The Development and Proliferation of Summer Algal Blooms in the Oligo/Poly-Haline Portion of the Chesapeake Bay - Observational and Numerical Modeling Studies

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The Development and Proliferation of Summer Algal Blooms in the Oligo/Poly-haline Portion of the Chesapeake Bay - Observational and Numerical Modeling Studies

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The College of William and Mary in Virginia

In Partial Fulfillment

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Doctor of Philosophy

by

Zhengui Wang

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<td>Integrated Compartment Model</td>
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<td>SCHISM</td>
<td>Semi-implicit Cross-scale Hydrosience Integrated System Model</td>
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<tr>
<td>HEM3D</td>
<td>A Three-Dimensional Hydrodynamic Eutrophication Model</td>
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<td>HAB</td>
<td>Harmful Algal Bloom</td>
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<tr>
<td>WWTP</td>
<td>Waste Water Treatment Plant</td>
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<td>NARR</td>
<td>North American Regional Reanalysis</td>
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<td>NDBC</td>
<td>National Data Buoy Center</td>
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<td>Total Nitrogen</td>
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<td>TP</td>
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Abstract

Algal blooms occur annually in many parts of the Chesapeake Bay. The causes of algal blooms are complex and can be different in different regions. In this study, we will conduct data analysis for the observed data and adopt various methods to investigate algal bloom phenomenon in three separate regions in the oligo/polyhaline portion of the Bay. Chapter 1 provides a general introduction of the algal bloom research in the Chesapeake Bay.

In Chapter 2, an observational analysis and a numerical study on the algal blooms in Back River were conducted. A hypothesis was made that high pH can trigger sediment phosphorus release, which in turn can enhance chlorophyll-a and further increase pH to form a positive feedback loop. To test this theory, water quality model ICM coupled onto SCHISM was applied in Back River to study the phenomenon. Moreover, a pH model was developed to describe the aquatic chemistry. The model results with and without pH model were compared with Bay Program observations for verifying our hypothesis. It proves the importance of sediment phosphorus release on the algal blooms in Back River.

In Chapter 3, a theoretical study combined with data analysis on cyanobacteria blooms dynamics was conducted in the upper tidal James River. The theory integrates the physical transport and biological effects, which leads to a simple governing equation composed of an advection term and a phytoplankton net growth term, in both linear and nonlinear forms. In this study, we derived a general analytic solution to the equation. Then, we applied the theory in the tidal freshwater portion of the James River. The theoretical predictions of chlorophyll concentrations were compared with observational data and verified the validity of the solution. In addition, the factors related to the local chlorophyll maximum in tidal freshwater rivers were discussed.

In Chapter 4, an observational analysis and numerical experiments were performed to investigate the algal bloom in the polyhaline of the Chesapeake Bay. This exploratory study is aimed to explain the broad distribution of *C. polykrikoides* blooms in the lower Bay and the sudden disappearance of the bloom in 2014. A hypothesis is made regarding the origin of *C. polykrikoides* cysts. In this hypothesis, the cysts are considered to be originated from coastal ocean and their transport is under the influence of wind patterns and gravitational circulation. In this study, the hydrodynamics in the lower Chesapeake Bay was first analyzed. Then, a series of particle tracking experiments were conducted for investigating the physical transport of *C. polykrikoides* cysts under different environmental conditions. Finally, water quality model ICM was used to simulate the algal blooms caused by *C. polykrikoides* in the lower Bay by incorporating the biological features of *C. polykrikoides*. The model can generate reasonable magnitude of the algal blooms in 2012, 2013 and simulate no algal bloom condition in 2014. The result indicates that *C. polykrikoides* cysts could be originated from the coastal ocean, while temperature and wind patterns play important roles in further controlling the subsequent development of the blooms.
The Development and Proliferation of Summer Algal Blooms in the Oligo/Poly-haline Portion of the Chesapeake Bay - Observational and Numerical Modeling Studies
Chapter 1 Introduction

Harmful Algal Bloom (HAB) is caused by the rapid proliferation of phytoplankton or microscopic algae (Anderson et al., 2012). It is affecting almost every region of the world as commonly called red tides (Anderson et al., 2008). Many phytoplankton species can potentially cause harmful blooms under favorable conditions. These conditions comprise many elements including cyst population, nutrients, temperature, salinity, light, sediment condition and physical transport (Sellner et al., 2003; Gentien et al., 2005; Ji 2008). HAB occurrence is increasing globally and becomes more frequently as well. There are many factors related to this trend. Human impact such as anthropogenic nutrient loading to the coastal ocean maybe a driver, climate change is likely to play a role as well. In addition, the global expansion of HAB species seeds through global trade, storms, and ocean currents enhance the HAB trend in general (Hallegraeff 1993; Sellner et al., 2003; Wood et al., 2013; Paerl et al., 2014; Qu et al., 2014). Depending on the species, HAB can be categorized as toxic or non-toxic blooms. For example, Alexandrium Monilatum bloom can produce toxins when concentration rises (Pease 2016) and becomes toxic to marine lives including all kinds of fishes and invertebrates. Non-toxic algal blooms can still be harmful to the local ecosystem when the concentration of phytoplankton cells gets high.

Generally, HAB has a negative impacts to both the environment and humans (Anderson et al., 2008). When HAB occurs, the bloom species usually outcompetes other phytoplankton species. It can prevent other phytoplankton species from growing by sucking all the available nutrients and shading the light with a canopy of bloom cells in the water surface. At the same time, the canopy shades the light to the beds. Consequently, the sea grass and benthic community may suffer as well. The accumulation of bloom cells can also discolor the water, and produce an unpleasant odor and noxious foams. This causes the loss of aesthetic and recreational values of waters, which often leads to events like water contamination and beach closure. Along with the HAB progression, the metabolism and death of bloom cells can produce plenty of organic matter. The degradation of this organic matter will deplete the dissolved oxygen in the water
column, which will suffocate marine animals and eventually cause mortality. In extreme cases, it can lead to massive fish and shellfish kills, large death occurrences of mammals and invertebrates, and death of other marine life whose biological activity is depending on dissolved oxygen. As a result, the HAB can cause a complete crash of the local ecosystem, commonly recognized as a “dead zone”. The ecological and economic loss can be huge, depending on the longevity and intensity of the HAB. For example, a single HAB happened in 1995 in Korea and caused a total loss of 95 million US dollar (Kim et al., 2004). On the other hand, toxic HAB can be even more harmful. Through the food chain, the biotoxin can be accumulated to a very high concentration in higher trophic level (eg. Shellfish). The consumption of these contaminated seafood with biotoxin can be fatal to fish, bird, marine mammals and humans. For example, in 1987, over one hundred human illnesses and several deaths related to the consumption of mussels has been reported from Atlantic Canada (Anderson et al., 2012).

In the last few decades, HAB is increasing around the world. However, the bloom mechanism in different regions can be very different. In addition, there are many bloom species and the dominant HAB species can be different in different regions. Even in the same location, the dominant HAB species can be shifted from one to another over time. Also, the nutrient dynamics that is responsible for the HAB can change greatly among different areas. Furthermore, the underlying hydrodynamics may play a significant role in regulating HAB development and can be dramatically different among different places. Therefore, it is difficult to provide a synthesis about the global HAB although there are some efforts trying to give a general picture. Hallegraeff (1993) described the global frequency and magnitude of HAB. Anderson et al., (2008) and Anderson et al., (2012) tried to provide a general picture of HAB about the global trend, scientific research and bloom dynamics. One problem is that it is hard to extrapolate the scientific findings about HAB in one region to another. Plus, there is always a lack sufficient long-term and comprehensive observational data. Along the United States East Coast, extensive studies were conducted in several regions including Gulf of Mexico, Mid-Atlantic Bight, and Gulf of Maine (Glibert et al., 2001; Anderson et al., 2005; Mulholland et al., 2009; Kudela and Gobler 2012; Morse et al., 2013; Egertonk et al., 2014;
Fitzpatrick et al., 2014). In Chesapeake Bay, Egertonk et al., (2014) summarized the various phytoplankton species that can cause HABs. Two major HAB species are Alexandrium and Cochlodinium. In this dissertation, one of the focuses of our studies will be on Cochlodinium Polykrikoides (C. polykrikoides) that blooms in Chesapeake Bay annually.

In the Chesapeake Bay, much research on algal blooms has been conducted in the mesohaline portion of the Bay. In the upper and mid-Chesapeake Bay, the annual phytoplankton bloom cycle is influenced by the winter-spring peak of freshwater input along with the external nutrients supplied by the Susquehanna River (EPA 1982; Malone et al., 1988). The nutrients are assimilated in the mesohaline reach of the Bay, which is downstream from the turbidity maximum. Therefore, the major algal bloom in the mesohaline region was dominated by the nutrients delivered by the Susquehanna River. There usually exhibits a local phytoplankton maximum along the mid-Bay and a positive relationship between algal concentration and the Susquehanna River discharge (Malone et al., 1986; Malone et al., 1988). The amounts of nutrients and suspended particulate matters carried by freshwater flows will modulate the nutrient abundance and light field, which further regulates the timing, position and magnitude of the spring bloom (Fisher et al., 1988; Malone 1992). Sellner and Kachur (1987) reported the phytoplankton species composition, productivity and pigment concentrations in the mesohaline waters along the shallow western shore of Chesapeake Bay over an 8-year period. It was found that diatoms dominate in the winter, spring and fall, while flagellates dominate in the summer months. Strong blooms were also observed in the mid-Bay region after rainfall events and major storms (Loftus et al., 1972; Miller et al., 2006). An annual, long range subsurface transport of the dinoflagellate Prorocentrum from the mouth of the Chesapeake Bay to its blooming locations in the upper Bay was reported by Tyler and Seliger (1978) and Tyler and Seliger (1981).

Compared to considerable literature existing in the mesohaline region, the research investigation conducted for algal blooms in the tidal fresh/oligohaline and polyhaline regimes of the Bay are only more recent. In the oligohaline regime of Potomac River, Fitzpatrick et al., (1992) found that the sediment phosphorus release triggered the extensively microcystic algal bloom during the summer of 1983. Sellner
et al., (1988a) reported that salinity affects freshwater phytoplankton by influencing the growth rate and species compositions. Bukaveckas et al., (2011) reported a high chlorophyll maximum dominated by *Microcystis aeruginosa* existing in the tidal freshwater James River as a result of morphological transition from a narrow deep channel to a broader expansive shallow area. In the polyhaline regime of the lower Chesapeake Bay, Marshall and Nesius (1996) and Marshall et al., (2005) documented the major phytoplankton species with a dominant diatom flora throughout the year and identified the toxic phytoplankton species. Reiss and McConaugha (1999) and Filippino et al., (2009) studied the phytoplankton dynamics in the inner shelf of the Bay. They found that wind speed and direction strongly influence the location and type of plumes and thus the biological uptake of nitrogen (N) and carbon (C). Also, the studies show that high freshwater does not necessarily translate into high productivity in the coastal zone; high productivity was observed during periods where the recycling process dominated. In the lower Chesapeake Bay, Mulholland et al., (2009) studied the dinoflagellate *C. polykrikoides* that regularly blooms from July to September. Morse et al., (2011) and Morse et al., (2013) studied the control factors responsible for *C. polykrikoides* blooms.

In this dissertation, we will study the algal blooms in Chesapeake Bay at three different separate locations in the oligohaline and polyhaline of the Chesapeake Bay. The observational analysis and numerical model methods will be used to investigate the algal bloom dynamics. Chapter 2 reports on a study in Back River of the upper Chesapeake Bay. This area belongs to oligohaline region and we will study how nutrient dynamics controls the algal bloom. Chapter 3 is a theoretical study for phytoplankton growth and how physical transport and biological processes are linked in the tidal fresh James River. In Chapter 4, we first conduct a data analysis on the algal bloom occurred in the polyhaline regime of the lower Chesapeake Bay. A hypothesis about the *C. polykrikoides* blooms in the polyhaline region of the Bay is proposed. It focuses on the transport of bloom cysts from the offshore into the lower Chesapeake Bay and modeling experiments were conducted to test the hypothesis.
Chapter 2 Coupling a pH model to Water Quality Model for Application in the Back River, Upper Chesapeake Bay

Abstract

Back River is located along the western shoreline of the upper Chesapeake Bay and is about 8 miles in length and 2-3 meters in average depth. Each summer, algal blooms with chlorophyll-a concentration exceeding 100 µg/L are regularly observed in Back River. This excessive primary production, exhibited by the high chlorophyll-a concentrations, is among the highest in the Chesapeake Bay and its tributaries. In order to explain the unusual phenomenon, a field survey was conducted in the low salinity water of Back River by Boynton and Ceballos (2014), which suggested that pH values exceeding 8.5 on average can trigger a release of phosphorus from the sediment. Based on the observation and related studies, a hypothesis was formulated that a pH-mediated feedback mechanism may exist in this system by which elevated phytoplankton growth can enhance pH and the increased pH, in turn, can trigger a phosphorus release from the sediment in Back River where phosphorus is normally limited. A numerical modeling approach was used to verify the hypothesis. In this study, we developed a dynamic pH model with four state variables and coupled it into “integrated compartment model” (ICM) water quality model with 19 state variables. The coupled model is then set up in the upper Chesapeake Bay including Back River. The calibrated model gives reasonable results for hydrodynamics and water quality variables. For testing our hypothesis, we applied the pH model kinetics in Back River and compared with the scenario “with” and “without” it. The results show a positive feedback loop interacting among phytoplankton, total inorganic carbon, pH and phosphate, which verifies that the effect of pH on sediment phosphorus release is important to sustain the high phytoplankton biomass during summer.
2.1 Introduction

Eutrophication is defined as nutrient over-enrichment of an aquatic system and it can be related to anthropogenic nutrient loading, internal nutrient recycling and urbanization pollution as well as other human related activities (Boynton et al., 1982; Ji 2008). In the last few decades, eutrophication is becoming an increasing issue for many waterbodies (Anderson et al., 2012; Carroll et al., 2013; Tsatsaros et al., 2013). It can cause water quality degradation characterized by reduced water clarity, frequent occurrences of algal blooms and hypoxic conditions (Kemp et al., 2005; Kemp et al., 2009).

In an eutrophication waterbody, phytoplankton can grow substantially because of the sufficient available nutrients. While a certain amount of phytoplankton concentration is necessary for the balance of the ecosystem, the excessive phytoplankton biomass accumulation can be a disaster. Excessive nutrient inputs can cause the degradation of water quality and the disruption of the ecosystem including: (1) increase of phytoplankton production (Boynton et al., 1982; Malone et al., 1988; Jordan et al., 1991), 2) decrease of dissolved oxygen (Taft et al., 1980; Officer et al., 1984), and (3) demise of submerged aquatic vegetation (Kemp and Boynton 1984). For several decades, the Back River and Patapsco River have shown signs of eutrophication (Magnien et al., 1993). Therefore, it is important to understand the factors that can influence the phytoplankton growth. In an ecosystem, there are many phytoplankton species coexisting in the same environment. Every species has a different growth rate, a different metabolism rate and reacts differently to ambient nutrient, light and temperature. In addition, hydrodynamic transport and water mixing can change the biomass distribution.

Back River is a small tributary in the Upper Chesapeake Bay along the western shoreline. It is a shallow water system and the average depth is about 2-3 meters. The tidal range in the area is about 0.4 meter. There is a Waste Water Treatment Plant (WWTP) that routinely discharges a large amount of waste water with over 100 MGD. The river is largely fresh in the upper portion and is normally within the range of 5 PPT in the lower Back River (Figure 2-2) depending on the Susquehanna River discharge. The WWTP discharge changes the local hydrodynamics and the associated nutrient loads promotes the phytoplankton
growth. The persistent elevated chlorophyll concentration within surface waters can last from the spring to fall season each year inside the Back River (Robertson 1977; Boynton et al., 1998). In summer months, the chlorophyll-a concentration can reach over 100 µg/L and some extreme values can be as large as 400 µg/L. Despite of the large algal biomass present in the river, hypoxia has rarely occurred in Back River due to the shallow water depth.

2.2 Observation and Hypothesis

The high chlorophyll-a concentration in Back River is fueled by the abundant nutrients. Thus, it is important to understand the nutrient dynamics in this region. In Figure 2-1, the upper panel shows the DIN/DIP ratio at Station WT4.1 in Back River from 2012 to 2014. The DIN/DIP ratio is very high in the winter and spring and low in the summer, which suggests a phosphorus limitation in the winter and spring and a nitrogen limitation in the summer (lower panel of Figure 2-1). However, the nitrogen limitation in near fresh to brackish water in the summer conflicts with past research which states that generally phosphorus should be the limiting element for low saline regions (Doering et al., 1995). Further examining the DIP concentration reveals that phosphorus concentration is very high in Back River in the summer time (Figure 2-2) when water temperature is also high. Therefore, there must be additional internal phosphorus sources besides watershed loading. In Back River, a plausible source is sediment phosphorus release. In Chesapeake Bay, it is well known that hypoxia/anoxia condition in the deep channel can trigger the sediment phosphorus release resulting in high phosphorus concentration in the water column. However, in Back River, the oxygen concentration in the summer is generally higher than 5 mg/L (Figure 2-2), which rules out the possibility of hypoxia/anoxia induced sediment phosphorus release.
Figure 2-1. The upper panel is DIN/DIP ratio at Station WT4.1 in Back River from 2012 to 2014. The lower panel shows the phosphorus and nitrogen limitation factors (smaller values suggest phytoplankton growth limiting). The data used in this figure are from the Chesapeake Bay Program.
Figure 2-2. Observational data for chlorophyll-a, pH, phosphorus, salinity and dissolved oxygen at Stations CB3.1 (left panels) and WT4.1 (right panels). WT4.1 is a station in Back River and CB3.1 is a station that is located in Chesapeake Bay Channel and is close to WT4.1. In summer months, both CHLA and pH are higher in Back River than in the open Bay. This indicates that the feedback of pH-induced sediment PO4 release may exist in Back River.
In order to explain the high sediment phosphorus release under aerobic conditions, a mechanism that is related to high pH has been proposed (Andersen 1975; Cerco 1988; Boers 1991; Seitzinger 1991; James et al., 1992; Gao et al., 2012; Cerco 2013). When pH is low, the phosphate ions are absorbed onto $[\text{Fe}^{3+}]$ particles and the phosphorus release from the sediment is blocked. As pH gets higher, the absorption of phosphate ions becomes weaker and the phosphorus release increases (Cerco 2013). This theory has successfully explained the large algal bloom that occurred in upper Potomac River in 1983. In Back River, Boynton and Ceballos (2014) conducted a field experiment and found that phosphorus can be released from the sediment (or on resuspended particles) when pH exceeds a threshold value about 8.5.

In Figure 2-3, the observational data for phosphorus release versus pH in Potomac River show that phosphorus flux increases dramatically when pH gets higher than 9.0. An exponential function is used to fit the relationship and this function will be used in our following study. Figure 2-2 shows chlorophyll-a and pH observations for Back River Station WT4.1 and a nearby Bay Channel Station CB3.1. By comparing the observations between these two stations, we found that the chlorophyll-a and pH are both much higher at WT4.1 than at CB3.1 in summer months although these two stations are geographically close to each other. The higher pH in Back River indicates the mechanism that a high pH-induced sediment phosphorus release may exist in this area.

After examining the observation data about chlorophyll-a, pH and nutrient concentrations in Back River, we made a hypothesis that a positive feedback mechanism may exist in Back River that is responsible for the observed high chlorophyll-a and high pH in summer months. The mechanism is illustrated in Figure 2-4. In the summer, the temperature gets higher and phytoplankton begin to grow. The phytoplankton assimilation will consume the dissolved inorganic carbon in the water column, which will lead to higher pH values. The increased pH will trigger sediment phosphorus release, which will, in turn, promote the phytoplankton growth. This comprises a positive feedback loop that high chlorophyll-a and high pH are linked. On the other hand, chlorophyll-a will continue to increase as long as the condition is favorable for phytoplankton growth. To prevent the phytoplankton concentration from increasing into infinity, the
phytoplankton growth will eventually be limited either by the nutrient availability or by dissolved inorganic carbon.

Figure 2-3. The relationship for pH induced Phosphorus release from sediment. The data are from (Bailey et al., 2006). An exponential function is used to fit the observation data with a pH base at 8.3.
To test our hypothesis, the following tasks were undertaken.

1. Developing a water quality model that includes the Back River area with reasonable calibration for the hydrodynamics and water quality variables.

2. Developing a pH dynamic model and coupling it into our water quality model.

3. Conducting sensitivity tests to verify our hypothesis.

2.3 Model Framework

Figure 2-5 shows the whole framework for the coupled SCHISM model plus the water quality model. Hydrodynamics is simulated in SCHISM model including temperature and salinity. The information is passed to the water quality model ICM. Additionally, nutrient loading from the watershed model that is provided by another group is used to drive the ICM. Water quality model simulates all the kinetic processes about phytoplankton, carbon, nitrogen, phosphorus, silica, chemical oxygen demand and dissolved oxygen. Inside the water quality model, a sediment flux model is also employed to simulate the diagenesis processes happening in the sediment and feedback sediment nutrient fluxes to water column. Finally, a pH model
based on aquatic chemistry is developed and coupled within our model. The following is the description about the individual parts of the whole model framework.

Figure 2-5. Model framework for SCHISM+ICM. SCHISM model provides the hydrodynamics to water quality model ICM. The watershed model provides nutrient loading for driving ICM. ICM also includes a submodule of sediment flux model for simulating the sediment kinetics. Recently, a pH model is developed and coupled with ICM.

