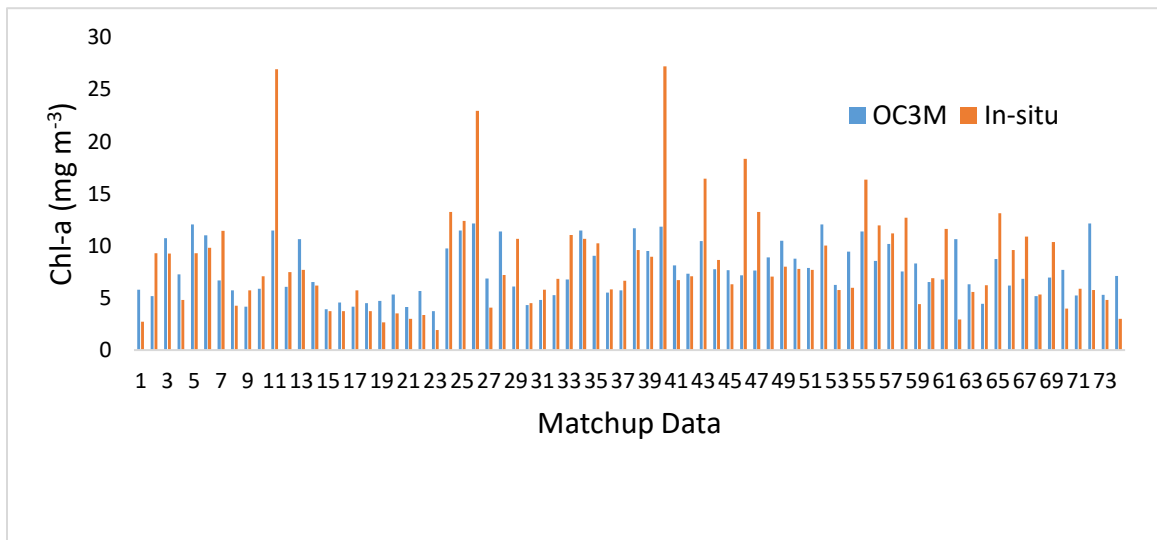


Figure 4.12 Clustered column compares the in-situ chlorophyll-a concentrations with concentrations derived using the novel algorithm developed in this study

The matchup data set was divided into four groups according to season. The algorithm derived and in-situ concentrations for each season were analyzed to understand the seasonal performance of the novel algorithm (Figure 4.13). Most accurate result was obtained for the spring season ($r^2=0.608$, $p<0.001$). The accuracy in summer ($r^2=0.206$, $p=0.044$) was also acceptable. The results obtained for autumn ($r^2=0.077$, $p=0.282$) and winter ($r^2=0.250$, $p=0.170$) were not good enough but still better than the performance of the OC3M algorithm in these seasons. Table 4.5 shows the result of different statistical analysis that has been performed to compare the accuracy of the novel algorithm in different seasons

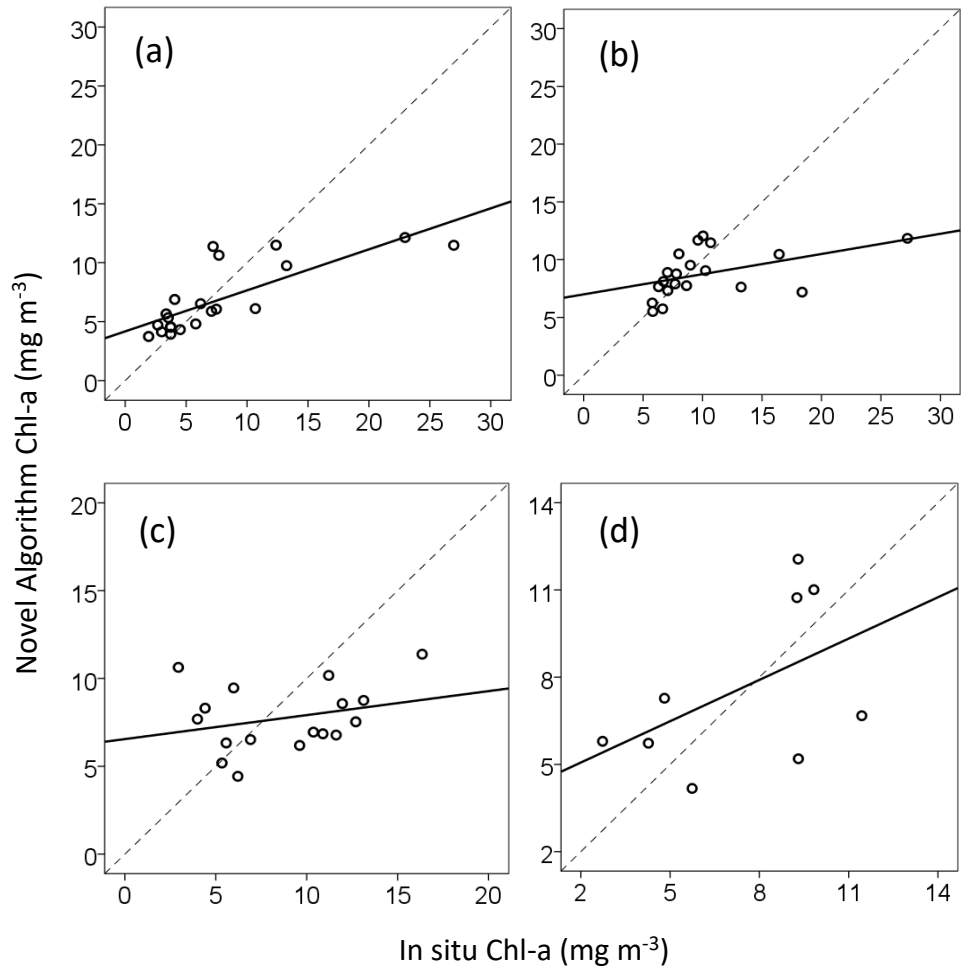


Figure 4.13 Seasonal comparison of In-situ and the novel algorithm derived chlorophyll-a in Chesapeake Bay for: (a) spring (b) summer (c) Autumn and (d) winter. Dotted lines represent 1:1 relationship

Table 4.5 Statistics showing the seasonal performance of the novel algorithm in Chesapeake Bay.

| Season | R ² | P-value | RMSE | MAE | MAPE |
|--------|----------------|---------|------|------|------|
| All | 0.323 | < 0.001 | 4.20 | 2.89 | 37.0 |
| Spring | 0.608 | < 0.001 | 4.61 | 2.86 | 37.4 |
| Summer | 0.206 | 0.044 | 4.77 | 2.79 | 20.9 |
| Autumn | 0.077 | 0.282 | 3.83 | 3.32 | 49.0 |
| Winter | 0.250 | 0.170 | 2.80 | 2.53 | 40.9 |

4.3.3 Test of the novel algorithm

The accuracy of the novel algorithm was evaluated and compared with the performance of OC3M algorithm using an independent test sample of match-up pairs. The novel algorithm developed using green-red band ratio performed better than the existing OC3M algorithm for the coastal water system of Chesapeake Bay. The correlation between the novel algorithm derived and in-situ chlorophyll-a, obtained for the test sample, is significantly ($p < 0.001$) higher as depicted by a R² of 0.435 as compared to the OC3M algorithm (R² 0.013, $p = 0.462$) (Table 4.6). Furthermore, other statistical analysis (RMSE, MAE and MAPE) performed to compare the accuracy of OC3M algorithm and the novel algorithm demonstrated the error in satellite estimation of chlorophyll-a using MODIS data is reduced by several folds if the novel algorithm is used (Table 4.6).