2.3.1 Hydrodynamic model

SCHISM stands for "Semi-implicit Cross-scale Hydroscience Integrated System Model" and is a derivative work from the original SELFE model (Zhang and Baptista 2008). SELFE was a product developed up to 2014 at the Oregon Health Sciences University, while SCHISM continued to be upgraded by Dr. Joseph Zhang of College of William & Mary and other developers around the world. SCHISM is an open-source community-supported modelling system based on unstructured grids, designed for seamless simulation of 3D baroclinic circulation across creek-lake-river-estuary-shelf-ocean scales. It uses a highly efficient semi-implicit finite-element/finite-volume method with Eulerian-Lagrangian algorithm to solve the Navier-Stokes equations (in either hydrostatic or non-hydrostatic form), in order to address a wide range
of physical and biological processes. The numerical algorithm judiciously mixes higher-order with lower-order methods, to obtain stable and accurate results in an efficient way. Mass conservation is enforced with the finite-volume transport algorithm. It also naturally incorporates wetting and drying of tidal flats.

The SCHISM system has been extensively tested against standard ocean/coastal benchmarks and applied to a number of bays/estuaries around the world, in the context of general circulation, tsunami and storm-surge inundation, water quality, oil spill, sediment transport, coastal ecology, and wave-current interaction. SCHISM now includes many upgrades from the original SELFE code (v3.1dc). The major characteristics of SCHISM include:

(1) Finite element/volume.

(2) Unstructured horizontal grid (pure triangles, quadrilaterals, or a mixture of them).

(3) Cross scale modeling from 1D, 2D to 3D

(4) Hybrid SZ coordinates or new LSC\textsuperscript{2} in the vertical dimension: LSC\textsuperscript{2} is a better terrain-following vertical coordinate.

(5) Semi-implicit time stepping with robust matrix solver: allowing very fine grids with large time stepping.

(6) Mass conservative transport methods: upwind, explicit and implicit TVD.

For more detailed information about SCHISM and downloading the source code, one can refer to SCHISM website [http://ccrm.vims.edu/schism/](http://ccrm.vims.edu/schism/).

2.3.2 Water Quality Model

Our water quality model is based on ICM and HEM3D. ICM is the abbreviation of “Integrated Compartment Model” originally developed by U.S. Army Corps of Engineering (ASCE) Research and Development Center (Cerco and Cole, 1994) as one of the component of the water quality model package to study eutrophication processes in the Chesapeake Bay. HEM3D stands for “A Three dimensional
Hydrodynamic Eutrophication Model” and its water quality portion was developed by Park et al., (1995) at Virginia Institute of Marine Science. ICM and HEM3D share similar kinetics and the numerical implementation employed is analogous to finite volume numerical method allowing an easy implementation on an unstructured grid system. Our water quality model is coupled onto the SCHISM model that computes the hydrodynamics as well as temperature and salinity. Our water quality model invokes temperature and salinity directly from SCHISM, while the original ICM calculate them inside its own module.

Our water quality model has 19 state variables for delineating the kinetics happening in the water column. Table 2-1 lists all the variables and symbols used in our model. There are 3 phytoplankton species, 3 carbon species, 5 nitrogen species, 4 phosphorus species, 2 silica species, 1 chemical oxygen demand and 1 dissolved oxygen. Figure 2-6 is a diagram showing the inter-relationships among water quality variables. For a certain variable, each term from the mass balance equation is put on the diagram along with an arrow representing its flow direction. In addition, a unique color is designed to each variable to distinguish itself from others. In the following, we will list the equations of kinetics for each variable.
Table 2-1. State variables in water column

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B_d$</td>
<td>Diatom</td>
</tr>
<tr>
<td>$B_g$</td>
<td>Green Algae</td>
</tr>
<tr>
<td>$B_c$</td>
<td>Cyanobacteria</td>
</tr>
<tr>
<td>RPOC</td>
<td>Refractory Particulate Organic Carbon</td>
</tr>
<tr>
<td>LPOC</td>
<td>Labile Particulate Organic Carbon</td>
</tr>
<tr>
<td>DOC</td>
<td>Dissolved Organic Carbon</td>
</tr>
<tr>
<td>RPON</td>
<td>Refractory Particulate Organic Nitrogen</td>
</tr>
<tr>
<td>LPON</td>
<td>Labile Particulate Organic Nitrogen</td>
</tr>
<tr>
<td>DON</td>
<td>Dissolved Organic Nitrogen</td>
</tr>
<tr>
<td>$NH_4$</td>
<td>Ammonium Nitrogen</td>
</tr>
<tr>
<td>$NO_3$</td>
<td>Nitrate+Nitrite Nitrogen</td>
</tr>
<tr>
<td>RPOP</td>
<td>Refractory Particulate Organic Phosphorus</td>
</tr>
<tr>
<td>LPOP</td>
<td>Labile Particulate Organic Phosphorus</td>
</tr>
<tr>
<td>DOP</td>
<td>Dissolved Organic Phosphorus</td>
</tr>
<tr>
<td>$PO_4^-$</td>
<td>Total Phosphate</td>
</tr>
<tr>
<td>SU</td>
<td>Particulate Biogenic Silica</td>
</tr>
<tr>
<td>SA</td>
<td>Available Silica</td>
</tr>
<tr>
<td>COD</td>
<td>Chemical Oxygen Demand</td>
</tr>
<tr>
<td>DO</td>
<td>Dissolved Oxygen</td>
</tr>
</tbody>
</table>
Figure 2-6. A schematic diagram for water column kinetics. Boxes represent state variables and different colors are used to distinguish among them. The arrows show the relationship among variables. $B_x$ represents three phytoplankton species ($B_d$, $B_g$, $B_c$). The various terms along the arrows are from the mass balance equations for state variables and one can refer to the kinetics parts below for more information.
2.3.2.1 Phytoplankton

There are 3 phytoplankton (algal) groups in our model including diatoms, green algae and cyanobacteria. The kinetics of phytoplankton includes growth, metabolism, predation, settling and external loads. The growth depends on nutrients, light and temperature. The growth of diatoms also depends on silica concentration. Additionally, salinity affects cyanobacteria growth. For metabolism and predation rates, these are largely influenced by temperature. Below are the questions related to phytoplankton:

$$\frac{\partial B_x}{\partial t} = (P_x - BM_x - PR_x)B_x + \frac{\partial(WS_x \cdot B_x)}{\partial z} + \frac{WB_x}{V}$$ (2.1)

$$P_x = \begin{cases} \frac{PM_x \cdot f_1(N) \cdot f_2(I) \cdot f_3(T)}{PM_x \cdot f_1(N) \cdot f_2(I) \cdot f_4(S)}, & \text{for diatom and green alage} \\ \frac{PM_x \cdot f_1(N) \cdot f_2(I) \cdot f_3(T) \cdot f_4(S)}, & \text{for cyanobacteria} \end{cases}$$ (2.2)

$$f_1(N) = \begin{cases} \min\left(\frac{NH_4 + NO_3}{KHN_x + NH_4 + NO_3}, \frac{PO_4_d}{KHP_x + PO_4_d}\right), & \text{for green alage and cyanobacteria} \\ \min\left(\frac{NH_4 + NO_3}{KHN_x + NH_4 + NO_3}, \frac{PO_4_d}{KHP_x + PO_4_d}, \frac{SA_j}{KHS + SA_d}\right), & \text{for diatom} \end{cases}$$ (2.3)

$$f_2(I) = \frac{2.718 \cdot (e^{-\alpha_T} - e^{-\alpha_B})}{Ke \cdot \Delta z}, \quad \alpha_T = \frac{I_0}{(I_0)_x} \cdot e^{-Ke(T + \Delta z)}, \quad \alpha_B = \frac{I_0}{(I_0)_x} \cdot e^{-Ke \cdot H}$$ (2.4)

$$Ke = Ke_b + Ke_{TSS} \cdot TSS + Ke_{chl} \cdot \sum_x \left(\frac{PB_x}{cchl_x}\right)$$ (2.5)

$$f_3(T) = \begin{cases} e^{-KTG_1(T - TM_x)}, & \text{if } T \leq TM_x \\ e^{-KTG_2(T, TM_x)}, & \text{if } T > TM_x \end{cases}$$ (2.6)

$$f_4(S) = \frac{STOX^2}{STOX^2 + S^2}$$ (2.7)

$$BM_x = BMR_x \cdot e^{KTB_1(T - TR_x)}$$ (2.8)

$$PR_x = PRR_x \cdot e^{KTB_1(T - TR_x)}$$ (2.9)

where

- $B_x$: algal biomass of algal species $x$ (mg[C]/l)
- $t$: time (day)
2.3.2.2 Carbon

There are 3 carbon species in our model including refractory particulate organic carbon (RPOC), labile particulate organic carbon (LPOC), and dissolved organic carbon (DOC). For particulate organic carbon, the source is from the phytoplankton predation, while the loss includes hydrolysis and settling of...
particulate organic carbon. For dissolved organic carbon, the source includes phytoplankton metabolism, predation and the hydrolysis of particulate organic carbon, while the loss includes heterotrophic respiration and denitrification. Below are the questions related to carbon:

\[
\frac{\partial \text{RPOC}}{\partial t} = \sum_x FCRP \cdot PR_x \cdot B_x - K_{\text{RPOC}} \cdot \text{RPOC} + \frac{\partial}{\partial z} (\text{WS}_{\text{RP}} \cdot \text{RPOC}) + \frac{\text{WRPOC}}{V} 
\]

(2.10)

\[
\frac{\partial \text{LPOC}}{\partial t} = \sum_x FCLP \cdot PR_x \cdot B_x - K_{\text{LPOC}} \cdot \text{LPOC} + \frac{\partial}{\partial z} (\text{WS}_{\text{LP}} \cdot \text{LPOC}) + \frac{\text{WLPOC}}{V} 
\]

(2.11)

\[
\frac{\partial \text{DOC}}{\partial t} = \sum_x \left[ FCD_x + (1 - FCD_x) \frac{K_{HR}}{K_{HR} + DO} \right] BM_x + FCDP \cdot PR_x \cdot B_x 
\]

\[+ K_{\text{RPOC}} \cdot \text{RPOC} + K_{\text{LPOC}} \cdot \text{LPOC} - K_{\text{HR}} \cdot \text{DOC} - \text{Denit} \cdot \text{DOC} + \frac{\text{WDOC}}{V} \]

(2.12)

\[
K_{\text{RPOC}} = \left( K_{RC} + K_{RCalg} \cdot \sum_x B_x \right) \cdot e^{K_{Tide}(T-TR_{tide})} 
\]

(2.13)

\[
K_{\text{LPOC}} = \left( K_{LC} + K_{LCalg} \cdot \sum_x B_x \right) \cdot e^{K_{Tide}(T-TR_{tide})} 
\]

(2.14)

\[
K_{\text{HR}} = \frac{DO}{K_{HORDO} + DO} K_{DOC} 
\]

(2.15)

\[
K_{\text{DOC}} = \left( K_{DC} + K_{DCalg} \cdot \sum_x B_x \right) \cdot e^{K_{TMLE}(T-TR_{MLE})} 
\]

(2.16)

\[
\text{Denit} = \frac{K_{HORDO}}{K_{HORDO} + DO} \cdot \frac{NO_3}{K_{HDN_x} + NO_3} AANOX \cdot K_{DOC} 
\]

(2.17)

where

FCRP: fraction of predated phytoplankton carbon produced as refractory particulate organic carbon
FCLP: fraction of predated phytoplankton carbon produced as labile particulate organic carbon
FCDP: fraction of predated phytoplankton carbon produced as dissolved organic carbon
FCDx: fraction of metabolism excluded as dissolved organic carbon at infinite dissolved oxygen concentration for algal group x
K_{RPOC}: dissolution rate of refractory particulate organic carbon (day^{-1})
K_{LPOC}: dissolution rate of labile particulate organic carbon (day^{-1})
K_{HR}: heterotrophic respiration rate of dissolved organic carbon (day^{-1})
WS_{RP}: settling velocity of refractory particulate organic carbon (m day^{-1})
WS_{LP}: settling velocity of labile particulate organic carbon (m day^{-1})
WRPOC: external loads of refractory particulate organic carbon (g[C] day^{-1})
WLPOC: external loads of labile particulate organic carbon (g\[C\] day\(^{-1}\))
WDOC: external loads of dissolved organic carbon (g[C] day\(^{-1}\))
KHR\(_x\): half saturation constant of dissolved oxygen for DOC for algal group x (mg [O\(_2\)]/L)
Denit: denitrification rate (day\(^{-1}\))
K\(_{RC}\): minimum dissolution rate of refractory particulate organic carbon (day\(^{-1}\))
K\(_{LC}\): minimum dissolution rate of labile particulate organic carbon (day\(^{-1}\))
K\(_{DC}\): minimum respiration rate of dissolved organic carbon (day\(^{-1}\))
K\(_{RCalg}\): constant that relates dissolution of refractory particulate organic carbon to phytoplankton biomass (day\(^{-1}\) mg\(^{-1}\)[C] L)
K\(_{LCalg}\): constant that relates dissolution of labile particulate organic carbon to phytoplankton biomass (day\(^{-1}\) mg\(^{-1}\)[C] L)
K\(_{DCalg}\): constant that relates respiration of DOC to phytoplankton biomass (day\(^{-1}\) mg\(^{-1}\)[C] L)
KT\(_{HDR}\): effect of temperature on hydrolysis of particulate organic matter (°C)
KT\(_{MNL}\): effect of temperature on mineralization of dissolved organic matter (°C)
TR\(_{HDR}\): reference temperature for hydrolysis of particulate organic matter (°C)
TR\(_{MNL}\): reference temperature for mineralization of dissolved organic matter (°C)
KHOR\(_{DO}\): oxic respiration half saturation constant for dissolved oxygen (mg[O\(_2\)] /L)
K\(_{DOC}\): heterotrophic respiration rate of DOC at infinite dissolved oxygen concentration (day\(^{-1}\))
KHDN\(_N\): denitrification half saturation constant for nitrate (mg[N]/L)
AANOX: ratio of denitrification rate to oxic dissolved organic carbon respiration rate

2.3.2.3 Nitrogen

There are 5 nitrogen species in our model including refractory particulate organic nitrogen (RPON), labile particulate organic nitrogen (LPON), and dissolved organic nitrogen (DON), ammonium nitrogen (NH\(_4\)), and nitrite-nitrate nitrogen (NO\(_3\)). For particulate organic nitrogen, the source is from the phytoplankton metabolism and predation, while the loss includes hydrolysis and settling of particulate organic nitrogen. For dissolved organic nitrogen, the source includes phytoplankton metabolism, predation and hydrolysis of particulate organic carbon, while the loss is from mineralization. For ammonium nitrogen, the source includes phytoplankton metabolism, predation and hydrolysis of particulate organic carbon, while the loss is from mineralization. For ammonium nitrogen, the source includes phytoplankton metabolism, predation, mineralization from DON and sediment ammonium flux, while the loss includes phytoplankton uptake and nitrification into nitrate. For nitrate nitrogen, the source includes nitrification from NH4 and sediment nitrate flux, while the loss includes phytoplankton uptake and denitrification to nitrogen gas. Below are the questions related to nitrogen:

\[
\frac{\partial \text{RPON}}{\partial t} = \sum \left( FNR_{ri} \cdot BM_x + FNRP \cdot PR_x \right) \cdot \text{ANC}_x \cdot B_i - K_{RPON} \cdot \text{RPON} + \frac{\partial}{\partial z} \left( WS_{RP} \cdot \text{RPON} \right) + \frac{WRPON}{V} \tag{2.18}
\]
\[ \frac{\partial \text{LPON}}{\partial t} = \sum_x \left( \text{FNL}_x \cdot \text{BM}_x + \text{FNL} \cdot \text{PR}_x \right) \cdot \text{ANC}_x \cdot B_x - K_{\text{LPON}} \cdot \text{LPON} - \frac{\partial}{\partial z} \left( \text{WS}_L \cdot \text{LPON} \right) + \frac{\partial}{\partial z} \left( \text{LPON} \right) + \frac{W\text{LPON}}{V} \]  

\[ \frac{\partial \text{DON}}{\partial t} = \sum_x \left( \text{FND}_x \cdot \text{BM}_x + \text{FNDP} \cdot \text{PR}_x \right) \cdot \text{ANC}_x \cdot B_x + K_{\text{RPON}} \cdot \text{RPON} + K_{\text{LPON}} \cdot \text{LPON} - K_{\text{DON}} \cdot \text{DON} + \frac{W\text{DON}}{V} \]  

\[ \frac{\partial \text{NH}_4}{\partial t} = \sum_x \left( \text{FNI}_x \cdot \text{BM}_x + \text{FNIP} \cdot \text{RP}_x - \text{PN}_x \cdot \text{P}_x \right) \cdot \text{ANC}_x \cdot B_x + K_{\text{DON}} \cdot \text{DON} - \text{Nit} \cdot \text{NH}_4 + \frac{\text{BFNH}_4}{\Delta z} + \frac{\text{WNH}_4}{V} \]  

\[ \frac{\partial \text{NO}_3}{\partial t} = -\sum_x \left( 1 - \text{PN}_x \right) \cdot \text{ANC}_x \cdot B_x + \text{Nit} \cdot \text{NH}_4 - \text{ANDC} \cdot \text{Denit} \cdot \text{DOC} + \frac{\text{BFNO}_3}{\Delta z} + \frac{\text{WNO}_3}{V} \]  

\[ P\text{N}_x = \text{NH}_4 \cdot \frac{\text{NO}_3}{(\text{KHN}_x + \text{NH}_4)(\text{KHN}_x + \text{NO}_3)} + \text{NH}_4 \cdot \frac{\text{KHN}_x}{(\text{NH}_4 + \text{NO}_3)(\text{KHN}_x + \text{NO}_3)} \]  

\[ K_{\text{RPON}} = \left( K_{\text{RN}} + \frac{\text{KHN}}{\text{KHN} + \text{NH}_4 + \text{NO}_3} K_{\text{RNalb}} \sum_x B_x \right) \cdot e^{K_{\text{Tmil}} (T - \text{Tmil})} \]  

\[ K_{\text{LPON}} = \left( K_{\text{LN}} + \frac{\text{KHN}}{\text{KHN} + \text{NH}_4 + \text{NO}_3} K_{\text{Lalb}} \sum_x B_x \right) \cdot e^{K_{\text{Tmil}} (T - \text{Tmil})} \]  

\[ K_{\text{DON}} = \left( K_{\text{D}} + \frac{\text{KHN}}{\text{KHN} + \text{NH}_4 + \text{NO}_3} K_{\text{Dalb}} \sum_x B_x \right) \cdot e^{K_{\text{Tmil}} (T - \text{Tmil})} \]  

\[ \text{Nit} = \frac{\text{DO}}{\text{KH} \text{Nit}_{{DO} + \text{DO}} \cdot \text{KH} \text{Nit}_{{x + \text{NH}_4}} \cdot \text{Nit}_m \cdot f_{\text{Nit}}(T) \]  

\[ f_{\text{Nit}}(T) = \begin{cases} e^{-K_{\text{Nit}}(T - \text{TNit})^2}, & \text{if } T \leq \text{TNit} \\ e^{-K_{\text{Nit}}2(\text{TNit} - T)^2}, & \text{if } T > \text{TNit} \end{cases} \]  

where

- FNR\(_X\): fraction of metabolized nitrogen by algal group \(x\) produced as refractory particulate organic nitrogen
- FNL\(_X\): fraction of metabolized nitrogen by algal group \(x\) produced as labile particulate organic nitrogen
- FND\(_X\): fraction of metabolized nitrogen by algal group \(x\) produced as dissolved organic nitrogen
- FNL\(_X\): fraction of metabolized nitrogen by algal group \(x\) produced as inorganic nitrogen
- FNRP: fraction of predated nitrogen produced as refractory particulate organic nitrogen
- FNLP: fraction of predated nitrogen produced as labile particulate organic nitrogen
- FNDP: fraction of predated nitrogen produced as dissolved organic nitrogen
- FNIP: fraction of predated nitrogen produced as inorganic nitrogen
- ANC\(_X\): nitrogen to carbon ratio for algal group \(x\) (g [N] per g[C])
- K\(_{\text{RPON}}\): hydrolysis rate of refractory particulate organic nitrogen (day\(^{-1}\))
- K\(_{\text{LPON}}\): hydrolysis rate of labile particulate organic nitrogen (day\(^{-1}\))
- K\(_{\text{DON}}\): mineralization rate of dissolved organic nitrogen (day\(^{-1}\))
- WRPON: external loads of refractory particulate organic nitrogen (g [N]day\(^{-1}\))
- WLPON: external loads of labile particulate organic nitrogen (g [N]day\(^{-1}\))
- WDON: external loads of dissolved organic nitrogen (g [N]day\(^{-1}\))
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WNH4: external loads of ammonium (g [N] day\(^{-1}\))
WNO3: external loads of nitrate (g [N] day\(^{-1}\))
PN\(_x\): preference for ammonium uptake by algal group \(x\) (0 ≤ PN\(_x\) ≤ 1)
Nitr: nitrification rate (day\(^{-1}\))
BFNH4: sediment-water exchange flux of ammonium (g [N] m\(^{-2}\) day\(^{-1}\))
BFNO3: sediment-water exchange flux of nitrate (g [N] m\(^{-2}\) day\(^{-1}\))
ANDC: mass of nitrate nitrogen reduced per mass of dissolved organic carbon oxidized (g [N] per g[C])
KRN: minimum hydrolysis rate of refractory particulate organic nitrogen (day\(^{-1}\))
KLN: minimum hydrolysis rate of labile particulate organic nitrogen (day\(^{-1}\))
KD: minimum mineralization rate of dissolved organic nitrogen (day\(^{-1}\))
KRNalg: constant that relates hydrolysis of RPON to algal biomass (day\(^{-1}\) per mg[C]/L)
KLNalg: constant that relates hydrolysis of LPON to algal biomass (day\(^{-1}\) per mg[C]/L)
KDalg: constant that relates mineralization of DON to algal biomass (day\(^{-1}\) per mg[C]/L)
KHN: mean half saturation constant for algal nitrogen uptake (mg [N]/L), \(KHN = \frac{1}{3} \sum_{x} KHN_x\)
KHNitr: nitrification half saturation constant for dissolved oxygen (mg [O\(_2\)]/L)
KHNit: nitrification half saturation constant for ammonium (mg [N]/L)
Nitr:\(_m\): maximum nitrification rate at temperature TNitr (day\(^{-1}\))
TNitr: optimal temperature for nitrification (°C)
K Nit1: effect of temperature below TNitr for nitrification rate (°C\(^{-2}\))
K Nit2: effect of temperature above TNitr for nitrification rate (°C\(^{-2}\))

2.3.2.4 Phosphorus

There are 4 phosphorus species in our model including refractory particulate organic phosphorus (RPOP), labile particulate organic phosphorus (LPOP), and dissolved organic phosphorus (DOP), and total phosphate (PO4). For particulate organic phosphorus, the source is from the phytoplankton metabolism and predation, while the loss includes hydrolysis and settling of particulate organic phosphorus. For dissolved organic phosphorus, the source includes phytoplankton metabolism, predation and hydrolysis of particulate organic carbon, while the loss is from mineralization. For total phosphate, the source includes phytoplankton metabolism, phytoplankton predation, mineralization from DOP and sediment phosphate flux, while the loss includes phytoplankton uptake and settling of sorbed phosphate. Below are the questions related to phosphorus:

\[
\frac{\partial RPOP}{\partial t} = \sum_{x} \left(FPR_{x} \cdot BM_{x} + FPRP \cdot PR_{x}\right) \cdot APC \cdot B_{x} - K_{RPOP} \cdot RPOP + \frac{\partial}{\partial z} \left(W_{RPOP} \cdot RPOP\right) + \frac{WRPOP}{V} \tag{2.29}
\]
\[
\frac{\partial LPOP}{\partial t} = \sum_x \left( FPL_x \cdot BM_s + FPDP \cdot PR_x \right) \cdot APC \cdot B_x - K_{LPOP} \cdot LPOP + \frac{\partial}{\partial z} (WS_{LPOP} \cdot LPOP) + \frac{WLPOP}{V} \tag{2.30}
\]

\[
\frac{\partial DOP}{\partial t} = \sum_x \left( FPDR_x \cdot BM_s + FPDP \cdot PR_x \right) \cdot APC \cdot B_x + K_{RPOP} \cdot RPOP + K_{LPOP} \cdot LPOP - K_{DOP} \cdot DOP + \frac{WDOP}{V} \tag{2.31}
\]

\[
\frac{\partial POA_x}{\partial t} = \sum_x \left( FPI_x \cdot BM_s + FPIP \cdot PR_x - P_x \right) \cdot APC \cdot B_x + K_{DOP} \cdot DOP + \frac{\partial (WS_{TSS} \cdot POA_x)}{\partial z} + BFPOA_x + \frac{WPOA_x}{V} \tag{2.32}
\]

\[
POA_x = \frac{K_{POA_x} \cdot TSS}{1 + K_{POA_x} \cdot TSS} \cdot POA_x, \quad POA_d = \frac{1}{1 + K_{POA_d} \cdot TSS} \cdot POA_d \tag{2.33}
\]

\[
K_{RPOP} = \left( K_{RP} + \frac{K_HP}{K_HP + POA_d} K_{RP_{alg}} \sum_x B_x \right) \cdot e^{KT_{max} (T - T_{thr})} \tag{2.34}
\]

\[
K_{LPOP} = \left( K_{LP} + \frac{K_HP}{K_HP + POA_d} K_{LP_{alg}} \sum_x B_x \right) \cdot e^{KT_{max} (T - T_{thr})} \tag{2.35}
\]

\[
K_{DOP} = \left( K_{DP} + \frac{K_HP}{K_HP + POA_d} K_{DP_{alg}} \sum_x B_x \right) \cdot e^{KT_{max} (T - T_{thr})} \tag{2.36}
\]

where

- **FPR**: fraction of metabolized phosphorus by algal group x produced as refractory particulate organic phosphorus
- **FPL**: fraction of metabolized phosphorus by algal group x produced as labile particulate organic phosphorus
- **FPD**: fraction of metabolized phosphorus by algal group x produced as dissolved organic phosphorus
- **FPI**: fraction of predated phosphorus produced as refractory particulate organic phosphorus
- **FLP**: fraction of predated phosphorus produced as labile particulate organic phosphorus
- **FPDP**: fraction of predated phosphorus produced as dissolved organic phosphorus
- **FPIP**: fraction of predated phosphorus produced as inorganic phosphorus
- **APC**: phosphorus to carbon ratio for algal group x (g [P] per g [C])
- **K_{RPOP}**: hydrolysis rate of refractory particulate organic phosphorus (day\(^{-1}\))
- **K_{LPOP}**: hydrolysis rate of labile particulate organic phosphorus (day\(^{-1}\))
- **K_{DOP}**: mineralization rate of dissolved organic phosphorus (day\(^{-1}\))
- **WRPOP**: external loads of refractory particulate organic phosphorus (g [P] day\(^{-1}\))
- **WLPOP**: external loads of labile particulate organic phosphorus (g [P] day\(^{-1}\))
- **WDOPO**: external loads of dissolved organic phosphorus (g [P] day\(^{-1}\))
- **WPOA**: external loads of total phosphate (g [P] day\(^{-1}\))
- **WS_{TSS}**: settling velocity of suspended solids (m day\(^{-1}\))
- **POA_d**: dissolved phosphate (mg [P]/L)
- **POA_e**: particulate phosphate (mg [P]/L)
- **BFPOA**: sediment-water exchange flux of phosphate (g [P] m\(^{-2}\) day\(^{-1}\))
- **K_{RP}**: minimum hydrolysis rate of refractory particulate organic phosphorus (day\(^{-1}\))
- **K_{LP}**: minimum hydrolysis rate of labile particulate organic phosphorus (day\(^{-1}\))
K_{DP}: minimum mineralization rate of dissolved organic phosphorus (day^{-1})

K_{RPalg}: constant that relates hydrolysis of RPOP to algal biomass (day^{-1} per mg P/L)

K_{LPalg}: constant that relates hydrolysis of LPOP to algal biomass (day^{-1} per mg [P]/L)

K_{DPalg}: constant that relates mineralization of DOP to algal biomass (day^{-1} per mg [P]/L)

K_{HP}: mean half saturation constant for algal phosphorus uptake (mg [P]/L), \( K_{HP} = \frac{1}{3} \sum K_{HP_i} \)

K_{PO4p}: empirical coefficient relating phosphate sorption to total suspended solid (per mg/L)

2.3.2.5 Silica

There are 2 silica species in our model including particulate biogenic silica (SU) and available silica (SA). For particulate biogenic silica, the source is from the phytoplankton metabolism and predation, while the loss includes dissolution and settling of particulate biogenic silica. For available silica, the source is from the phytoplankton metabolism, predation, dissolution of particulate biogenic silica and sediment available silica flux, while the loss includes phytoplankton uptake and settling of particulate biogenic silica.

Below are the questions related to silica:

\[
\frac{\partial SU}{\partial t} = (FSP_d \cdot BM_d + FSPP \cdot PR_d)ASC_d \cdot B_d - K_{SUd} \cdot SU + \frac{\partial (WS_d \cdot SU)}{\partial z} + \frac{WSU}{V} \tag{2.37}
\]

\[
\frac{\partial SA}{\partial t} = (FSI_d \cdot BM_d + FSIP \cdot PR_d - P_d)ASC_d \cdot B_d + K_{SUd} \cdot SU + \frac{\partial (WS_{TSS} \cdot SA_p)}{\partial z} + \frac{BFSAd}{\Delta T} + \frac{WSA}{V} \tag{2.38}
\]

\[
SA_p = \frac{K_{SAP} \cdot TSS}{1 + K_{SAP} \cdot TSS} \cdot SA_d, \quad SA_d = \frac{1}{1 + K_{SAP} \cdot TSS} \cdot SA_d \tag{2.39}
\]

\[
K_{SUd} = K_{SU} \cdot e^{KT_{SUd}(T - TR_{SUd})} \tag{2.40}
\]

where

FSP_d: fraction of metabolized silica by diatom produced as particulate biogenic silica

FSI_d: fraction of metabolized silica by diatom produced as available silica

FSPP: fraction of predated diatom silica produced as particulate biogenic silica

FSIP: fraction of predated diatom silica produced as available silica

ASC_d: silica to carbon ratio for diatom (g [Si] per g[C])

K_{SUd}: dissolution rate of particulate biogenic silica (day^{-1})

WSU: external loads of particulate biogenic silica (g [Si] day^{-1})

WSA: external loads of available silica (g [Si] day^{-1})

SA_d: dissolved available silica (mg [Si]/L)

SA_p: sorbed available silica (mg [Si]/L)

BFSAd: sediment-water exchange flux of available silica (g [Si] m^{-2} day^{-1})

K_{SAP}: empirical coefficient relating available silica sorption to total suspended solid (per mg/L)

K_{SU}: dissolution rate of particulate biogenic silica at TR_{SUd} (day^{-1})

KT_{SUd}: effect of temperature on dissolution of particulate biogenic silica (°C^{-1})
TR\textsubscript{SUA}: reference temperature for dissolution of particulate biogenic silica (°C)

2.3.2.6 Chemical Oxygen Demand

In the model, there is chemical oxygen demand that represents the reduced substances. The source is from chemical oxygen demand from sediment, while the loss is through oxidization. Below are the questions related to chemical oxygen demand:

\[
\frac{\partial \text{COD}}{\partial t} = \frac{\text{DO}}{K_{\text{COD}} + \text{DO}} \cdot \text{COD} \cdot \frac{\text{BFCOD}}{\Delta z} + \frac{\text{WCOD}}{V} \\
\]

(2.41)

where

\[K_{\text{COD}} = K_{\text{CD}} \cdot e^{K_{\text{TRCOD}}(T - TR_{\text{COD}})}\]  

(2.42)

where

\[K_{\text{COD}}: \text{half saturation constant of dissolved oxygen required for oxidation of chemical oxygen demand (mg[O}_2/L)\]

\[K_{\text{CD}}: \text{oxidation rate of chemical oxygen demand (day}^{-1})\]

\[\text{BFCOD: sediment-water exchange flux of chemical oxygen demand (g [O}_2 m^{-2} \text{ day}^{-1})}\]

\[\text{WCOD: external loads of chemical oxygen demand (g [O}_2 \text{ day}^{-1})}\]

\[K_{\text{TRCOD}}: \text{effect of temperature on oxidation of chemical oxygen demand (°C}^{-1})\]

\[TR_{\text{COD}}: \text{reference temperature for oxidation of chemical oxygen demand (°C)}\]

2.3.2.7 Dissolved Oxygen

There is one dissolved oxygen (DO) species in our model. The source includes photosynthesis and surface reaeration, while the loss includes phytoplankton metabolism, nitrification, heterotrophic respiration, oxidation of chemical oxygen demand, and sediment oxygen demand. Below are the questions related to dissolved oxygen:

\[
\frac{\partial \text{DO}}{\partial t} = \sum \left[ (1.3 - 0.3 \cdot P_{N_s}) P_s - (1 - FCD_s) \cdot \frac{\text{DO}}{K_{HR_s} + \text{DO}} \cdot \text{BM}_s \right] \cdot \text{AOCR} \cdot B_s - \text{AONT} \cdot \text{Nit} \cdot \text{NH}_4 \\
- \text{AOCR} \cdot K_{\mu_k} \cdot \text{DOC} - \frac{\text{DO}}{K_{HR_s} + \text{DO}} \cdot \text{KCOD} \cdot \text{COD} + K_s (DO_s - DO) + \frac{\text{SOD}}{\Delta z} + \frac{\text{WDO}}{V} \\
\]

(2.43)

\[K_s = Area \cdot Rv \cdot WMS^{1.5}\]  

(2.44)

\[Rv = 0.54 + 0.0233 \cdot T - 0.0020 \cdot S\]  

(2.45)

\[DO_s = 14.6244 - 0.367134 \cdot T + 4.497 \times 10^{-3} \cdot T^2 - (9.66 \times 10^{-2} - 2.05 \times 10^{-3} \cdot T - 2.739 \times 10^{-4} \cdot S) \cdot S\]  

(2.46)
where
AOCR: dissolved oxygen to carbon ratio in respiration (g [O₂] per g [C])
AONT: mass of dissolved oxygen consumed per unit mass of ammonium nitrogen nitrified (g [O₂] per g[N])
Kᵣ: reaeration coefficient (day⁻¹)
DOₕ: saturated concentration of dissolved oxygen (mg [O₂]/L)
SOD: sediment oxygen demand (g [O₂] m² day⁻¹)
WDO: external loads of dissolved oxygen (g [O₂] day⁻¹)
Area: empirical constant
Rᵥ: ratio of kinematic viscosity of pure water at 20 °C to kinematic viscosity of water at specified temperature and salinity
WMS: wind speed measured at 10 m above water surface (m/s)

2.3.3 Sediment Flux Model

One significant component of our water quality model is the coupling of the water column process with a sediment flux sub-model. The sediment flux model is based on the principle of mass conservation. It is consisted of three primary features. First, there are three fluxes: the depositional fluxes of particulate matters from the water column to the benthic bed, the diagenesis fluxes from the decay of particulate matter in the bed and the sediment fluxes of dissolved nutrient from the bed back into the overlying water. Second, there is a two-layer structure of the benthic bed: a thin aerobic/anaerobic upper layer and a permanently anaerobic lower layer. Third, particulate organic matter is presented in three G classes in the benthic sediments: they are split into three fractions (G classes) based on their decay rates. The details can be found in (DiToro and Fitzpatrick 1993).

2.3.4 pH Model

We have developed a pH model based on aquatic chemical equilibrium. In the water column, there are many acids/bases among which many processes happen. Some processes are due to the chemical reactions or transformations of chemical substances, while some other processes are related to biological activities. These processes affect the pH variations. The pH model aims to simulate these processes and we further have incorporated this model into our water quality model.
2.3.4.1 Aquatic Chemistry

In order to calculate the pH value in real environment, it is important to consider the major ions/anions and key processes that influence water PH. Although the rates of chemical reactions are important in aquatic chemistry, most aquatic chemical processes are regarded as in equilibrium state in our model since the timescales of most chemical reactions are much shorter than the biological processes considered. In the estuarine and open ocean, the carbonate system is the primary factor that determines the PH. In the water, carbon dioxide exists in three forms: aqueous carbon dioxide (CO₂ or H₂CO₃), bicarbonate (HCO₃⁻) and carbonate (CO₃²⁻). The carbonate system also includes the dissociation of water where water (H₂O) is ionized into hydrogen ion (H⁺) and hydroxide (OH⁻). For a quantitative calculation of PH, it is also necessary to take some major chemical species into consideration. For simplicity, our model will take boric acid (B(OH)₃) into account, which can represent the salinity effect. Below are the four chemical reactions that are considered in our pH model:

\[
H_2CO_3 \rightleftharpoons HCO_3^- + H^+ \quad (2.47)
\]

\[
HCO_3^- \rightleftharpoons CO_3^{2-} + H^+ \quad (2.48)
\]

\[
H_2O \rightleftharpoons OH^- + H^+ \quad (2.49)
\]

\[
B(OH)_3 + H_2O \rightleftharpoons B(OH)_4^- + H^+ \quad (2.50)
\]

where
CO₂ or H₂CO₃: aqueous carbon dioxide
HCO₃⁻: bicarbonate
CO₃²⁻: carbonate
H⁺: hydrogen ion
H₂O: water
OH⁻: hydroxide
B(OH)₃: boric acid
B(OH)₄⁻: borate
K₁, K₂, K₃, and K₄: thermodynamic equilibrium constants for chemical reactions
The thermodynamic equilibrium constants are used to describe the chemical reactions. They represent the relationship between the concentrations of reactants and the concentrations of products under equilibrium. These constants are affected by temperature, salinity and pressure. In saline water, the concentrated solutions will interact with each other because of the ionic strength. Therefore, the concentrations of reaction particles are somehow compromised and the concept of activity coefficient is used to account for this effect. The expressions for calculating these constants can be referred to (Weiss 1974; Dickson and Goyet 1994; Millero 1995; Keeling et al., 1998; Zeebe and Wolf-Gladrow 2003). The equations below show how the equilibrium constants are related to the concentrations of chemical substances. Here, square bracket means the concentration of a certain kind of particles:

\[
K_1 = \frac{[H^+][HCO_3^-]}{[H_2CO_3]} \quad (2.51)
\]

\[
K_2 = \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]} \quad (2.52)
\]

\[
K_w = [H^+][OH^-] \quad (2.53)
\]

\[
K_b = \frac{[H^+][B(OH)_4^-]}{[B(OH)_3]} \quad (2.54)
\]

Figure 2-7 gives an example for the water equilibrium constant \( K_w \) (dissociation coefficient). In the figure, the definition of \( pK_w \) is \( pK_w = -\log_{10} K_w \). As we can see, both salinity and temperature can influence the \( K_w \). Generally, \( K_w \) increases when salinity/temperature increases.
In order to calculate the pH, we also need relationships among the chemical substances. For the carbonate system, TIC refers to the total inorganic carbon concentration as the sum of the concentrations of aqueous carbon dioxide, bicarbonate and carbonate. For borate system, $B_T$ refers to the total boron concentration as the sum of the concentrations of boric acid and borate. In addition, alkalinity is needed for pH calculation. Alkalinity represents the water capacity to accept H$^+$ ions. Generally, a water of higher alkalinity is associated with a higher pH and larger ability to contain inorganic carbon. Alkalinity is an important property of water and can be regarded as a measure of water fertility. The full expression of alkalinity is composed of many kinds of ion species. For our pH model, only the carbonate and borate species are considered for their dominant effects on pH dynamics in estuarine, but the algorithm employed in our model allows the extension to easily include other ion species:

\[
TIC = [H_2CO_3] + [HCO_3^-] + [CO_3^{2-}] \quad (2.55)
\]

\[
B_T = [B(OH)_3] + [B(OH)_4^-] = 4.16 \times 10^{-4} \cdot \frac{S}{35} \quad (2.56)
\]

\[
ALK = [HCO_3^-] + 2[CO_3^{2-}] + [B(OH)_4^-] + [OH^-] - [H^+] \quad (2.57)
\]
TIC: the concentration of total inorganic carbon (mg[C]/L)
B_T: the concentration of boron (mg/L)
ALK: alkalinity (mg [CACO3]/L)

With some algebraic manipulation of Equations (2.51)-(2.56), we get the following relationships with the expression of TIC, H^+, B_T and equilibrium constants:

\[ [H_2CO_3] = \frac{[H^+]^2}{K_1[H^+] + K_1K_2 + [H^+]^2} \text{TIC} \]  \hspace{1cm} (2.58)

\[ [HCO_3^-] = \frac{K_1[H^+]}{K_1[H^+] + K_1K_2 + [H^+]^2} \text{TIC} \]  \hspace{1cm} (2.59)

\[ [CO_3^{2-}] = \frac{K_1K_2}{K_1[H^+] + K_1K_2 + [H^+]^2} \text{TIC} \]  \hspace{1cm} (2.60)

\[ [OH^-] = \frac{K_w}{[H^+]} \]  \hspace{1cm} (2.61)

\[ [B(OH)_4] = \frac{K_b}{[H^+] + K_b} B_T \]  \hspace{1cm} (2.62)

Substitution of Equations (2.58)-(2.62) into Equation (2.57) gives the following Equation (2.63). This is an equation of [H^+] and can be solved when alkalinity and total inorganic carbon are known. The other terms for B_T and equilibrium constants can be computed using empirical equations when temperature and salinity are known. Pressure effects on equilibrium constants are neglected because of the shallow depth in our model domain:

\[ ALK = \frac{K_1[H^+] + 2K_1K_2}{K_1[H^+] + K_1K_2 + [H^+]^2} \text{TIC} + \frac{K_b}{[H^+] + K_b} B_T + \frac{K_w}{[H^+]^2} - [H^+] \]  \hspace{1cm} (2.63)

pH is defined as \[ pH = -\log_{10}[H^+] \]. Figure 2-8 is a theoretic curve for pH versus alkalinity to TIC ratio. The result is consistent with (DiToro 2001), which states that pH is largely determined by the ratio of alkalinity to TIC concentration. Figure 2-9 shows how pH varies when alkalinity concentration changes
under different TIC concentration. Generally, pH goes up as alkalinity concentration increases under constant TIC concentration, while pH goes down as TIC concentration increases under constant alkalinity concentration.

Figure 2-8. Theoretic pH curve with alkalinity to total inorganic carbon ratio based on our pH model. The temperature used for the calculation is 15 °C and the salinity is 1.5 ppt. There are four curves for different total inorganic carbon concentrations and the difference is minor.
2.3.4.2 pH Model Kinetics

In our pH model, there are four state variables: total inorganic carbon (TIC), alkalinity (ALK), dissolved calcium ion Ca$^{2+}$ (CA), and solid-phase calcium carbonate (CaCO$_3$). Besides TIC and ALK, calcium species are introduced into our model because calcium usually has high concentration in commonly found water systems and can impact the pH system. Calcium plays an important role in many biogeochemical processes. In addition, calcium species comprise a buffer system. For instance, acid water with too much aqueous CO$_2$ will dissolve calcium carbonate and the acidity of the water will be reduced (pH will increase). The reverse reaction will form calcium carbonate and will cause CO$_2$ to be lost from the water (pH will decrease).