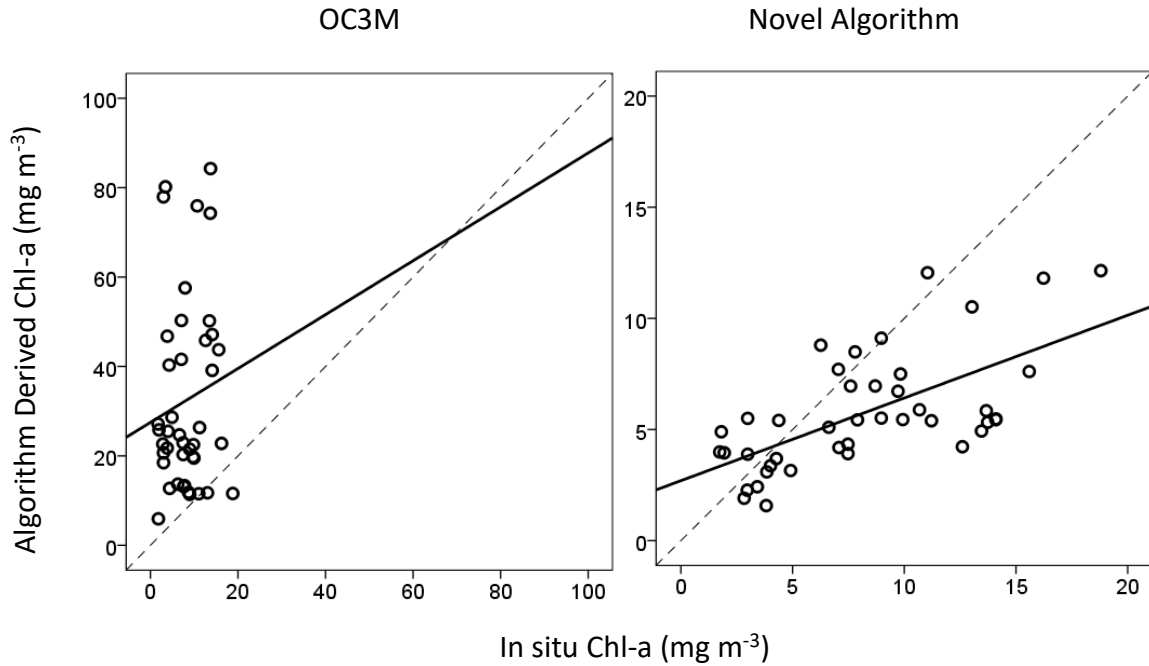


Figure 4.14 Scatter plots show the comparison between in-situ and algorithm derived chlorophyll-a for test samples. Solid lines represent linear regression fit. Dashed lines are 1:1 lines.

Table 4.6 Statistics comparing the performance of the novel and OC3M algorithms

| Algorithm | R ² | P-value | RMSE | MAE | MAPE |
|-----------|----------------|---------|--------|--------|--------|
| Novel | 0.435 | <0.001 | 4.228 | 3.267 | 42.66 |
| OC3M | 0.013 | 0.462 | 32.125 | 24.630 | 458.03 |

The OC3M algorithm is blue-green band ratio algorithm, which is prone to the presence of color dissolved organic matter (CDOM) and bottom reflectance, common in coastal water (Blondeau-Patissier et al., 2014). Red bands are less sensitive to the presence of CDOM (Gilerson et al., 2010). Furthermore, due to its early attenuating tendency, red band is less

affected by bottom reflectance (Carder et al., 2005b). Therefore, the use of red-band in the current algorithm might have reduced the error in chlorophyll-a estimation by reducing the noise due to CDOM and bottom reflectance.

Chapter 5

5 Conclusions and Recommendations

In this study, the spatial and temporal variability of chlorophyll-a in Chesapeake Bay is analyzed. Mean annual chlorophyll-a concentration at CB monitoring stations located in Upper Bay, Mid Bay and Lower Bay were estimated for the years from 2003 to 2017 to understand the annual variation in chlorophyll-a. The chlorophyll-a concentration at 285 monitoring stations were interpolated to produce chlorophyll-a map of the Chesapeake Bay for spring and summer seasons. The performance of OC3M algorithm was assessed in deep ocean water and coastal water and finally a novel algorithm was developed based on reflectance in green and red bands, and its performance in the coastal water system of Chesapeake Bay was tested using an independent data set.

In-situ chlorophyll-a data from Chesapeake Bay and Sargasso Sea were used for the study. MODIS reflectance data were downloaded from the Ocean Color Web and satellite derived concentrations were obtained by applying OC3M algorithm using SeaDAS software. The results obtained in the study suggest that water quality of Chesapeake Bay is degraded; the OC3M algorithm is performing poor in coastal water while its performance in deep ocean water is satisfactory; novel algorithm based on green-red band ratio performs better in the coastal water.

5.1 Conclusions

The annual variability in chlorophyll-a concentration in Chesapeake Bay is high. Mean annual chlorophyll-a concentrations at the CB stations employed for this study ranged between 4.31-18.06 mg m⁻³ from 2003 to 2017. The production of algal biomass is driven by the availability of nutrient, intensity of light and temperature condition (Cerco, 2000). Nutrients are present in the watershed from agricultural activities, urban activities and atmospheric deposition (Ator et al., 2011). However, the transport of nutrient to the bay is dependent on run-off from the watershed, which depend on the precipitation in the watershed. So, it could be said the chlorophyll-a dynamics in Chesapeake Bay is governed by natural factors, but it is aided by anthropogenic activities. Therefore, any management action plan to control the algal blooms in Chesapeake Bay should focus on reducing nutrient accumulation in the watershed and prevention of run-off to the bay.