For TIC, the source terms include oxic respiration of phytoplankton, heterotrophic respiration of DOC, oxidation of organic matter in the sediment, while the loss term is phytoplankton uptake in photosynthesis. Also, the gas exchange between water and air can alter the CO$_2$ concentration in the water.
Moreover, the formation/dissolution of calcium carbonate can decrease/increase CO2 concentration. For alkalinity, we will consider the effect of NH₄ and NO₃ uptake by phytoplankton. Cerco (2013) noted that alkalinity will decrease 15/14 mole when 1 mole of NH₄ is utilized, and will increase 17/16 mole when 1 mole of NO₃ is utilized. Plus, nitrification and the formation/dissolution of calcium carbonate can change alkalinity concentration. The only process that influences CA concentration is the formation/dissolution of calcium carbonate. The CACO₃ concentration can be altered by the formation/dissolution of calcium carbonate as well as its settling. The following shows the mass balance equations for these four variables:

\[
\frac{\partial TIC}{\partial t} = \sum_x \left[ \left( 1 - FC_D \right) \frac{DO}{K_{HR} + DO} B_M - P_x \right] B_s + \frac{r_{Ka} (C_{O2_{sat}} - C_{O2})}{\Delta z} + K_{HR} \cdot \Delta z \cdot \Delta C \cdot \frac{m_{C}}{m_{CACO3}} + \frac{SOD}{\Delta z \cdot AOC} \cdot r_{KCACO3} \cdot \left( C_{A_{sat}} - C_{A} \right) \frac{m_{C}}{m_{CACO3}}
\]

\[
\frac{\partial ALK}{\partial t} = \sum_x \left[ -\frac{15}{14} P_{N_x} P_x B_s + \frac{17}{16} \left( 1 - P_{N_x} \right) P_x B_s \right] A_{NC_x} \cdot \frac{m_{CACO3}}{2 \cdot m_N} - N_{it} \cdot \frac{m_{CACO3}}{m_N} + r_{KCACO3} \cdot \left( C_{A_{sat}} - C_{A} \right)
\]

\[
\frac{\partial CA}{\partial t} = r_{KCACO3} \cdot \left( C_{A_{sat}} - C_{A} \right)
\]

\[
\frac{\partial CACO3}{\partial t} = -r_{KCACO3} \cdot \left( C_{A_{sat}} - C_{A} \right) + \frac{\partial \left( W_{CACO3} \cdot CACO3 \right)}{\partial Z}
\]

where

- r_{Ka}: reaeration rate for CO₂ (m/day)
- CO₂_{sat}: saturation concentration of CO₂ (mg/L)
- CO₂: aqueous carbon dioxide concentration (mg/L)
- r_{KCACO3}: the dissolution/formation rate of calcium carbonate (day⁻¹)
- CA_{sat}: the saturation concentration of dissolved calcium (mg [CACO₃]/L)
- CA: the concentration of dissolved calcium (mg [CACO₃]/L)
- mC: mole weight for carbon (=12.011 g)
- m_{CACO3}: mole weight for calcium carbonate (=100.086 g)
- m_N: mole weight for calcium carbonate (=14.007 g)
- CACO₃: the concentration of calcium carbonate (mg [CACO₃]/L)
- W_{CACO3}: the settling velocity of calcium carbonate (m/day)
2.4 Model Set-up

In SCHISM, the basic computation unit is prism based on triangle or quadrilateral. For all the water quality variables including temperature and salinity, they are defined in the prism center where their concentration is specified. The finite volume method is applied for the physical processes including advection and diffusion, and for the kinetic processes such as phytoplankton growth. Figure 2-10 shows two types of prisms that are used in SCHISM. Each prism is either a triangular prism or a quadrilateral prism.

Figure 2-10. Basic computation unit in SCHISM: triangular prism (left) and quadrilateral prism (right). Here Ci represents the variable concentration at the prism center.

For modeling the algal bloom phenomenon in Back River, the model domain needs to be larger because Back River is largely influenced by the main Bay. Also, Back River is only ~50 km downstream of Susquehanna River, which affects the Back River as well as the whole Chesapeake Bay because of the large river flow. In order to include all the potential effects from outside on the Back River, our model domain contains Upper Chesapeake Bay (Figure 2-11) that extends from the Patuxent River mouth to Susquehanna River mouth. The whole domain is about 180 km long, 5 to 20 km wide. The depth ranges from 2 meters in shallow areas to 48 meters in deep holes (Figure 2-12).
Figure 2-11 shows our model grid which consists of 18,110 elements and 11,692 nodes in the horizontal. The elements are mixed triangles and quadrilaterals. Typically, quadrilaterals with high resolution are placed along the channel to the better represent bathymetry, while triangles are placed in shallow areas to better fit the geometry and shorelines. The quadrilaterals are very economical in term of computation cost and can also improve the accuracy because it uses bilinear shape functions for the calculation instead of linear shape functions for triangles. For the entire domain, the grid size can vary from 100m inside the Bay channel to 2km in some shallow areas. High grid resolution is also placed in Back River since it is our area of interest. In Back River, the grid size varies from 100m to 200m. Another characteristic about SCHISM is that it does not need the grid to be orthogonal. Instead, the model is very robust and can tolerate very skewed elements which do exist for some areas in our model grid.

For the vertical grid, we use Localized Sigma Coordinates with Shaved Cell (LSC$^2$). The detail about LSC$^2$ can be found in (Zhang et al., 2015). Fundamentally, LSC$^2$ allows the number of vertical layers to vary in space based on the local water depth. More layers are used in deep regions and fewer layers are used in shallow regions. This characteristic not only saves computation time, but also avoids the crowding of layers in shallow areas as for traditional sigma coordinates. The benefit of the shaved prisms placed in the bottom is the improvement of the model accuracy. Also, this feature prevents the hydrostatic inconsistency problem faced by many other models since it makes the slope of coordinate plane milder and shut down unrealistic mass exchange among some bottom cells. For our model, the maximum number of vertical layers is 35, while the average number for the entire domain is 14. Figure 2-12 shows the bathymetry of our model. The bathymetry data is from NOAA and one can download these from https://maps.ngdc.noaa.gov/viewers/bathymetry. Imbedded in the middle right of the Figure 2-12 is a vertical transect showing the structure of our vertical grids. In the deep, the number of vertical layers is over 30, but there are only 9 layers on the bank. In addition, we can see that there are degenerated prisms placed in the bottom which fits the bathymetry slope well. In fact, the NOAA bathymetry data are directly interpolated into our model grid with no smoothing technique applied.
Figure 2-11 also shows all the monitoring stations we used for our model calibration. There are five NOAA elevation stations (triangles), two NOAA velocity measurement stations (squares), and 24 water quality stations (dots) from Chesapeake Bay Program. The elevation and velocity data can be downloaded from [https://www.co-ops.nos.noaa.gov/](https://www.co-ops.nos.noaa.gov/), and water quality data can be downloaded from [http://www.chesapeakebay.net/data/](http://www.chesapeakebay.net/data/). Please note the elevation data from Solomons Island and the water quality data from Station CB5.1 are used for preparing boundary conditions for our model. The measurements from water quality stations include water quality variables as well as temperature and salinity observations, which are used to verify our hydrodynamic results. The stations with names beginning with ‘CB’ refer to channel stations and most of them are deep stations. The stations with names beginning with ‘WT’ and ‘ET’ refer to stations on the west bank and on the east band, respectively, and most of the stations are shallow stations.

Our model runs from 2012 to 2014 with a time step of 120 seconds. On the high performance parallel computing system at the College of William & Mary, it will take about 72 hours to complete a 3-year simulation with 84 vortex cores. The simulation is about 365 times faster than real time.
Figure 2-11. The horizontal grid for Upper Chesapeake Bay with monitoring stations for elevation (triangles), velocity profiles (squares), and water quality (dots). The region around Back River is zoomed in and shown on the upper left.
Figure 2-12. The bathymetry for the Upper Chesapeake Bay. In the middle left is a transect across the Bay from west to east showing the vertical grid profile.
2.4.1 Hydrodynamics

2.4.1.1 Surface Forcing

Surface forcing plays an important role for the hydrodynamics and water quality. For instance, wind affects the hydrodynamics in the Upper Chesapeake Bay by influencing the mixing and water circulation. SCHISM provides several options for how to specify the surface forcing. In a simple case, one can provide a time series of wind for the entire domain. In our case, we invoke a surface flux module of SCHISM which take surface flux inputs in NETCDF format. These inputs include wind, air pressure, air temperature, specific humidity, precipitation rate, and radiation fluxes. They are provided by North American Regional Reanalysis (NARR) which can be downloaded from http://www.emc.ncep.noaa.gov/mmb/rra1/. However, for wind, we use hybrid sources by blending NARR wind dataset with high-resolution wind dataset from National Data Buoy Center (NDBC). The NARR wind has a spatial resolution of 0.3 degrees (32 km) and a temporal resolution of 3 hours. NDBC has many measurement stations (circles in Figure 2-13) in Upper Chesapeake Bay with high temporal resolution and the data can be downloaded from http://www.ndbc.noaa.gov/. The resulting hybrid wind dataset has a spatial resolution of 0.1 degrees and a temporal resolution of 1 hour. Figure 2-13 is a snapshot for wind field on October 1st, 2013 by comparing the hybrid wind (black arrows) to NARR wind (red arrows). It can be seen that the two datasets are consistent, but the hybrid wind provides more variabilities.

2.4.1.2 Initial Condition

For hydrodynamics, the model needs the initial condition of elevation, velocity, temperature and salinity. Usually, elevation at zero referring to the mean sea level (MSL) and velocity with zero (still water) are used for the initial conditions. Based on experiment, it often takes a short time, normally less than one day, for the model to spin-up for elevation and velocity. However, it takes much longer for the model to spin up for temperature and salinity. In Upper Chesapeake Bay, there exists a gravitational circulation pattern characterized by a layer of fresher surface water flowing seaward over a layer of saltier bottom water flowing landward. In order to make our model to set up a relatively stable circulation structure in a
short time, the initial conditions for temperature and salinity are important. The measurement data for salinity and temperature from Bay Program were used to generate the initial conditions. The resulting initial conditions includes spatial distribution and vertical distribution for both temperature and salinity.

2.4.1.3 Boundary Condition

The open boundary of the model is located around the Bay Monitoring Station CB5.1 (Figure 2-11). The Bay Program provides monthly observation data at CB5.1 for temperature and salinity. The data covers the depth from surface (0.5 m) to bottom (33–36 m). Usually, each vertical profile has more than 20 measurements. By assuming there is no lateral variation, we interpolated the observation data in time and space and constructed boundary conditions for temperature and salinity. For the elevation boundary condition, we used the measurement from the NOAA station at Solomons Island (Figure 2-11). A time series with a temporal resolution of one hour is provided to drive the model. The input for the velocity boundary condition is not provided and we allowed the model adjust by itself.

For the river boundary, river flow discharge is usually specified as the boundary condition. However, SCHISM provides a more consistent method to add these incoming flows by treating them as local volume sources. A benefit of this method is that it can easily avoid a double count of river flow when the watershed loading for our water quality model also includes volume discharge, which is our case. Our watershed loading is provided by the Environmental Protection Agency (EPA) and the fresh water discharge is distributed along our model boundaries. Traditionally, river flow data are from United States Geological Survey (USGS) and the boundary condition out of it is applied to the river boundary. For our model, we use EPA loading to replace this river flow by adding the discharge to the model boundary elements. Figure 2-14 shows the comparison of flow discharge between these two sources. Generally, they are consistent in term of magnitude and long-term variation. However, for Susquehanna River, the EPA watershed loading has larger short-term variability than USGS data. For Choptank River, the flow from EPA watershed loading is generally larger than USGS data. The difference may be caused by that EPA
watershed loading contains additional non-point sources flow and point sources flow from land, besides the apparent surface river runoff.

Figure 2-13. Wind forcing comparison between hybrid wind (black arrows) and NARR wind (red arrows). The green line is Chesapeake Bay boundary and blue circles are meteorology stations from the National Data Buoy Center.
Figure 2-14. The comparison for river flow discharge between EPA watershed loading (red line) and USGS measurement (green line). For Upper Chesapeake Bay, the river flows from Susquehanna River (upper panel) and Choptank River (lower panel) are shown.

2.4.2 Water Quality

2.4.2.1 Initial Condition

The initial condition for the water quality model is based on the observational data from Chesapeake Bay Program around the beginning of 2012. The concentrations for phytoplankton species, organic carbon species, nutrient species, and dissolved oxygen are interpolated in the horizontal to generate a spatially varying initial condition for water quality variables. In addition, an assumption that concentration is uniform in the vertical is made since the overturning in the winter will mix the water column. For chemical oxygen demand, we prescribe its initial concentration as zero for the entire domain.
2.4.2.2 Boundary Condition

For the open boundary condition of the water quality model, the observational data from Station CB5.1 from Chesapeake Bay Program is used. The observational data are first interpolated in the vertical to get water quality variable concentrations from surface to bottom. Then, the monthly or bi-weekly data are interpolated in time to provide the temporal variation from 2012 to 2014. Furthermore, the boundary condition is applied across the entire open boundary. If the local depth at a particular point on the boundary is shallower than maximum depth of the boundary condition, the interpolation result for the lower depth is discarded. For most water quality variables, this method gives a good estimation in terms of vertical distribution and temporal coverage. Figure 2-15 shows an example using the interpolation. The variable is dissolved oxygen. Overall, we can see that the interpolation result is consistent with the observation and serves well for the purpose of providing the water quality boundary condition.

For the water quality model, the river boundary condition is also very important because a large amount of nutrient loading is associated with the river discharge. Traditionally, the river flow is assumed to be well-mixed and time series for all water quality variables are used as the river boundary conditions for every river. For instance, in Upper Chesapeake Bay, the time series based on measurements at Station CB1.1 or Station CB1.0 is often used as the boundary condition for Susquehanna River. However, in the current model setup, the river boundary condition is implicitly included in the watershed loading which is consistent with the way the river flow is added in the model. In fact, the way of adding river flow is also implicit as mentioned in Section 2.5.1.3. In order to specify the boundary condition, times series of concentrations of water quality variables are specified for every volume source (flow) around the river boundary, instead of for the river boundary directly. In this way, the river boundary conditions for water quality variables are provided to the model when the river flow is added.
Figure 2-15. The upper panel shows dissolved oxygen measurements at Station CB5.1 from the Chesapeake Bay Program from 2012 to 2015. The lower panel shows the interpolation results based on measurement, providing both the vertical distribution and the temporal variation dissolved oxygen, which is then used as the water quality boundary condition.

2.4.2.3 Nutrient Loading

The nutrient loading is included in the watershed loading that the EPA provided to us. Besides the nutrient loading, watershed loading also contains the fresh water discharge from all watersheds in the Upper Chesapeake Bay. The lower limit of the loading is Patuxent River. EPA group simulate the non-point source loadings for every watershed based on their watershed model from 2012 to 2014. Then, they combine all the point source loading into the simulated results. In addition, the watershed loading is partitioned into every boundary elements of model grid based on the location of watersheds. The final product we received is combined loading for all nutrient species and for every boundary elements. SCHISM treats watershed flows (including river flows) as local volume sources. The nutrient loading represents a property that is associated with the water masses from watersheds. Therefore, it is a natural way to add nutrient loading into our water quality model by specifying the concentrations for all nutrients species for each water mass. Figure 2-16 shows the total watershed loading for our model from 2012 to 2014. The loading varies little among the three years with a slightly larger loading in 2014. The average flow for the entire Upper
Chesapeake Bay is around 1116 m³/s. The mean yearly loading for Total Organic Carbon (TOC) is about 5.68×10⁵ Kg/Day; the mean yearly loading for Total Nitrogen (TN) is about 1.83×10⁵ Kg/Day; and the mean yearly loading for Total Phosphorus (TP) is about 8.28×10³ Kg/Day.

Figure 2-16. Watershed loading for Upper Chesapeake Bay above Patuxent River from 2012 to 2014. The upper left is yearly averaged flow and the other three subplots are Total Organic Carbon (TOC), Total Nitrogen (TN) and Total Phosphorus (TP).

Apart from the watershed loading, atmospheric loading is also an input to the water quality model, which is also provided by the EPA. Due to the small size of our model, a uniform atmospheric loading in the horizontal is specified. The nitrogen deposition of atmospheric loading can be in two forms: wet deposition (that is associated with precipitation) and dry deposition (that enters water without the aid of precipitation). The data EPA provides include the dry and wet components of deposition nitrogen and the wet component of deposition phosphorus. We sum up these two forms of loading as they are not distinguished in our water quality model. Figure 2-17 shows the atmospheric loading of nitrogen and
phosphorus from 2012 to 2014. On average, atmospheric loading of nitrogen is about 2.85 mg/(m²·day), while atmospheric loading of phosphorus is 0.196 mg/(m²·day).

Figure 2-17. Atmospheric loading for nitrogen (left panel) and phosphorus (right panel). For nitrogen deposition, dry deposition and wet deposition are also shown. The unit is mg/(m²·day).

In Back River, the most important nutrient source is from a Waste Water Treatment Plant (WWTP), which is located in the northern part of Back River. The WWTP has the capability to process waste water 180 million gallons per day (MGD) of which about 130 MGD is discharged into Back River. The discharged water from the WWTP contains high concentration organic and inorganic nutrients which promotes the phytoplankton growth in the local. The City of Baltimore provides detailed daily information about the Back River WWTP. Figure 2-18 summarizes the nutrients loading. On average, the WWTP flow is about 4.62 m³/s. For nitrogen, the total loading is about 3.08×10³ Kg/Day with a mean concentration of about 7.72 mg/L. For phosphorus, the total loading is about 67.0 Kg/Day with a mean concentration of about 0.168 mg/L.
Figure 2-18. Nutrient loading from Back River Waste Water Treatment Plant (WWTP). The upper left panel is the mean flow discharge from 2012 to 2014. In the upper/lower middle is total nitrogen loading/concentration. In the upper/lower right is total phosphorus loading/concentration.

2.4.2.4 Sediment Initial Condition

The sediment flux model plays an important role for water quality simulation because many kinetic processes happening inside the sediment can significantly affect the nutrient dynamics in the water column. Here, its initial condition refers to the initial concentration of sediment variables such as the concentrations of particular organic matter in the sediment. The initial condition represents the history of interaction between water column and sediment. In practice, there is no such data for model application. In some cases, a “stand-alone” sediment model is used to estimate the initial conditions (Park et al., 1995). Here, we adopt another approach by running the model for multiple years until equilibrium reaches for sediment processes. Then, the sediment state at this point is used for the initial condition of sediment fluxes model. This method has been applied in several other applications (e.g., shallow river simulation in Chester River in the Upper Chesapeake Bay) and works well.
2.4.2.5 Additional Issues

There is still one problem for water quality model referring to Equation (2.5), which shows that total suspended solids (TSS) concentration needs to be known for computing the light attenuation coefficient for phytoplankton. In order to get TSS, there are two methods available in our model. The first one is to launch a full 3D dynamic sediment transport model which resides in the SCHISM modeling system and is coupled it into our water quality model. This approach has been tried and is now an option for our water quality model. However, to calibrate the sediment transport for the Upper Chesapeake Bay needs much efforts before it can be used for computing light attenuation. Moreover, it increases model runtime. The second method is to estimate TSS by using available water quality variables. From data analysis, it is found that TSS has a good correlation with particulate organic carbon in Upper Chesapeake Bay. Coynel et al., (2005) shows that there is a correlation between TSS and particulate organic matter (POC). For each station in Chesapeake Bay, the least squares regression analysis gives a conversion coefficient from POC to TSS (Figure 2-19). We further interpolate this relation to the entire domain and the result is shown in Figure 2-20. It is interesting that the coefficient is generally larger in the upper part below Susquehanna River and smaller in the lower part. This approach is simple and straightforward, usually giving a reasonable good estimation of TSS in the model application. We also tested this approach in Chester River and the result was satisfactory. Therefore, for the current study we will adopt this approach to compute TSS for our model.
Figure 2-19. Correlation between total suspended solids (TSS) and particulate organic carbon (PC) in Upper Chesapeake Bay.

Figure 2-20. Horizontal distribution of POC to TSS conversion coefficient in Upper Chesapeake Bay.
2.4.3 pH model

For specifying the pH model in Upper Chesapeake Bay, one difficulty is the lacking of data for the input of the four variables TIC, ALK, Ca and CaCO$_3$. For example, the watershed loading doesn’t provide any information about these four variables, whereas in reality water flow from watershed does have certain concentration of them. Thus, some assumption needs to be made regarding the input of the pH model.

2.4.3.1 Alkalinity

Alkalinity plays a key role in calculating water PH, but in some situation alkalinity data are not available. Fortunately, there is a way to estimate the alkalinity based on water salinity. Lee et al., (2006) mentioned that the variation of alkalinity and the variation of salinity in surface water are closely related. For example, freshwater addition such as precipitation reduces water alkalinity and at the same time reduces the water salinity. Therefore, in cases where alkalinity is not available, an estimate of alkalinity based on the empirical relationship between salinity and alkalinity is applied. Figure 2-21 shows the correlation between alkalinity and salinity based on observation data from CB3.3C. A linear regression: ALK=35.6761+2.3058*SAL is used to approximate alkalinity.
Figure 2-21. Correlation between alkalinity and salinity. The observation data from station CB3.3C are used for the linear regression. The correlation coefficient for the regression is about 0.66.

2.4.3.2 Total Inorganic Carbon

TIC is necessary for computing pH according to the aquatic chemistry in 3.4.1. However, TIC is not among the variables that are routinely measured in regular water quality monitoring programs such as Chesapeake Bay Program. On the other hand, pH is a variable that can be easily measured and is normally available. As discussed by Zeebe and Wolf-Gladrow (2001) about carbonate system, one can calculate all the six variables (CO$_2$, HCO$_3^-$, CO$_3^{2-}$, H$^+$, TIC, and ALK) if any two of them are given. According to the aquatic chemistry, we can get the following equation after some algebraic manipulation of Equation (2.63).

Here, we calculate TIC based on pH and ALK:

$$TIC = \frac{K_i[H^+] + K_iK_2 + [H^+]^2}{K_i[H^+] + 2K_iK_2} \left( \text{ALK} + [H^+] \right) - \frac{K_b}{[H^+] + K_b} B_T - \frac{K_w}{[H^+]}$$  \hspace{1cm} (2.68)
2.4.3.2 Dissolved Calcium and Calcium Carbonate

In order to couple the pH model with the water quality model, we also need to take CA and CaCO$_3$ into consideration. In Upper Chesapeake Bay, the largest freshwater source is from Susquehanna River (Figure 2-14) and the calcium measurement is available from 2012 to 2014 (Figure 2-22). Figure 2-22 also shows the temporal variation of ALK for Susquehanna River and the correlation between CA and ALK. It is shown that CA and ALK have a good correlation in freshwater. Therefore, in case that CA measurement is missing, estimation based ALK would be a good choice. CaCO$_3$ is solid phase by our definition and for the sake of simplicity we regard its concentration in watershed loading is zero.

2.4.3.3 Initial Condition and Boundary Condition

In order to generate initial/boundary condition, the four variables (ALK, TIC, CA, CaCO$_3$) need to be known. ALK can be estimated using salinity based on 4.3.1 in the horizontal (for initial condition) and in the open boundary (for boundary condition). Chesapeake Bay Program provides abundant pH measurements in the whole Bay. Therefore, we can compute TIC based on Equation (2.68). Because CA has a good relation with ALK and CaCO$_3$ is assumed to be zero, it is now sufficient to specify the initial/boundary condition for the pH model.

2.4.3.4 Back River

Because studying the bloom phenomenon in Back River is one of our focuses, in this part, we will discuss how to apply the pH model in Back River.

As mentioned before, the biggest freshwater source in Back River is the WWTP. Besides the nutrient loading, the City of Baltimore also provides the information of alkalinity and pH on daily basis about the discharge water from the WWTP. Figure 2-23 shows the time series of flow, alkalinity and pH for the Back River WWTP. A similar approach to the preparation of initial/boundary condition in 2.5.3.3 is employed here to estimate the three variables (TIC, CA, CaCO$_3$) of the pH model. Because of the daily
measurements of WWTP data which are quite abundant compared to water quality measurements from Chesapeake Bay Program, our purpose of the pH model application in Back River was well satisfied.

For Susquehanna River, its water quality data ([https://water.usgs.gov/owq/data.html](https://water.usgs.gov/owq/data.html)) includes ALK, pH and CA. This enables us to calculate all the inputs for pH model for the watershed of Susquehanna River. However, watershed loading EPA provided does not includes any of these information for other watersheds. For current model setting, we apply the pH model input derived from Susquehanna River to all the other watersheds except in Back River (Figure 2-11). There are several reasons that justify this approach. First, the focus of our pH model application is in Back River where detailed pH model input is available. Second, because Susquehanna River is responsible for a large part of freshwater discharge to Upper Chesapeake Bay and it is close to Back River, the disturbance effect from other watersheds loading should be small. Third, to further reduce the uncertain effects of watershed loading on pH model in Back River, pH model kinetics described in 3.4.2 are only applied in Back River. Outside the Back River, we will nudge the ALK and TIC to the values calculated based on local pH and salinity. Since kinetics are missing outside Back River, only physical processes (advection and diffusion) control the distribution of pH model variables.

When inorganic carbon is depleted, the photosynthesis process will be hampered. In order to account for this phenomenon in our model, we modify phytoplankton growth rate $P_x$ in Equation (2.2) by multiplying it with a limiting function of TIC. The revised phytoplankton growth rate is

$$P_x = \begin{cases} PM_x \cdot f_1(N) \cdot f_2(I) \cdot f_3(T) \cdot f_5(TIC), & \text{for diatom and green alage} \\ PM_x \cdot f_1(N) \cdot f_2(I) \cdot f_3(T) \cdot f_4(S) \cdot f_5(TIC), & \text{for cyanobacteria} \end{cases} \tag{2.69}$$

where

$$f_5(TIC) = \frac{TIC^2}{TIC^2 + TIC_{RF}^2}, \tag{2.70}$$

and $TIC_{RF}$ is concentration when the growth rate is halved.
Figure 2-22. The upper panel shows the measurements of water calcium and alkalinity in Susquehanna River from 2012 to 2014. The lower panel is the linear regression between calcium and alkalinity. The correlation coefficient is about 0.96.
Figure 2-23. Time series of Back River WWTP flow (upper panel), alkalinity (middle panel) and pH (lower panel) from 2012 to 2014.
2.5 Comparison Between Model Results and Observation

In this section, we will present our model results about hydrodynamics, water quality and pH model. The observation data from all the monitoring stations (Figure 2-11) are used for the comparison. For temperature, salinity and water quality variables, the surface and bottom model results are displayed against observation data. Also, we will present the results for all the stations from Chesapeake Bay Program from 2012 to 2014. This allows us to view the overall spatial variation and temporal variability. It also enables us to evaluate the model results in both deep and shallow regions of Upper Chesapeake Bay. In this way, one can get a complete picture about our model behavior for certain variables. This is important because the kinetics in the water quality model are complicated and many state variables are involved. If results are shown only for particular stations or in certain periods, the conclusion may be misleading even if the result is good for these stations and periods.

2.5.1 Hydrodynamics

2.5.1.1 Elevation

In order to evaluate model elevation, four stations (Cambridge, Annapolis, Baltimore, and Tolchester) are selected for the comparison. The spatial distribution of these four stations covers from the lower part of the model domain to the upper part. Figure 2-24 shows three-year time series from 2012 to 2014 for all stations. Although it is difficult to discern the details from the clustered time series, we still can see that the model elevation matches observation well in terms of subtidal signals and tidal amplitude for all stations. Correlation coefficients between model and observation time series are 0.97 for Cambridge, 0.92 for Annapolis, 0.87 for Baltimore, and 0.90 for Tolchester. In addition, a harmonic analysis is done at each station. In Figure 2-25, the upper panels are tidal amplitudes for both observation and model outputs. Five tidal constituents (O₁, K₁, M₂, S₂, N₂) are presented. Overall, tidal amplitudes of model results match those of the observations well for all tidal components. For the largest tidal constituent M2 tide, a large model to observation difference about 4 cm occurs at Station Annapolis. The lower panels are the tidal
phases and the model results are close to observations with very small differences. In addition, from the south to north, we can see that there is a tidal phase shift.

2.5.1.2 Velocity

Two NOAA stations with current measurements (cb1101, cb1201) are selected for velocity comparison. At these two stations (Figure 2-11), Acoustic Doppler Current Profilers (ADCPs) are used to measure water currents from surface to bottom. The final product of ADCP gives velocity profiles in the vertical direction with intervals in one meter. For simplicity, we plotted observed and modeled along channel velocity profiles together for comparison in Figure 2-26 and Figure 2-27. Our simulation is from 2012 to 2014, and only the results in July 2012 at both stations are shown as an example. As we can see, velocity is well-simulated for most layers. A slightly larger discrepancy between observed and modeled velocities exists for the surface layer (depth=0.2 meter) at cb1201, which is probably due to the insufficient specification of wind forcing (Ye et al., 2016). Overall, the model is fairly accurate regarding the velocity amplitude and phase.
Figure 2-24. Elevation time series from 2012 to 2014. The model results (green dashed lines) are displayed with observation data (red lines). There are four stations (Cambridge, Annapolis, Baltimore, and Tolchester) from downstream to upstream.
Figure 2-25. Harmonic analysis for elevation results of the four stations in Upper Chesapeake Bay (Cam. (Cambridge), Ann. (Annapolis), Bal. (Baltimore), and Tol. (Tolchester)). The upper panels are tidal amplitudes and the lower panels are tidal phases. Five tidal components (O₁, K₁, M₂, S₂, N₂) are shown. In all the diagrams, observation data (asterisk) and model results (circles) are displayed for the comparison.
Figure 2-26. The comparison of observed (blue) and modeled (red) along channel velocity profiles at Station cb1101 in July 2012. The direction of channel is 25.0° true north obtained from NOAA website.
Figure 2-27. The comparison of observed (blue) and modeled (red) along channel velocity profiles at Station cb1201 in July 2012. The direction of channel is 12.0° true north obtained from NOAA website.
2.5.1.3 Temperature

Temperature is a quantity that is modeled by SCHISM. For Upper Chesapeake Bay, we have 24 gauge stations and the calibration result is shown in Figure 2-28. As we can see, the surface and bottom temperatures are well-reproduced by the model for most stations. There is some discrepancy between observational and modeled temperature for CB1.1 and CB2.1. These two stations are in the very upstream and are largely influenced by Susquehanna River flow. The discrepancy is probably because the temperature specification in the watershed loading may have some errors and its effect on water quality should be negligible for the whole system. In addition, it is interesting to notice that for all deep stations the bottom temperature has a phase lag from the surface temperature, while for all shallow stations the water column is well-mixed.

2.5.1.4 Salinity

In Figure 2-29, bottom and surface salinity of model results from 2012 to 2014 are shown against observations. For all the stations along the bay channel, the model well captured the bottom and surface salinity variabilities. In the shallow areas, the model results also match the observation well although there is a slight underestimation at certain stations such as ET4.2 and ET5.2. At station WT4.1 in Back River, the salinity is generally less than 5 PPT and well mixed. Our model results are very close to the observations with large differences only at the beginning in 2012 when the model is still spinning up.

For the coupled model, it is important to have a reasonable salinity result. This not only represents that the model hydrodynamics is reasonable, but also guarantees that the salinity effect on water quality is correct. To evaluate the model performance on salinity prediction, stratification is often employed. In Chesapeake Bay, it is a challenge to obtain a good stratification. Here, we use bottom and surface salinity difference to represent the salinity stratification. Figure 2-30 shows the result. Although there is plenty of temporal and spatial variability, the model catches the mean of stratification and spatial variation from upstream to downstream.
Figure 2-28. Model calibration results for temperature in the Upper Chesapeake Bay from 2012 to 2014. There are 11 channel stations with the names starting with ‘CB’, 3 shallow stations on the eastern banks with the names starting with ‘ET’, and 9 shallow stations and 1 deep station (WT5.1) on the western banks with the names starting with ‘WT’. The stations are ordered from upstream to downstream. Model results for surface values (green lines) and bottom values (red lines) are shown against observations (black dots). The same format is applied to plots for salinity and water quality variables.
Figure 2-29. Model calibration results for salinity in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-30. Time series of bottom-surface salinity difference for deep stations in the Upper Chesapeake Bay. The model results are in red line and observation are in circles.
2.5.2 Water Quality

In this section, we will describe the calibration results of the water quality model. The parameters used in the calibration are mainly from literature (Park et al., 1995; Cerco and Noel 2004). For the model setup, one can refer to 4.2. However, at this point the pH model has not been fully coupled into water quality model. For this reason, the pH model does not feedback its effects to water column kinetics such that high pH does not trigger sediment phosphorus release in Back River as mentioned in our hypothesis. For the model comparison, we only show the results of variables that have measurements in Chesapeake Bay Program.

Figure 2-31 shows the chlorophyll-a result in the Upper Chesapeake Bay from 2012 to 2014. For channel stations, the model catches the mean concentration and the overall seasonal variation. The model is also able to show the chlorophyll-a concentration difference between bottom and surface. However, the model does not fully reproduce the spring bloom at some stations such as CB3.2 and CB3.3C and there seems to be a lag for bloom timing. For shallow area stations, our model performs well in capturing the mean variation and the chlorophyll-a magnitude is close to the observation. At Back River Station WT4.1, the summer chlorophyll-a can reach over 120 µg/L, but the model concentration is generally below 60 µg/L. Thus, chlorophyll-a is under-predicted in Back River.

The kinetics of phytoplankton are very complexed as they are influenced by many factors. In addition, our model uses fixed carbon to chlorophyll ratio for simplicity, but it can be varying in estuary (De Jonge 1980). Therefore, it is always a challenge for the water quality model to reproduce chlorophyll-a variation. For testing our hypothesis, experiments based on calibration should be fine since the model captures the mean chlorophyll-a variation.

DO is an important water property and Figure 2-32 shows the bottom and surface DO. The results are reasonable. For deep stations, the model captures the seasonal variation and clearly shows the bottom hypoxia/anoxia in the summer time. For shallow area stations, the seasonal variation is also well-captured.
At certain times, the calibration results tend to give lower DO. For instance, the summer DO at WT4.1 is too low in 2012.

For nitrogen concentration, TN is shown in Figure 2-33. Our model captures the mean concentration for most stations. For channel stations, our model performs well in capturing the overall variation. For some shallow stations, some details are missing, but it should not impair the entire nitrogen dynamics. Generally, we regard that TN is reasonable. Moreover, nitrogen species (PON, DON, NH4 and NO23) are shown in from Figure 2-43 to Figure 2-46. Here PON is total particulate organic nitrogen as the sum of LPON and PPON. As we can, the results for all nitrogen species are reasonable in capturing the mean variation for most stations. In addition, for dissolved inorganic nitrogen (NH4+NO23) that can directly influence phytoplankton growth, the results are satisfactory in that the high/low concentration in summer/winter is well reproduced.

For phosphorus, TP is shown in Figure 2-34. Again, the model captures the mean concentration for most stations. For channel stations, our model reproduces the seasonal variation that has low phosphorus concentration during the winter and high phosphorus concentration at the bottom during the summer. For shallow stations, the model generally catches the mean. Overall, we regard that TP is also reasonable. The phosphorus species (POP, DOP and PO4) are shown in from Figure 2-47 to Figure 2-49. Here POP is total particulate organic phosphorus as the sum of LPOP and PPOP. The model tends to under-estimate the POP concentration. However, DOP and PO4 are still reasonable. PO4 can directly influence the phytoplankton growth and the model is doing well in simulating the seasonal variation for channel stations. However, for shallow area stations, there is some large peak of PO4 appearing occasionally. At Back River Station WT4.1, the model underestimates the high PO4 concentration in the summer time since pH effects is off on sediment phosphorus release.
Figure 2-31. Model calibration results for Chlorophyll-a in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-32. Model calibration results for dissolved oxygen in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-33. Model calibration results for total nitrogen in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-34. Model calibration results for total phosphorus in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2.35. pH values in Upper Chesapeake Bay. For Station WT4.1, the kinetics of pH model are invoked. For other stations outside of Back River, the kinetics are skipped. Instead, pH is calculated based on ALK and TIC that are nudged to local observations.
2.5.3 pH Model

2.5.3.1 Without pH feedback mechanism

The focus of our pH model is on Back River. The pH model kinetics are applied only inside Back River (Figure 2-11). Outside of Back River, pH model kinetics are skipped, which means the ALK and TIC outside of Back River are not calculated through the dynamic pH model. Instead, ALK and TIC are nudged to local values that are computed based on observations. This treatment ensures reasonable exchanges of ALK and TIC between Back River and the Bay.

For calibration, the positive feedback mechanism illustrated in Figure 2-4 is off. This leads to the low PO4 at Station WT4.1 (Figure 2-49) which limits phytoplankton growth as shown in Figure 2-31. Figure 2-35 shows the pH values in Upper Chesapeake Bay. Due to nudging (ALK and TIC are from inputs), the pH values outside of Back River match the observation. However, for Station WT4.1, the pH is under-estimated. This is consistent with our hypothesis for low chlorophyll-a and low PO4.

2.5.3.2 With pH feedback mechanism

In this part, we will turn on the pH feedback mechanism inside Back River. The assumption is that high pH values will increase the sediment PO4 fluxes. There are two methods for implementing this idea. The first method was introduced by Cerco (2013) by incorporating a pH effect on the phosphorus partition coefficient in the sediment diagenesis model. The other one is described in (Liu 2002) by using an exponential function between phosphorus flux and pH values:

\[ BF_{PO4} = BF_{BFM} \cdot e^{K_{PH}(PH_{R} - PH)} \]  

(2.71)

Where:
- BF_{PO4}: enhanced phosphorus release (g [P] m^{-2} day^{-1})
- BF_{BFM}: calculated phosphorus release without pH effect (g [P] m^{-2} day^{-1})
- K_{PH}: the pH effect on phosphorus release
- PH_{R}: reference pH value.
The second method is simple and straightforward. In addition, the exponential relation between phosphorus flux and pH can be justified using the observational data as shown in Figure 2-3. Therefore, we will adopt the second method for testing our hypothesis. Based on the observational data from (Bailey et al., 2006), one can estimate $K_{PH}$ by fitting data using Equation (2.71). However, our trials show that the value of $K_{PH}$ depends on the choice of $PH_R$ if $BF_{BFM}$ is kept constant. A larger $PH_R$ leads to a larger $K_{PH}$. For instances, $K_{PH}=1.75$ if $PH_R$ is 8.0; and $K_{PH}=2.8$ if $PH_R$ is 9.0. Cerco (2013) mentions that release of phosphorus begins to be blocked under aerobic conditions and $PH=8.3$. Therefore, we will use $PH_R=8.3$ as the criterion, which yields a relation:

$$BF_{PO4} = BF_{BFM} \cdot e^{2.0(PH-8.3)}$$

and Figure 2-3 shows the fitted curve by a blue line.

Figure 2-36 gives the comparison between the model results with and without the pH effect on sediment phosphorus release. The location is at WT4.1 in Back River. There are four variables: chlorophyll-a, TIC, $PO_4$ and pH.

For chlorophyll-a, we can see that the concentration is enhanced in summer months with the pH effect. In 2012, the surface values can approach around 100 µg/L while the calibration value is generally below 60 µg/L. The summer chlorophyll-a is slightly higher in 2013 than in 2012, while the chlorophyll-a in 2014 is highest and can reach over 120 µg/L. Overall, the model with the pH effect gives high chlorophyll-a concentration for all three simulation years. The model result matches the observational data much better than the calibration result. The model reproduces the summer time algal blooms observed in Back River from 2012 to 2014.

Corresponding to chlorophyll-a, TIC also changes. For the calibration result without the pH effect, TIC is over 10 mg/L for the whole simulation period with higher TIC concentration in winter and lower TIC concentration in summer. With pH effect, TIC drops in summer months. TIC has lowest values in 2012 with values below 5 mg/L in summer months. As we know, phytoplankton growth consumes inorganic
carbon. Therefore, the TIC drop in summer is consistent with the high chlorophyll-a concentration in summer.

In Back River, pH values increase in summer with the pH effect. The calibration pH without the pH effect also increases in summer, but normally stays below 8.5. With pH effect, the pH can easily exceed 9.5 and can even approach 10 in 2012. It is worth noticing that the model simulates higher pH values than the observed. However, the pH increase well reproduces the phenomenon of high pH values observed in Back River in warm period. Overall, we can see that the variation in pH is generally related with the variation in TIC. This can be understood in that adding CO₂ into water means increasing water acidity. When inorganic carbon is taken out of water by phytoplankton, the water acidity is reduced, which leads to pH increase.

In Figure 2-36, we can see that the PO₄ concentration with the pH effect is much higher than the concentration without the pH effect. Without the pH effect on sediment phosphorus release, PO₄ presents as a limiting nutrient for phytoplankton with values generally smaller than \(5 \times 10^{-3}\) mg/L in summer months. However, with the pH effect, PO₄ concentration in water can reach over 0.1 mg/L with peak values around 0.2 mg/L in summer. The high concentration is not limiting phytoplankton growth and this explains the high chlorophyll-a in Back River. In addition, the modeled high PO₄ is consistent with the monthly PO₄ measurements that have large values in summer.

According to our hypothesis, the PO₄ increase in summer is due to a sediment phosphorus release. Figure 2-37 compares the sediment phosphorus release with and without the pH effect. As we can see, the high PO₄ fluxes appear in summer when there is the pH effect. Without the pH effect, the PO₄ fluxes is very limited. The magnitude of PO₄ fluxes is consistent with those from a previous study by Liu (2002). Additionally, there is one measurement of PO₄ flux at WT4.1 on 08/23/2014. It was collected by Boynton and Ceballos (2014). For diagnostics, the value of measured PO₄ flux is within the range of values of the modeled PO₄ fluxes. After summer, the temperature begins to drop, which suppresses the phytoplankton
growth resulting in lower consumption of TIC. On the other hand, the air-water exchange of CO₂ will replenish the TIC in the water (shown in the TIC variation in Figure 2-36). The increase of TIC leads to lower pH, which eventually shut down the feedback loop when pH value is below the threshold.