The seasonal comparison in chlorophyll-a concentration demonstrates that algal growth is higher in spring than that of summer in all three sections of Chesapeake Bay. The spring phytoplankton bloom is a regular phenomenon in Chesapeake Bay that results in elevated chlorophyll-a throughout the bay water. The over abundant algal bio-mass die and decay at the end of their life cycle resulting in a hypoxia condition during summer, which is a recurrent phenomenon in the bay. The hypoxia condition becomes stable since the density stratification inhibits the downward mixing of oxygenated water at the surface (Ator et al.,

2011). To check the hypoxia condition during summer, it is important to focus on strategies that would control the algal production during spring.

The spatial analysis of chlorophyll-a in the bay water during spring and summer demonstrated that in both seasons, concentrations in the Upper Bay was highest, followed by the Mid Bay and it was lowest in the Lower section of Chesapeake Bay. During spring, the concentration in the Upper Bay was more than 15 mg m^{-3} ; in the Mid Bay, it varied from 10 to 20 mg m^{-3} , and in the Lower Bay the concentration was less than 10 mg m^{-3} . The summer concentration in the Lower Bay was generally higher than that of the spring. The chlorophyll-a in the Upper, Mid and Lower Bay during summer ranged between >15 , 6-10, and $<6 \text{ mg m}^{-3}$, respectively. Standard deviations of chlorophyll-a during spring and summer across different locations of Chesapeake Bay demonstrated higher variance during spring as compared to summer, which can be justified by the dynamicity in algal growth during spring.

The uncertainties in satellite estimation of chlorophyll-a using OC3M algorithm in Sargasso Sea (Case1 water) and Chesapeake Bay (Case 2 water) has been evaluated. The algorithm worked well for case 1 water (RMSE= 0.016). However, the error of estimation was very high in case 2 waters (RMSE=23.14). The algorithm was found to be overestimating the chlorophyll-a concentrations in Chesapeake Bay. The blue-green band ratio based algorithms are susceptible to noise due to bottom reflectance and CDOM. Both factors are present in the coastal water that leads to the overestimation. The result of the

analysis demonstrates that OC3M algorithm is useful for synoptic mapping of chlorophyll-a in the deep ocean region. However, the high error of estimation in Chesapeake Bay shows that the algorithm is unsuitable for satellite estimation of chlorophyll-a in the coastal water.

The novel algorithm developed in this study is a green-red band ratio algorithm. The red band has been used in the algorithm because it is less sensitive to bottom reflectance and CDOM that are sources of error in satellite estimation of chlorophyll-a in coastal water. The novel algorithm performed significantly better than the OC3M algorithm in the coastal water of Chesapeake Bay. The RMSE reduced from of 32.12 mg m^{-3} to 4.22 mg m^{-3} when novel algorithm was used instead of the OC3M algorithm for the same validation data set. The evaluation of seasonal performance of the algorithm demonstrated that the algorithm performed best for the winter season (RMSE=2.80).

5.2 Recommendations

It has been more than 40 years since the ocean color research began in 1970. Sufficient accuracy has been achieved in satellite estimation of chlorophyll-a in mid ocean water but the error in satellite estimation of chlorophyll-a in coastal region is still substantial. The coastal water is of great importance to human civilization and therefore a robust ocean color algorithm for coastal water is desired. The present study demonstrates the importance of red-band in development of ocean color algorithm for complex coastal water. Although,

the novel algorithm reduced the error in deriving chlorophyll-a by a significant margin but still the following limitations exist. The matchup data set used for the development of the algorithm is small (74 pairs). Most of the pixels in the MODIS imagery of the study area are Nan Pixels where reflectance data is not available and frequency of in-situ observations are low. It would be better to utilize a larger set of matchup pixels in order to develop an algorithm with a greater accuracy. Furthermore, the satellite estimation of chlorophyll-a in coastal water is severely affected by the operational atmospheric correction procedures that are known to be inefficient. Therefore, the most encouraging prospect for enhancement in satellite estimation of chlorophyll-a in coastal water is improvement in atmospheric correction procedure and development of red band based algorithm with a larger set of matchup pixels.

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