Figure 2-36. Model results (CHLA, TIC, PO₄ and PH) at Station WT4.1 in Back River with and without the pH effect on phosphorus release from 2012 to 2014. Surface and bottom results are compared with observation data.
2.6 Discussion

2.6.1 Water Quality Modeling

Our water quality model is grounded on unstructured grid. The flexibility of grid allows fine resolution in areas of interest. The successful coupling of water quality model into SCHISM provides a way to simulate regions of complex geometry where traditional structured grid models may have difficulty in resolving the geographic features. We applied the model in Upper Chesapeake Bay. The model gives reasonable chlorophyll-a, DO, TN and TP (from Figure 2-31 to Figure 2-34). We compared the results at 24 gauge stations that spans from upstream to downstream, and from deep regions to shallow areas, and the results are satisfactory. The model performance gives us confidence regarding our water quality model. In Back River, high resolution is applied. Figure 2-38 shows the spatial distribution of monthly averaged surface chlorophyll-a in Back River in 2013. An algal bloom appears from June to September, mainly in the middle reach of the River.

Figure 2-37. Sediment PO4 flux at Station WT4.1 in Back River with and without the pH effect on phosphorus release from 2012 to 2014. There is only one observation data point for diagnostics.
2.6.2 pH Effect in Back River

In order to verify the hypothesis about the pH effect in Back River, we coupled a dynamic pH model into the water quality model and compared the results with and without the pH effect in Figure 2-36 and Figure 2-37. The results prove that high chlorophyll-a and high pH values as observed in Back River are connected. The positive feedback mechanism suggested by Figure 2-4 is clearly shown in Figure 2-36 and Figure 2-37. This theory was initially proposed to explain the algal bloom happened in Potomac River (James et al., 1992; Bailey et al., 2006; Cerco 2013). Furthermore, Liu (2002) did a sensitivity study about the pH effect on phosphorus release, which suggested that the same theory can explain to algal blooms in Back River. Within our model, pH is computed and then incorporated into the water quality model to construct a positive feedback loop. This loop comprises chlorophyll-a, TIC, PH, PO₄ and sediment PO₄ flux. With the pH effect, the model gives rise to reasonable results when compared with observations. In addition, Figure 2-39 shows nitrogen species, phosphorus species and DO. For nitrogen species, the model results for PON, DON and NO₃ are slightly improved with the pH effect. For phosphorus species with the pH effect, DOP is much better and POP is slightly improved. In addition, the model gives better DO with the pH effect. Overall, it proves that the pH effect plays an important role in the water quality simulation in Back River.
Figure 2-38. Monthly averaged surface chlorophyll-a of Back River in 2013.
Figure 2-39. Model results for nitrogen, phosphorus and DO at Station WT4.1 in Back River with and without the pH effect on phosphorus release from 2012 to 2014. Surface and bottom results are compared with observation data.

2.6.3 Sensitivity Analysis to $K_{\text{PH}}$

In the model, we used Equation (2.71) to simulate the pH effect on sediment phosphorus release. We chose a reference pH value $PH_R=8.3$ from the literature. For $K_{\text{PH}}$, we estimate its value $K_{\text{PH}}=2.0$ by fitting the exponential function to the data. In order to test the model sensitivity of $K_{\text{PH}}$, we run the model with $K_{\text{PH}}=1.0$ and compare the results to the ones with $K_{\text{PH}}=2.0$ in Figure 2-40. With smaller $K_{\text{PH}}=1.0$, chlorophyll-a, pH and PO$_4$ are depressed, while TIC is enhanced. The largest comparison difference happens to PO$_4$. As we can see, the PO$_4$ concentration with $K_{\text{PH}}=1.0$ is dramatically reduced due to lower sediment fluxes. Therefore, the model seems very sensitive to $K_{\text{PH}}$ and the choice of $K_{\text{PH}}$ influences the PO$_4$ concentration in the water column. However, when compared to the calibration results, the values of chlorophyll-a and pH with $K_{\text{PH}}=1.0$ are still improved. This suggests that the positive feedback mechanism is still working, but with a weaker magnitude. It is also interesting to notice that pH values with $K_{\text{PH}}=1.0$ match observation better than the ones with $K_{\text{PH}}=2.0$, though PO$_4$ is much lower.
2.6.4 Back River WWTP

In Back River, the largest loading is from the WWTP. In order to investigate how it influences the hydrodynamics and nutrient budget inside Back River, we conducted a sensitivity run by shutting down the WWTP input. Figure 2-41 shows the comparison of Salinity and TN with and without WWTP loading. The salinity intrusion becomes larger without WWTP because of the reduced freshwater input. This implies that the flow pattern is changed inside Back River if WWTP is removed. In addition, TN is much reduced without WWTP, which suggests the importance of WWTP loading on nutrient dynamics inside Back River. Thus, Back River WWTP plays an important role for our water quality model and an appropriate treatment is necessary.
2.6.5 Inorganic Carbon Limitation on Phytoplankton

In the model, inorganic carbon limitation on phytoplankton is applied using Equation (2.70). This function represents the fact that algal bloom cannot grow unlimited and eventually it will be limited by the water fertility (Manahan 2000). In order to see its influence on phytoplankton dynamics, a scenario with no carbon limitation was studied. Figure 2-42 shows the model results with and without carbon limitation. As expected, TIC concentration can approach zero (e.g., in 2012) with no carbon limitation. Chlorophyll-a also becomes higher and the maximum was shown to reach over 200 µg/L in 2014. Because of the low TIC concentration, pH can increase to around 11 when the TIC limitation is off. This leads to very large sediment PO\textsubscript{4} flux resulting in high PO\textsubscript{4} concentration in the water column.
Figure 2-42. Model results comparison for chlorophyll-a, TIC, PO_4 and pH between pH effects with and without carbon limitation.

2.7 Summary

In this work, we have developed a fully coupled model composed of a water quality model ICM, a pH model and SCHISM. The model was applied in the upper Chesapeake Bay to simulate the water quality condition from 2012 to 2014 and tested the hypothesis regarding the algal blooms recurring in Back River. We summarize the following findings:

1). The model yields an excellent calibration results for elevation, velocity, salinity and temperature for the entire upper Chesapeake Bay including both shallow and deep regions.

2). Our water quality model gives reasonable results for water quality variables including chlorophyll-a, DO, TN and TP. The calibration results for nitrogen and phosphorus species are also reasonable for most stations in upper Chesapeake Bay.
3). The pH model is applied in Back River to verify the positive feedback mechanism. The feedback loop composed of chlorophyll-a, TIC, pH and PO₄ clearly shows how these variables are linked. The result proves our hypothesis that the pH can affect sediment phosphorus release and drive high chlorophyll-a. The high chlorophyll-a in turn increases pH even higher. This positive feedback mechanism can explain the extreme high summer chlorophyll-a concentration regularly observed in Back River.
Appendix A: Additional figures and Tables for Chapter 2

Figure 2-43. Model calibration results for particulate organic nitrogen in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-44. Model calibration results for dissolved organic nitrogen in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-45. Model calibration results for ammonia nitrogen in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-46. Model calibration results for nitrite-nitrate nitrogen in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-47. Model calibration results for particulate organic phosphorus in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-48. Model calibration results for dissolved organic phosphorus in the Upper Chesapeake Bay from 2012 to 2014.
Figure 2-49. Model calibration results for phosphate in the Upper Chesapeake Bay from 2012 to 2014.
Chapter 3 A conceptual phytoplankton model and its application in the tidal freshwater James River

Abstract

The James River from the City of Williamsburg to Hopewell where James River meets the Appomattox River is a long stretch of a tidal river. The salinity in this section varies from freshwater to a few ppt of brackish water. A local chlorophyll maximum dominated by cyanobacteria was found to be persistent each summer here. Statistical analysis also found that the temporal variation of the chlorophyll-a is inversely proportional to the upstream river discharge. Based on these observations, a semi-analytic model was proposed to describe the phenomenon derived for a well-mixed, one-dimensional partial differential equation composed of an advection term and a phytoplankton net growth term, that can be parameterized in both linear and nonlinear forms. In this study, we derive a general analytic solution to the equation. The various forms of the solution for different parameterization for the net growth rate are applied in the tidal freshwater region (TFR) of James River to explain the temporal and spatial variabilities of phytoplankton biomass. It is found that the physical and biological factors which influence the phytoplankton dynamics are closely linked. In the TFR of James River, boundary condition becomes important. Under high flow condition, river discharge controls the phytoplankton biomass by limiting the retention time, while under low flow condition, biological effects may dominate. Given the assumption that phytoplankton is originated from upstream and phytoplankton net growth rate can vary in time and space, chlorophyll-a concentration may reach local maxima/minima at a location where the local phytoplankton net growth rate equals zero. As river flow increases, this location of local chlorophyll-a maxima/minima goes downstream.
3.1 Introduction

The Tidal freshwater region (TFR) is a part of an estuary that is influenced by tide and river flow, but beyond the influence of saline water. Phytoplankton blooms are often observed in this region (Filardo and Dunstan 1985; James et al., 1992; Muylaert et al., 2005). The high phytoplankton production may play an important role for the whole ecosystem. For example, it may impact on the higher level heterotrophs (Bukaveckas et al., 2011; Anderson et al., 2012). Phytoplankton growth is related to many factors such as nutrient abundance, salinity, phytoplankton species compositions and flow conditions (Sellner et al., 1988b; James et al., 1992; Marshall and Affronti 1992). Watershed runoff brings nutrients into TFR and high nutrient concentrations can be found in many of these areas (Heisler et al., 2008; Carroll et al., 2013). Different phytoplankton species may react very differently due to their different biological behaviors (Anderson et al., 2012). In addition, river flow may influence phytoplankton concentration largely by controlling its transit time in TFR (Borsuk et al., 2004; Lucas et al., 2009).

For phytoplankton biomass to increase, the growth rate must be larger than the loss rate, or in other words, the net growth rate must be positive (Lucas et al., 2009). The factors affecting growth rate include temperature, nutrients and light, while the factors affecting loss rate include respiration, grazing and settling (Park et al., 1995; Cerco and Noel 2004). An appropriate amount of phytoplankton biomass is necessary to maintain a healthy aquatic ecosystem. However, excessive accumulation of phytoplankton can be harmful (Cloern 1996). For phytoplankton to bloom in a certain region, the local retention time must be longer than the cell doubling time (Ralston et al., 2015). Otherwise, phytoplankton will be flushed out before it can bloom.

The physical and biological controls on phytoplankton growth are closely linked (Filardo and Dunstan 1985; Lucas et al., 2009; Bukaveckas et al., 2011). A deep understanding on this is the key to explain the temporal and spatial phytoplankton variabilities as observed in many TFRs. Lucas et al., (2009) depict a conceptual phytoplankton model for a one-dimensional, uniform and steady state system. By combining the physical transport process and phytoplankton kinetic processes, this theory can largely explain many
observed relationships between transport time and phytoplankton biomass, namely whether phytoplankton biomass is positively or negatively, or not at all, correlated with the transport time. In real environment, hydrodynamic condition can change dramatically due to large variation of physical forcing such as river discharge and winds (Du and Shen 2015). In addition, phytoplankton growth and loss are modulated by many factors as mentioned above and has inherited inter-annual, seasonal and daily cycles. How these complexities are interacted in term of time and space is a question that needs to be addressed. In this work, we considered one dimensional system with variable velocity field, net growth rate and boundary condition and presented a complete explicit solution to the question. The solution is then applied in the TFR of James River to study its temporal and spatial variations of phytoplankton biomass.

3.2 Method

3.2.1 General solution

In many estuaries, there exists an upstream section extending longitudinally in TFR that has a more or less regular shape and is homogenous both vertically and laterally. Thus, a one-dimensional model is sufficient to describe the hydrodynamics for this river section. Assuming there is no diffusivity and phytoplankton is purely advected along the water movement (Lucas et al., 2009), the problem for phytoplankton dynamics can be described by the following equations with an initial condition and a boundary condition:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \left(\mu_{\text{grow}} - \mu_{\text{loss}}\right) \cdot C = \mu_{\text{net}} C$$

(3.1)

$$C(t, x = 0) = a(t), \text{ for } t \geq 0$$

(3.2)

$$C(t = 0, x) = b(x), \text{ for } x \in [0, L]$$

(3.3)

where, \( C(t, x) \) (mg/L) is phytoplankton biomass concentration (can also be represented by chlorophyll concentration \( \mu g[\text{Chl}]/L \)), \( t \) is time, \( x \) is the downstream distance from the head of this river section,
$u(t,x)$ (m/s) is velocity, $\mu_{\text{grow}}$ (day$^{-1}$) and $\mu_{\text{loss}}$ (day$^{-1}$) are phytoplankton growth rate and total loss rate, $\mu_{\text{net}}(t,x)$ is net growth rate and $L$ is the length of the river section. In addition, $a(t)$ and $b(x)$ are respectively the boundary and initial conditions. There are two processes controlling the local change rate $\frac{\partial C}{\partial t}$ of phytoplankton biomass. First, phytoplankton is transported by the flow with velocity $u$. Second, phytoplankton is growing simultaneously at the rate $\mu_{\text{net}}$ while being transported. Here, the phytoplankton source is assumed to be upstream originated and no local sources such as benthic algal cysts resuspension are considered.

The solution to Equations (3.1)-(3.3) is:

$$C(t,x) = a(t - T(t,x)) \cdot e^{G(t,x)}, \quad t \geq 0, \ x \in [0,L] \quad (3.4)$$

where $T(t,x)$ and $G(t,x)$ are implicitly expressed using the equations below

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = 1 \quad (3.5)$$

$$\frac{\partial G}{\partial t} + u \frac{\partial G}{\partial x} = \mu_{\text{net}} \quad (3.6)$$

$$T(t, \ x = 0) = 0 \quad (3.7)$$

$$G(t, \ x = 0) = 0 \quad (3.8)$$

For Equations (3.5)-(3.8), the underlying assumptions are: 1) all water parcels are originated from upstream, 2). flow field $u$ is known, 3) the upstream boundary conditions are known, and 4) reaction term $\mu_{\text{net}}$ is known. Therefore, downstream $T$ and $G$ can determined by upstream boundaries since every water parcel can be traced back to the boundary and all flow conditions are known. By comparing the water age concept (Deleersnijder et al., 2001; Shen and Lin 2006) and Equations (3.5) and (3.7), we can see that $T(t,x)$ is actually the water age when the diffusion term is neglected. More specifically for our problem, $T(t,x)$
represents the time elapsed since a water parcel is released from the river head \((x = 0)\). Hereafter, we call \(T(t, x)\) water age for simplicity. \(G(t, x)\) is denoted as an amplification factor. It has a physical meaning representing the overall net growth/dampening effect of phytoplankton that is accumulated within time period \(T(t, x)\) and over the path the water parcel undergoes after it is released from \((x = 0)\). At this point, Equation (3.3) is not used in our solution. On the other hand, by examining the solution of Equation (3.4), we noticed that it requires the value of \(a(t)\) for the period \(t \in [-T(t = 0, x = L), 0]\). To resolve this conflict, we substitute \(C(t, x)\) into Equation (3.3), which leads to the following relationship between boundary condition \(a(t)\) and initial condition \(b(x)\):

\[
b(x) = a(-T(t = 0, x)) \cdot e^{G(t = 0, x)}, \quad x \in [0, L],
\]

or

\[
a(x) = b(T^{-1}(-x)) \cdot e^{-G(t = 0, T^{-1}(-x))}, \quad x \in [-T(t = 0, x = L), 0],
\]

where \(T^{-1}(x)\) is the inverse function of \(T(t = 0, x)\). The relationship that Equation (3.9) indicates that a water parcel at \((t = 0, x)\) is derived from the one released at \((t = -T(t = 0, x), x = 0)\) and the associated phytoplankton biomass is changed by a factor of \(e^{G(t = 0, x)}\) relative to the initial concentration when released.

To summarize, the combination of Equations (3.4)-(3.8) and (3.10) comprises the complete solution to our problem Equations (3.1)-(3.3).

3.2.2 \(\mu_{\text{net}}\) is replaced by \(\mu_{\text{net}}(1 + kC)\)

The general solution Equation (3.4) should work well when reasonable velocity field \(u(t, x)\) and net growth rate \(\mu_{\text{net}}(t, x)\) are provided. However, in reality it is always difficult to estimate \(\mu_{\text{net}}(t, x)\) because the physical and biological information in time and space is demanding. In addition, diffusion is playing a role in smoothing the variations of phytoplankton concentration in space. An alternative form of net growth rate \(\mu_{\text{net}}(t, x) \cdot (1 + kC)\) is proposed to better estimate the real situation for the net growth rate of phytoplankton. This form of net growth rate provides a negative feedback mechanism when
phytoplankton biomass concentration $C$ is too high. The rationale for this modification is explained later.

With the alternative form of net growth rate, Equation (3.1) becomes:

$$\begin{align*}
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} &= \mu_{\text{net}} \cdot (1 + kC) \cdot C
\end{align*}$$

(3.11)

Here, $(1 + kC)$ is used to account for the factors that are not considered in $\mu_{\text{net}}(t,x)$. For example, shading effect tends to reduce the growth rate when phytoplankton biomass is high, but is hard to quantify. For another example, in some cases, zooplankton is an important contribution to phytoplankton reduction and its grazing may increase when phytoplankton biomass increases (Filardo and Dunstan 1985; Cerco and Noel 2004). In addition, the term $(1 + kC)$ plays a similar effect as physical mixing from tide and turbulence to dampen the local peaks of phytoplankton concentration. The solution to Equations (3.2), (3.3) and (3.11) are

$$C(t,x) = \frac{a(t - T(t,x)) \cdot e^{G(t,x)}}{1 + k \cdot a(t - T(t,x)) \cdot (1 - e^{G(t,x)})}, \quad t \geq 0, \quad x \in [0, L]$$

(3.12)

where $T(t,x)$ and $G(t,x)$ remain the same as Equation (3.4). The relationship between $a(t)$ and $b(x)$ is

$$b(x) = \frac{a(-T(t = 0, x)) \cdot e^{G(t = 0, x)}}{1 + ka(-T(t = 0, x)) \cdot (1 - e^{G(t = 0, x)})}, \quad x \in [0, L]$$

(3.13)

and

$$a(\xi) = \frac{b(T^{-1}(\xi))}{(1 + kb(T^{-1}(\xi))) \cdot e^{G(t = 0, T^{-1}(\xi))} - kb(T^{-1}(\xi))}, \quad \xi \in [-T(t = 0, x = L), 0].$$

(3.14)

### 3.2.3 Constant $\mu_{\text{net}}$ and $u(x)$

Considering a simple case when net grow rate $\mu_{\text{net}}$ can be regarded as a constant and the velocity field $u(x)$ does not change with time, then, we can get the expression of $T$ and $G$ by solving Equations (3.5)-(3.8):
\[ T(x) = \int_{x}^{L} \frac{d\eta}{u(\eta)}, \quad x \in [0, L] \]  
\[ G = \mu_{\text{net}} \cdot T. \]  

The solutions of Equations (3.4), (3.9), and (3.10) become:

\[ C(t, x) = a(t - T) \cdot e^{\mu_{\text{net}} T}, \quad t > 0, \quad x \in [0, L] \]  
\[ b(x) = a(-T) \cdot e^{\mu_{\text{net}} T}, \quad x \in [0, L]. \]  
\[ a(\xi) = b(T^{-1}(\xi)) \cdot e^{\mu_{\text{net}} \xi}, \quad \xi \in \left[ -\int_{0}^{t} \frac{d\eta}{u(\eta)}, 0 \right]. \]

Here, Equations (3.17)-(3.18) merely reflect the relationship that every water parcel can be traced back to the upstream boundary. If boundary condition \( a \) is known for the period \( t \in \left[ -\int_{0}^{t} \frac{d\eta}{u(\eta)}, 0 \right] \), the downstream condition \( C(t = 0, x) = b(x), \quad x \in [0, L] \) can be known through Equation (3.17). In reverse, if downstream condition \( C(t = 0, x) = b(x), \quad x \in [0, L] \) is known, we can trace back to the corresponding boundary condition \( a(t), \quad t \in \left[ -\int_{0}^{t} \frac{d\eta}{u(\eta)}, 0 \right] \). The simple solution Equation (3.17) shows that the temporal and spatial variation are controlled by the boundary condition \( a(t) \) and velocity field \( u(x) \). It merely represents that the phytoplankton biomass is increasing exponentially when \( \mu_{\text{net}} > 0 \) or is decreasing exponentially when \( \mu_{\text{net}} < 0 \). When \( \mu_{\text{net}} \) is replaced by \( \mu_{\text{net}} \cdot (1 + kC) \), Equations (3.12)-(3.14) become:

\[ C(t, x) = \frac{a(t - T(x)) \cdot e^{\mu_{\text{net}} T}}{1 + ka(t - T(x)) \cdot (1 - e^{\mu_{\text{net}} T(x)})}, \quad t > 0, \quad x \in [0, L] \]  
\[ b(x) = \frac{a(-T) \cdot e^{\mu_{\text{net}} T}}{1 + ka(-T(x)) \cdot (1 - e^{\mu_{\text{net}} T(x)})}, \quad t = 0, \quad x \in [0, L]. \]  
\[ a(\xi) = \frac{b(T^{-1}(\xi)) \cdot e^{\mu_{\text{net}} \xi}}{e^{\mu_{\text{net}} \xi} \cdot (1 + kb(T^{-1}(\xi)) - kb(T^{-1}(\xi)))}, \quad \xi \in \left[ -\int_{0}^{t} \frac{d\eta}{u(\eta)}, 0 \right]. \]
3.3 Comparison between results and observation

3.3.1 Observation in James River

For many estuaries, the tidal freshwater portions share many common features in hydrology, geomorphology and water chemistry (Bukaveckas et al., 2011). For example, the river often has a regular shape in the longitudinal direction and a constricted cross section. The hydrodynamics are usually under fluvial influence resulting in a transit time changing with river discharges. Also, the water is usually in abundance of nutrients and suspended particulate matters. These characteristics make the interaction between hydrodynamics and phytoplankton dynamics in tidal freshwater different from those in mesohaline and polyhaline regions. In particular, the physical transport may play an important role in regulating the phytoplankton distribution. Several studies have shown the hydrodynamic control on the phytoplankton variations, phytoplankton populations and distributions (Sze 1981; Filardo and Dunstan 1985; Sellner et al., 1988b).

James River is located in the state of Virginia, in the southwest portion of Chesapeake Bay (Figure 3-4). It is about 170 km long from the fall line to the river mouth (Shen and Lin 2006). The average river discharge is about 200 m³/s and can vary from below 10 m³/s to over 8000 m³/s (Fang et al., 1973). The James River is considered to be tidal and characterized by complex hydrodynamics (Shen et al., 1999). High chlorophyll-a concentration is often observed in the TFR of James River and river flow may play an important role in modulating the variation (Filardo and Dunstan 1985; Bukaveckas et al., 2011). Filardo and Dunstan (1985) conducted a field experiment in the upper James River and found that there exists an inverse relationship between river discharge and chlorophyll-a concentration, as shown in Figure 3-1. Bukaveckas et al., (2011) reported a local chlorophyll-a maximum reoccurring each summer in the downstream of the confluence of tidal James and Appomattox Rivers, as shown in Figure 3-2. The study shows that the chlorophyll-a maximum coincides with low salinity and a high turbidity zone, while the location is related to the river geomorphology. Below the confluence of the tidal James and Appomattox
Rivers, the river has a broader cross-section with shallower depth, which provides longer residence time and favorable light conditions for phytoplankton production.

The water quality model simulation result for the upper James River by CE-QUAL-ICM, the EPA Chesapeake Bay Program’s official model, is shown in Figure 3-3. The time series of chlorophyll concentrations at the surface from 1991-2000 is compared with the observation at Station TF5.5 in the upper freshwater portion of the tidal James. The CE-QUAL-ICM result underestimates chlorophyll-a in five out of ten years in the calibration period. It may be related to the lack of spatial resolution of the model, which cannot represent a reasonable hydrodynamic field to account for the longer water residence times. In addition, the insufficient resolution to resolve the shallow shoal or deep regions in the lateral direction may result in unreasonable light limitation on algal growth. The shortcoming of the current phytoplankton simulation in the Upper James River motivates us to consider an in-depth study on the controlling mechanism of the algal growth. A conceptual model governed by advection term, and linear/nonlinear reaction terms is built to investigate the temporal and spatial variabilities of the algal bloom in the tidal freshwater James River. Specifically, a one-dimensional system with a variable velocity field, net growth rate and boundary condition is considered. The conceptual model, although simple, is a complete explicit solution to the problem when transformed to a set of first order partial differential equations. The solution with realistic parameters is then applied in the TFR of James River to study the temporal and spatial patterns of phytoplankton biomass.
Figure 3-1. The upper panel is the mean river discharge and the lower panel is the chlorophyll-a concentration in the upper James River. This figure is from (Filardo and Dunstan 1985)
Figure 3-2. Longitudinal patterns of turbidity, salinity and chlorophyll-a in the James River Estuary (distance from the confluence with Chesapeake Bay). Data are average values for 1999-2004 based on monthly sampling for Chesapeake Bay Program by the Virginia Department of Environmental Quality. This figure is from (Bukaveckas et al., 2011).

Figure 3-3. Historical observations at Station TF5.5 from EPA water quality monitoring program (blue dots). Plot comparing of Chesapeake Bay WQSTM-simulated surface chlorophyll-a values (red line) from 1991-2000. This figure is from (Cerco and Noel 2004).
In this section, we will apply the various solutions to Equation (3.1) in the TFR of James River. Three different kinds of water quality observations are used (available at VIMS website http://web2.vims.edu/vecos/) including continuous monitoring data, dataflow and long-term monitoring data. We will focus on the spatial and temporal patterns of phytoplankton biomass.

3.3.2 Constant \( \mu_{net} \) under low flow condition

In cases when river discharge is low, we can assume the velocity doesn’t change with time when only the tidal average variabilities of phytoplankton are considered. If the net growth rate is also assumed to be constant, the solution shown in Equations (3.17)-(3.19) can be used. Here, we will use Equation (3.18) to verify our model predictability, which means that the phytoplankton boundary condition will be used to estimate the spatial variation.

Figure 3-4. The TFR of James River. The triangle refers to the location of Continuous Monitoring Station JMS073.37 and the color lines show chlorophyll distribution from dataflow measurement on 08/13/2008 in the upper James River. The red line shows our model axis starting around Station JMS073.37.
In the TFR of James River, there is a Continuous Monitoring Station JMS073.37 (triangle in Figure 3-4) where the chlorophyll observation is available as a proxy of phytoplankton biomass. Our model axis origin $x = 0$ is near this station and the axis (red line in Figure 3-4) is along the river channel. If we regard every water parcel is from upstream and the lateral variation can be neglected, the chlorophyll measurements at Station JMS073.37 can represent mean chlorophyll concentration for the river cross section. The chlorophyll observation at this station provides the boundary condition $a(t)$ in Equation (3.2). Figure 3-5 shows the time series of $a(t)$ for the period 06/01/2008-08/15/2008 and the moving average with a 12-hour window is used for our calculation by eliminating the sporadic points. Chlorophyll dataflow data were also available on 08/13/2008 which provides the spatial variation of phytoplankton biomass (color lines in Figure 3-4). The dataflow is interpolated along the model axis and the result serves as the initial condition $b(x)$ in Equation (3.3). The flow discharge (available on United States Geological Survey website) in James River can change over three orders of magnitude annually. However, in the two months prior to 08/13/2008, the river flow variation is relatively small with an average about 37 m$^3$/s and a standard deviation about 16 m$^3$/s. Therefore, we regard the river flow as a constant 37 m$^3$/s. Based on continuity equation $Q = A \cdot u$ where $Q$ (m$^3$/s) is the flow rate and $A$ (m$^2$) is the cross-sectional area, the velocity $u(x)$ can be approximated. Here, the effect of tidal excursion is neglected as we are focusing the residual velocity field. The values of $A(x)$ and $u(x)$ are shown in Figure 3-6. Here, the 10-meter resolution bathymetry data from Federal Emergency Management Agency are used to calculate $A(x)$. 
Figure 3.5. Chlorophyll observation (dots) at Station JMS073.37 for the period 06/01/2008-08/15/2008. The red line is the moving average using a 12-hour window.

Figure 3.6. Blue line shows the cross-section area of James River in the TFR. The red line is mean flow velocity when river flow equals 37 m$^3$/s.
With the boundary condition $a(t)$ and velocity $u(x)$ known, we can use Equation (3.18) to compute $C(t=0,x)$ or $b(x)$ if $\mu_{\text{net}}$ is further given. Here, $b(x)$ represents the spatial variation of phytoplankton biomass and its observation derived from dataflow is displayed in Figure 3-7a as a black line. It shows that the phytoplankton concentration slowly decreases moving downstream, which suggests that the net growth rate $\mu_{\text{net}}$ should be negative. Here, four $\mu_{\text{net}}$ values (0.0, -0.01, -0.03, -0.05 day$^{-1}$) are assigned and each corresponding calculated $b(x)$ is shown in Figure 3-7a. When $\mu_{\text{net}} = 0.0$ day$^{-1}$, the modeled $b(x)$ merely represents the result of advection of the boundary condition (Figure 3-5). When $\mu_{\text{net}} = -0.01$ day$^{-1}$, the chlorophyll concentration is overestimated and advection still explains the general feature of observed $b(x)$, while when $\mu_{\text{net}} = -0.05$ day$^{-1}$, the chlorophyll concentration is underestimated and the biological attenuation dominates. When $\mu_{\text{net}} = -0.03$ day$^{-1}$, the modeled $b(x)$ matches the observation well, except that there are several peaks.

There peaks in Figure 3-7a correspond to the peaks in the boundary condition $a(t)$. In a real situation, these peaks dissipate very quickly as shown in the observation. This suggests a larger negative net growth rate or physical dissipation associated with these high phytoplankton concentration periods. Therefore, it is appropriate to use Equation (3.21) to estimate $b(x)$. Here, the two sets of parameters ( $\mu_{\text{net}} = -0.015$ day$^{-1}$, $k = 0.05$ $\mu$g$^{-1}$.L) and ( $\mu_{\text{net}} = -0.0075$ day$^{-1}$, $k = 0.2$ $\mu$g$^{-1}$.L) are used and the modeled $b(x)$ based on Equation (3.21) is shown in Figure 3-7b. We can see that the overall pattern matches the observation much better and the peaks are depressed. The maximum deviation of $b(x)$ from observation is less than 5 $\mu$g/L for the second parameter set. Here, the combination of $\mu_{\text{net}}$ and $k$ reflects a variation of phytoplankton growth rate which is related to the present phytoplankton biomass concentration.
Figure 3-7. Model results with constant net growth rate under a low flow condition. The upper panel (a) shows model results using four different net growth rates: 0.0 day\(^{-1}\) (red), -0.01 day\(^{-1}\) (blue), -0.03 day\(^{-1}\) (green), and -0.05 day\(^{-1}\) (magenta). The lower panel (b) shows model results using two sets of parameters: \((\mu_{\text{net}} = -0.015 \text{ day}^{-1}, k = 0.05 \text{ } \mu g^{-1}\text{L})\) and \((\mu_{\text{net}} = -0.0075 \text{ day}^{-1}, k = 0.2 \text{ } \mu g^{-1}\text{L})\). The dataflow observation \(b(x)\) on 08/13/2008 is shown in black lines in both (a) and (b).
3.3.3 Constant $\mu_{net}$ under high flow condition

For high flow condition, we selected 07/06/2006 when chlorophyll dataflow data are available and the flow rate is large. In the period 06/29/2006-07/06/2006, the flow changes from over 2000 m$^3$/s to below 200 m$^3$/s with an average about 435 m$^3$/s and a standard deviation about 452 m$^3$/s. Here, we regard the river flow as a constant 435 m$^3$/s. Since the flow rate is pretty large, the retention time of water parcel in our computation domain $x \in [0, L]$ is short, about one week. Figure 3-8 shows the spatial distribution of chlorophyll on 07/06/2006 and Figure 3-9 shows the chlorophyll time series in the period 07/01/2006-07/07/2006 obtained from Continuously Monitoring Station JMS073.37.

![Figure 3-8](image)

**Figure 3-8.** Same as Figure 3-4 except chlorophyll distribution from dataflow measurement is on 07/06/2008.
Figure 3-9. Chlorophyll observation (dots) at Station JMS073.37 for the period 07/01/2006-07/07/2008. The red line is the moving average using a 12-hour window.
Figure 3-10. Model results with constant net growth rate under high flow condition. The upper panel (a) shows model results using four different net growth rates: 0.0 day\(^{-1}\) (red), -0.1 day\(^{-1}\) (blue), -0.2 day\(^{-1}\) (green), and -0.4 day\(^{-1}\) (magenta). The lower panel (b) shows model results using two sets of parameters: \(\mu_{net}=-0.008 \text{ day}^{-1}, k=0.25 \mu g^{-1}.L\) and \(\mu_{net}=-0.008 \text{ day}^{-1}, k=0.5 \mu g^{-1}.L\). The dataflow observation \(b(x)\) on 07/06/2006 are shown as black lines in both (a) and (b).
Similar to the procedure as for the low flow condition, we use Equation (3.18) and Equation (3.21) to compute \( b(x) \) and the results are shown in Figure 3-10a-b. The results with constant \( \mu_{\text{net}} \) differ a lot from the observation for the four trial values \((0.0, -0.1, -0.2, -0.4 \text{ day}^{-1})\) and the results with \( \mu_{\text{net}} \cdot \left(1 + kC\right) \) still fail to match the observation well. The reason for this mismatch may be because the constant flow assumption does not hold under the high flow condition since the flow change dramatically in a very short period. In addition, there is a big mismatch at \((t = 0, x = 0)\) between the chlorophyll dataflow observation and continuously monitoring chlorophyll data as shown in Figure 3-10. It is impossible for our model to work properly if this mismatch exists for the whole simulation period. This mismatch maybe the real case if there exists a lateral variation under high flow condition and the Continuously Monitoring Station JMS073.37 cannot represent the true boundary condition \( a(t) \).

3.3.4 Spatially and temporally varying velocity \( u \) and net growth rate \( \mu_{\text{net}} \)

For a more general situation, we apply Equation (3.4) to the TFR of James River with more realistic velocity and net growth rate. The hydrodynamics in James River is well studied and its 3D velocity field is also well-simulated (Shen et al., 2016b). Here, we will use the velocity output from the SCHISM hydrodynamic model (Zhang et al., 2017) in the TRF of James River. The velocity is tidal averaged over the river cross section resulting in a one-dimensional velocity field \( u(t, x) \) varying with time and space along our model axis (red line in Figure 3-11) which is along the river channel and starts from water quality Station TF5.2A.
Figure 3-11. The TFR of James river with 5 long-term monitoring stations (triangles): TF5.2A, TF5.3, TF5.5, TF5.5A and TF5.6. The red line is our model axis starting from Station TF5.2A.

3.3.4.1 Calculation of phytoplankton net growth rate

In this part, the phytoplankton net growth rate is calculated based on long-term monitoring nutrients, light and temperature assuming there is only one species. The long-term monitoring systems from Chesapeake Bay Program provides various kinds of water quality measurement data for Stations (TF5.2A, TF5.3, TF5.5, TF5.5A and TF5.6) on a monthly basis. The measured Nitrite+Nitrate, Ammonium, Phosphate, Water Temperature and Light Attenuation are interpolated in space and time (Figure 3-12). The results are used to calculate the net growth rate. The radiation data from NARR (North American Regional Reanalysis) database is used to estimate the daily mean PAR (Photosynthetically Available Radiation). The daytime is calculated based on latitude and day of year (Forsythe et al., 1995) and a sinusoidal function is used for the daily PAR variation.
Figure 3-12. The interpolated Nitrite+Nitrate (mg/L), Ammonium (mg/L), Phosphate (mg/L), Water Temperature (°C) and Light Attenuation coefficient (1/m) in time and space. The dots represent the measurements. The lower right panel is daily mean Photosynthetically Available Radiation (ly/day).

The interpolated variables above are used to calculate phytoplankton net growth rate \( \mu_{\text{net}}(t,x) \). Below are the detailed formulations which are from the water quality model (Park et al., 1995; Cerco and Noel 2004). The net growth rate \( \mu_{\text{net}} \) is composed of three parts: growth rate \( P \) (day\(^{-1}\)), basal metabolism rate \( BM \) (day\(^{-1}\)) and predation rate \( PR \) (day\(^{-1}\)):

\[
\mu_{\text{net}} = P - BM - PR .
\]  
(3.23)

The growth rate represents how phytoplankton will grow under the effects of nutrients, light and temperature and its formulation is:

\[
P = PM \cdot f_1(N) \cdot f_2(I) \cdot f_3(T) ,
\]  
(3.24)

and

\[
f_1(N) = \min\left( \frac{NH4 + NO23}{KHN + NH4 + NO23}, \frac{PO4}{KHP + PO4} \right) ,
\]  
(3.25)

\[
f_2(I) = \frac{1}{H} \int_0^H \int_{I_m}^{I_{m+1}} e^{-\frac{K_e \cdot z}{I_m}} dz = \frac{1}{H} \int_0^H \frac{I_0 e^{-\frac{K_e \cdot z}{I_m}}}{I_m} e^{-\frac{K_e \cdot z}{I_m}} dz
\]  
(3.26)
where $PM$ (day$^{-1}$) is the maximum growth rate, $NH4$ (mg/L) is ammonium concentration, $NO23$ (mg/L) is nitrite+nitrate concentration, $PO4$ (mg/L) is phosphate concentration, $KHN$ (mg/L) and $KHP$ (mg/L) are half-saturation constants for nitrogen and phosphorus, respectively, $I$ (ly/day) is light intensity and $I_0$ (ly/day) is solar radiation at water surface, $I_m$ (ly/day) is optimal light intensity for phytoplankton growth radiation, $K_e$ (m$^{-1}$) is light extinction coefficient, $H$ (m) is water depth, $T$ ($^\circ$C) is temperature and $TM$ ($^\circ$C) is the optimal temperature for phytoplankton growth, and $KTG1$ ($^\circ$C$^{-1}$) and $KTG2$ ($^\circ$C$^{-1}$) are, respectively, temperature effect coefficients for temperature below and above $TM$. The basal metabolism rate represents phytoplankton decrease due to respiration and excretion and its formulation is:

$$BM = BMR \cdot \exp(KTB \cdot [T - TR])$$  

(3.28)

where $BMP$ (day$^{-1}$) is the reference basal metabolism rate at reference temperature $TR$ ($^\circ$C) and $KTB$ ($^\circ$C$^{-1}$) is temperature effect coefficient of metabolism. The predation rate stands for the effect of zooplankton grazing and the formulation is:

$$PR = PRR \cdot \exp(KTB \cdot [T - TR])$$  

(3.29)

where $PRR$ (day$^{-1}$) is the reference predation rate at reference temperature $TR$ ($^\circ$C). Table 3-1 shows the parameter values used to calculate net growth rate $\mu_{net}(t,x)$.

Using Equation (3.23)-(3.29), we compute the net growth rate $\mu_{net}(t,x)$. Figure 3-13 shows the time series of net growth rate at 4 water quality stations at noon time when $\mu_{net}$ is maximum during the daytime. During the nighttime, $\mu_{net} < 0$, since the absence of light will limit phytoplankton
growth. As we can see, $\mu_{\text{net}}$ has an evident seasonal variation. It has larger values in summer times when temperature is high than in winter times when temperature is low. Also, it varies inter-annually, probably due to change of the nutrients and light availabilities in different years. In addition, we can see that $\mu_{\text{net}}$ is large at upstream stations TF5.3, while it is small at downstream stations. The larger $\mu_{\text{net}}$ at TF5.3 value may be due to the shallow depth we used to calculate the light condition in the upstream.

Table 3-1. Parameter values used to calculate phytoplankton net growth rate

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PM</td>
<td>3.0 day$^{-1}$</td>
</tr>
<tr>
<td>KHN</td>
<td>0.01 mg/L</td>
</tr>
<tr>
<td>KHP</td>
<td>0.001 mg/L</td>
</tr>
<tr>
<td>KTG1</td>
<td>0.001 °C$^{-1}$</td>
</tr>
<tr>
<td>KTG2</td>
<td>0.001 °C$^{-1}$</td>
</tr>
<tr>
<td>$I_m$</td>
<td>40 ly/day</td>
</tr>
<tr>
<td>BMP</td>
<td>0.04 day$^{-1}$</td>
</tr>
<tr>
<td>KTB</td>
<td>0.069 °C$^{-1}$</td>
</tr>
<tr>
<td>TM</td>
<td>25 °C</td>
</tr>
<tr>
<td>TR</td>
<td>20 °C</td>
</tr>
<tr>
<td>PRR</td>
<td>0.01 day$^{-1}$</td>
</tr>
</tbody>
</table>

Figure 3-13. Phytoplankton net growth rate at 4 water quality monitoring stations at noon time.
3.3.4.2 Results with varying $u$ and $\mu_{net}$

Provided with $u(t,x)$ and $\mu_{net}(t,x)$, we solve the Equations (3.5)-(3.8) numerically to get water age $T(t,x)$ and amplification factor $G(t,x)$. The solutions of $T(t,x)$ and $G(t,x)$ give more information about the system by relating the all the downstream phytoplankton distribution to upstream phytoplankton conditions. Finite difference method is used to discretized Equations (3.5)-(3.6). Figure 3-14 shows the water age at four downstream stations below TF5.2A. As we can see, the water retention time is fairly short, usually below 3 days between Station TF5.2 and Station TF5.3. This is mainly because of the narrow river morphology resulting in large velocity. However, within the river section from Station TF5.5 to TF5.6, the river has a broad open shape, which slows down the water and increases the retention time. The retention time can last for months during certain years and this will give phytoplankton enough time to grow. Figure 3-15 shows the time series of the amplification factor at 4 stations. Since amplification factor represents the accumulated growth effect, the positive values mean that the phytoplankton biomass will increase when it leaves our boundary and moves down along the water parcel. The phytoplankton biomass increase is small at Station TF5.3, while it is larger for Stations TF5.5, TF5.5A and TF5.6. However, the variation of amplification factor is relatively small from Station TF5.5 to TF5.6, given the long retention time in this region. The plausible explanation is that a sort of balance is achieved for phytoplankton dynamics, which limits phytoplankton to grow constantly.
Figure 3-14. Time series of water age $T(t, x)$ at 4 stations in the TFR of James River.

Figure 3-15. Time series of amplification factor $G(t, x)$ at 4 stations in the TFR of James River.
The long-term monitoring station TF5.2A provides chlorophyll-a observation (upper left panel in Figure 3-16), which is then interpolated in time and serves as the boundary condition for the one-dimensional phytoplankton model. As suggested by the results above, Equation (3.12) performs better than Equation (3.4). By substituting the values of \( T(t, x) \) and \( G(t, x) \) into Equation (3.12), we get the solution \( C(t, x) \) to Equation (3.1) in time and space. The red lines in Figure 3-16 shows the result for the 4 stations below TF5.1A. Overall, the results reproduce the seasonal and inter-annual variabilities. For a comparison, the green lines in Figure 3-17 are the results from Equation (3.4). As we can see, there are many high peaks in summer times. The results from Equation (3.12) match the chlorophyll-a observation much better and most of the peaks are depressed. Because the calculation of net growth rate \( \mu_{net}(t, x) \) and our boundary condition are based on the monthly information, we regard our result as a good example for our model predictability.

Figure 3-16. Conceptual model results with \( u(t, x) \) and \( \mu_{net}(t, x) \). The upper left panel is chlorophyll-a observation at Station TF5.2A used for boundary condition. In the other 4 panels, the model result using Equation (3.12) is displayed in red lines (\( k=-0.015 \)).
Figure 3-17. Conceptual model results with $u(t,x)$ and $\mu_{\text{net}}(t,x)$. The upper left panel is chlorophyll-a observation at Station TF5.2A used for boundary condition. In the other 4 panels, the model result using Equation (3.4) is displayed in green lines, while the model result using Equation (3.12) is displayed in red lines ($k=-0.015$).
3.4 Discussion

1. With appropriate information about velocity field, phytoplankton net growth rate and boundary condition, our conceptual model can explain the phytoplankton temporal and spatial patterns observed in the TFR of James River. The form of solution Equation (3.4) shows that physical control and biological effects on phytoplankton dynamics are closely linked. Phytoplankton as a passive tracer in the water (this is true in most cases) not only grow locally, but also is being transported. The phytoplankton biomass we observed is an accumulative growing/damping effect of phytoplankton. For example, if a high phytoplankton concentration is detected in one place, the reason may be a large local growth $G(t, x)$ or a large amount of phytoplankton transported to this area from other places. Additionally, large local growth $G(t, x)$ may be due to a large net growth rate or long retention time. Retention time can be regarded as the time that allow phytoplankton to growth. When it fixed, larger net growth rate means phytoplankton can grow faster resulting larger phytoplankton biomass. On the other hand, if net growth rate is fixed, longer retention time can also result in larger phytoplankton biomass because they can grow longer. Therefore, two different scenarios can lead to the same phytoplankton concentration. The solution Equation (3.4) or (3.12) composed of $T(t, x)$ and $G(t, x)$ can better describing the system by separating the effects of net growth rate and retention time. Equation (3.4) is the general solution to the one-dimensional phytoplankton dynamics with variable velocity, net growth rate and boundary condition. If all these factors are assumed to be constant, then Equation (3.4) degenerated to the solution of a steady state and uniform system as discussed by Lucas et al., (2009). However, Equation (3.4) tells us more information about how the phytoplankton evolve in time and space when being transported downstream. $T(t, x)$ related a certain water parcel back to the upstream boundary, while $G(t, x)$ is the accumulation of net growth rate in time/space.

2. Because local phytoplankton sources are not considered in our conceptual model and all phytoplankton is originated from upstream, the boundary condition becomes important. The signal contained in the boundary such as the peaks in Figure 3-5 will largely influence the downstream
phytoplankton concentration as we can see from Figure 3-7. This is particularly true when net growth rate is assumed to be constant. However, this doesn’t mean that boundary condition completely determines the temporal and spatial patterns of phytoplankton in the downstream because physical and biological factors are also important in real environment. For example, when phytoplankton is abundant, its growth is likely to be limited by self-shading, nutrients and zooplankton grazing. The solution Equation (3.4) does not provide this kind of feedback, while Equation (3.12) can account for it, which is why the results based on Equation (3.12) are better than those based on Equation (3.4). Therefore, the nonlinear second order reaction term is better than the first order reaction term because an additional feedback mechanism is added.

3. There exists an inter-annual variation of phytoplankton concentration in the TFR of James River (Figure 3-17) The chlorophyll-a is relatively low for 2003 and 2004 for all stations including TF5.2A. This is due to the high flow condition in 2003 and 2004. In these two years, the average flow rates were respectively, 413 m$^3$/s and 269 m$^3$/s, and the peak flow could have been more than 3000 m$^3$/s in 2003. The inverse relationship between high river flow and low phytoplankton concentration is because transit time decreases as flow rates goes high (Lucas et al., 2009). The short transit time restricts the accumulation of phytoplankton biomass. Here, transit time is represented by water age $T(t, x)$ and Figure 3-18 shows that water age decreases exponentially as James River discharge increases. The correlation is best at TF5.3, while it becomes worse as it goes downstream with more complex river morphology and more hydrodynamic processes involved.

4. In the TFR of James River, chlorophyll-a maximum is often observed around the river section with a broad and shallow river channel (Bukaveckas et al., 2011) where Stations TF5.5 and TF5.5A are located. Bukaveckas et al., (2011) points out that the river morphology and biological factors may contribute to the chlorophyll-a maximum. However, the criterion of phytoplankton maximum is unknown. If assuming that the boundary condition $a$ is constant, net growth rate $\mu_{net}$ and velocity $u$ do not change with time, then Equation (3.4) becomes:

$$ \frac{\partial x}{\partial t} + u \frac{\partial x}{\partial x} - \mu_{net} x = 0 $$
By using the necessary condition $\frac{\partial C}{\partial x} = 0$ where $C$ gets maximized/minimized, we get the following conclusion

$$\mu_{net}(\eta) = 0$$

This relation simply says that phytoplankton will have one local maxima/minima where the net growth rate equals zero. It means that phytoplankton biomass will not increase or decrease in the region where the total growth is balanced by the total loss. In a river system, there may be multiple local maxima/minima. If there is a chlorophyll maximum, it should be at one of the local maxima. The may explain why the net growth rates at noon time for Stations TF5.5 and TF5.5A are similar in Figure 3-13 if they are in the region where phytoplankton maximizes. The necessary condition $\mu_{net}(\eta) = 0$ means that phytoplankton maximum is biological controlled. At the point of phytoplankton maximum, the maximum phytoplankton biomass is reached and phytoplankton biomass stops increasing beyond this point. It implies that the net growth rate $\mu_{net}(\eta)$ will become negative beyond the point of phytoplankton maximum. If this is not the case and $\mu_{net}(\eta)$ keeps positive beyond the point of phytoplankton maximum, the phytoplankton will continue to grow during being transported downstream and maximum phytoplankton must be at further downstream.

The net growth rate equaling zero means that the loss terms of phytoplankton surpass the growth term at the point of phytoplankton maximum. For example, when the retention time is long enough and net growth rate is positive, phytoplankton will grow continuously until it is limited by some factors such as nutrients and light, and the net growth rate then becomes zero. In addition, the necessary condition $\mu_{net}(\eta) = 0$ does not means that physical transport is irrelevant to the location of phytoplankton maximum. Instead, it can influence the distribution of $\mu_{net}(\eta)$ in space, which in turn influence the location. For example, when river flow increases, the location will shift downstream because longer transport distance is needed before
phytoplankton reach its maximum. The longer distance is translated to the same length of growth time compared to the original smaller river flow. In a case when flow is very large, the retention time is fairly short and the maximum condition $\mu_{net}(\eta) = 0$ may never be reached. For example, in 2003 and 2004 in the TRF of James River, the chlorophyll-a keeps low (Figure 3-17).

Figure 3-18. Water age VS. Flow rates at 4 stations in the TFR of James River

5. About the chlorophyll-a maximum, there are two more questions that remain regarding 1) its location, 2) how factors such as river flow influence the location. For a simple analysis, we list some assumptions:

a) River channel has a shape $A = A_0(1 + kx)$ and the velocity profile is $u = \frac{Q}{A_0(1 + kx)}$, where $A$ is the river cross section area, $A_0$ is the area at the head, $Q$ is a constant river flow rate and $k$ is a coefficient to reflect river cross section changes longitudinally and can be positive, zero or negative
b) Constant net phytoplankton growth rate $\mu_{net}$ and boundary condition $a$

c) The phytoplankton concentration at chlorophyll-a maximum is $C_m$. It should be determined by some environment factors such as nutrients concentration in the system and it represents the capacity of the system that allows phytoplankton to grow. Beyond the chlorophyll-a maximum, $\mu_{net}$ cannot be regarded as constant. The corresponding amplification factor at chlorophyll-a maximum is $G_m = \ln(C_m / a)$.

With these assumptions, we can determine the amplification factor based on Equations (3.6) and (3.8):

$$G = \begin{cases} 
\mu_{net} \cdot \int_0^x \frac{d\eta}{\mu(\eta)} = \mu_{net} \cdot \int_0^x \frac{A(1+k\eta)d\eta}{Q} = \mu_{net} \cdot A_0 \frac{(1+kx)^2 - 1}{2kQ} & k \neq 0 \\
\frac{\mu_{net} \cdot A_0}{Q} x, & k = 0
\end{cases}$$

At the location of chlorophyll-a maximum, we have $G(x_m) = G_m$. This leads to:

$$x_m = \begin{cases} 
\frac{1}{k} \left( \sqrt{1 + \frac{2kG_mQ}{A_0\mu_{net}}} - 1 \right), & k \neq 0 \\
\frac{G_mQ}{A_0\mu_{net}}, & k = 0
\end{cases}$$

where $x_m$ is the location where chlorophyll-a maximum will happen. Figure 3-19 shows the position of chlorophyll-a maximum predicated by Equation (3.33) when river cross-sections changes. As we can see, the location $x_m$ increases when $\frac{G_mQ}{A_0\mu_{net}}$ increases. It is interesting that the curvatures of lines changes for different values of $k$. When $k > 0$, the line curves upward; When $k < 0$, the line curves downward; when $k = 0$, it is a straight line. From Equation (3.33), we can see that when river flow $Q$ increases, $x_m$ will increase if other factors are kept constant. Figure 3-20 shows how the location of the chlorophyll maximum changes as river flow increases in the TFR of the James with the assumption that $G_m = 2$, $A_0 = 4 \times 10^3$ m$^2$. 

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, $k = 1.5 \times 10^{-3} \text{ m}^{-1}$, and $\mu_{net} = 0.1 \text{ day}^{-1}$. The estimation of $x_m$ based on Equation (3.33) matches the observation well, though the approach is highly simplified. In TFR of James River, the river cross-section increases with a positive $k$. The upward curvature of the location $x_m$ is consistent with the James River morphology, which again verifies our model. In addition, when $\mu_{net}$ becomes smaller, $x_m$ will be larger meaning that the chlorophyll-a maximum tends to be at further downstream when net growth is small. Furthermore, $x_m$ will increase if $G_m$ increases, which implies that the chlorophyll-a maximum tends to be at further downstream when the capacity of the system that allows phytoplankton to grow increases.
Figure 3-19. Location of chlorophyll maximum predicted by Equation (3.33).
Figure 3-20. How the location of the chlorophyll maximum shifts as river flow changes in the TFR of James River. Red circles are locations of the chlorophyll maximum extracted from dataflow observations. Blue line is an estimation from Equation (3.33) when $G_m = 2$, $A_0 = 4 \times 10^3 \text{ m}^2$, $k = 1.5 \times 10^{-3} \text{ m}^{-1}$, and $\mu_{net} = 0.1 \text{ day}^{-1}$.

6. Our conceptual model is only applied to one phytoplankton species, but in theory it should work individually for multiple species as long as they don’t interact with each other in the same environment. In addition, it is a one-dimensional system. However, the concept should hold more generally for a three-dimensional system if diffusion can be neglected. Assuming the three-dimensional velocity field and net growth rate are known, the corresponding three-dimensional solution is:

$$C(t, \bar{x}) = a(t - T(t, \bar{x}), \bar{x}_o) \cdot e^{G(t, \bar{x})}, \ t \geq 0, \ \bar{x} \in V$$  \hspace{1cm} (3.34)$$

and water age $T$ and amplification factor $G$ are determined by the following equations:

$$\frac{\partial T}{\partial t} + u \cdot \nabla T = 1, \ t \geq 0, \ \bar{x} \in V$$  \hspace{1cm} (3.35)$$
\[
\frac{\partial G}{\partial t} + u \cdot \nabla G = \mu_{\text{net}}, \quad t \geq 0, \quad \bar{x} \in V
\]

(3.36)

\[
T(t, \bar{x}) = 0, \quad \bar{x} \in \Omega
\]

(3.37)

\[
G(t, \bar{x}) = 0, \quad \bar{x} \in \Omega
\]

(3.38)

where \( \Omega \) represents the boundary of domain \( V \), \( \partial \) is the boundary condition on \( \Omega \) and \( \bar{x}_0 \) determines the original point on the boundary from which the water parcel originates.

### 3.5 Summary

A theoretical combined with data analysis studies on cyanobacteria blooms dynamics was conducted in the upper tidal James River. The governing equation includes the physical transport and biological effects, which leads to a simple partial differential equation composed of an advection term and a phytoplankton net growth term, in linear and nonlinear forms. The general solution, which has an implicit analytic form, integrates the boundary condition, net growth rates and velocity field to explain the phytoplankton dynamics. Various forms of the solution are then constructed and discussed under different assumptions. To show its predicative capability of the solution, we apply the analytic theory in the tidal freshwater portion of the James River. The theoretical predictions of chlorophyll concentrations are compared with observational data and verified the validity of the solution. In addition, the factors for the formation of chlorophyll maximum in tidal freshwater rivers are discussed and the criteria and location of chlorophyll maximum are given based on our theory. The application of the analytic model in the TFR of the James demonstrates that it can simulate the temporal and spatial patterns of phytoplankton biomass in a simple setting of one dimensional case. The results show that physical and biological factors are both important and are closely linked in regulating phytoplankton biomass.
Appendix B: Proof for the Conservation of Equation (3.1)

This section provides proof that the Equation (3.1) regarding phytoplankton dynamics is conservative.

Below are definitions of some variables.

\( C(t, x) \): Phytoplankton concentration

\( A(t, x) \): River Cross-Sectional Area

\( U(t, x) \): Velocity

\( \mu(t, x) \): Net growth rate

In a river system, the following conservative form equation for phytoplankton always holds:

\[
\frac{\partial (CA)}{\partial t} + \frac{\partial (CAU)}{\partial x} = \mu CA. \tag{3.39}
\]

By rearranging the above equation, we get the following equations:

\[
A \frac{\partial C}{\partial t} + C \frac{\partial A}{\partial t} + AU \frac{\partial C}{\partial x} + C \frac{\partial (AU)}{\partial x} = \mu CA \tag{3.40}
\]

and

\[
A \left( \frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} \right) + C \left( \frac{\partial A}{\partial t} + \frac{\partial AU}{\partial t} \right) = \mu CA \tag{3.41}
\]

In Equation (3.41), \( \left( \frac{\partial A}{\partial t} + \frac{\partial AU}{\partial x} \right) = 0 \) as it is the one-dimensional continuity equation. Therefore, we have the following equation accounting for phytoplankton dynamics.

\[
\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = \mu C
\]
Appendix C: proofs of the solution method to the advection reaction equation in Chapter 3

In Chapter 3, we discussed the equation of phytoplankton dynamics with two types of reaction terms: (1) linear form and (2) nonlinear form. Instead of solving the original equation, we transformed the problem into a set of quasi-linear partial differential equations, which lead to an elegant solution in implicit form. This appendix gives the proofs.

1 Linear reaction term

The equations for the problem are listed below:

\[
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \left( \mu_{\text{grow}} - \mu_{\text{loss}} \right) C = \mu_{\text{net}} C \tag{3.42}
\]

\[C(t, x = 0) = a(t), \quad \text{for } t \geq 0 \tag{3.43}\]

\[C(t = 0, x) = b(x), \quad \text{for } x \in [0, L] \tag{3.44}\]

and the solution to Equations (3.42)-(3.44) can be expressed as:

\[C(t, x) = a(t - T(t, x)) \cdot e^{G(t, x)}, \quad t \geq 0, \ x \in [0, L] \tag{3.45}\]

\[\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = 1 \tag{3.46}\]

\[\frac{\partial G}{\partial t} + u \frac{\partial G}{\partial x} = \mu_{\text{net}} \tag{3.47}\]

\[T(t, x = 0) = 0 \tag{3.48}\]

\[G(t, x = 0) = 0 \quad . \tag{3.49}\]

\[a(\xi) = b \left( T^{-1}(-\xi) \right) \cdot e^{-G(t = 0, \ T^{-1}(-\xi))}, \quad \xi \in \left[ -T(t = 0, \ x = L), 0 \right] . \tag{3.50}\]

Here, Equations (3.45)-(3.50) comprise a complete solution to the problem: Equations (3.42)-(3.44).

1.1 Proof: Equations (3.45)-(3.50) are solutions to Equation (3.42)

Substituting Equation (3.45) into Equation (3.42), we have:
\[
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = a \cdot \left(1 - \frac{\partial T}{\partial t}\right) \cdot e^G + a \cdot e^G \cdot \frac{\partial T}{\partial t} + u \cdot a \cdot \left(- \frac{\partial T}{\partial x}\right) \cdot e^G + u \cdot a \cdot e^G \cdot \frac{\partial T}{\partial x}
\]
\[
= a \cdot \left(1 - \frac{\partial T}{\partial t} - u \frac{\partial T}{\partial x}\right) \cdot e^G + a \cdot e^G \cdot \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x}\right)
\]
\[
= a \cdot 0 + a \cdot e^G \cdot \mu_{net} = \mu_{net} \cdot C
\]

Note that Equations (3.46)-(3.47) are used in the derivation. Substituting Equation (3.45) into Equations (3.43)-(3.44), we have:
\[
a(t - T(t, x = 0)) \cdot e^{G(t, x=0)} = a(t).
\]
\[
a(- T(t = 0, x)) \cdot e^{G(t=0, x)} = b(x).
\]

Note that the relations of Equations (3.48)-(3.50) are used. Therefore, Equations (3.45)-(3.50) comprise the solutions to Equations (3.42)-(3.44).

1.2 Proof: Equations (3.48)-(3.50) are the unique solutions

Assuming there is another solution \( \psi \) satisfying Equation (3.42):
\[
\frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} = \mu_{net} \cdot \psi.
\]

Then, \( C + \psi = a(t - T(t, x)) \cdot e^{G(t, x)} + \psi \) also satisfy Equation (3.42). Substituting \( C + \psi \) into Equations (3.43)-(3.44), we get:
\[
\psi(t, x = 0) = 0.
\]
\[
\psi(t = 0, x) = 0.
\]

This states that the initial and boundary conditions of \( \psi \) are all zeros. From the Lagrangian point of view, Equation (3.42) can be expressed as \( \frac{d\psi}{dt} = \mu_{net} \cdot \psi \). Its initial condition \( \psi(t, x = 0) = 0 \) and boundary condition \( \psi(t = 0, x) = 0 \) mean:
\[
\psi = 0,
\]
in time and space. Here, the flow direction is from \( x = 0 \) to \( x = L \). Therefore, Equations (3.48)-(3.50) are the unique solutions.
2 Nonlinear reaction term

If the reaction term of Equation (3.42) has a nonlinear form as shown below, the problem becomes:

\[
\begin{align*}
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} &= \mu_{net} \cdot (1 + k C) \cdot C \\
\text{note: } k \text{ is negative when } \mu_{net} > 0 \text{ and is positive when } \mu_{net} < 0.
\end{align*}
\] (3.58)

\[C(t, x = 0) = a(t), \text{ for } t \geq 0 \] (3.59)

\[C(t = 0, x) = b(x), \text{ for } x \in [0, L] \] (3.60)

Then, the solution to Equations (3.58)-(3.60) can be expressed as:

\[C(t, x) = \frac{a(t - T(t, x)) \cdot e^{G(t, x)}}{1 + ka(t - T(t, x)) \cdot (1 - e^{G(t, x)})}, \quad t \geq 0, \ x \in [0, L] \] (3.61)

\[\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = 1 \] (3.62)

\[\frac{\partial G}{\partial t} + u \frac{\partial G}{\partial x} = \mu_{net} \] (3.63)

\[T(t, x = 0) = 0 \] (3.64)

\[G(t, x = 0) = 0 \] (3.65)

\[a(\xi) = \frac{b(T^{-1}(-\xi))}{(1 + kb(T^{-1}(-\xi))) \cdot e^{G(t = 0, T^{-1}(-\xi))} - kb(T^{-1}(-\xi))}, \quad \xi \in [-T(t = 0, x = L), 0]. \] (3.66)

Here, Equations (3.61)-(3.66) comprise a complete solution to the problem: Equations (3.58)-(3.60).

2.1 Proof: Equations (3.61)-(3.66) are the solutions to Equation (3.58)

Substituting Equation (3.61) into (3.58), we have:
\[
\frac{a \cdot \left(1 - \frac{\partial e^G}{\partial t}\right) \cdot e^G + a \cdot e^G \cdot \frac{\partial G}{\partial x}}{1 + k \cdot a \cdot (1 - e^G)} - \frac{ka \cdot e^G \cdot \left[ a \cdot \left(1 - \frac{\partial e^G}{\partial t}\right) \cdot \left(1 - e^G\right) - a \cdot e^G \cdot \frac{\partial G}{\partial x}\right]}{1 + k \cdot a \cdot (1 - e^G)^2}
\]

+ \frac{u}{1 + k \cdot a \cdot (1 - e^G)} \cdot \frac{ka \cdot e^G \cdot \left[ a \cdot \left(1 - \frac{\partial e^G}{\partial t} - u \frac{\partial T}{\partial x}\right) \cdot \left(1 - e^G\right) - a \cdot e^G \cdot \left(\frac{\partial G}{\partial t} + u \frac{\partial G}{\partial x}\right)\right]}{1 + k \cdot a \cdot (1 - e^G)}

= \frac{a \cdot e^G \cdot \mu_{net}}{1 + k \cdot a \cdot (1 - e^G)} + \frac{ka \cdot e^G \cdot a \cdot e^G \cdot \mu_{net}}{1 + k \cdot a \cdot (1 - e^G)^2}

= \mu_{net} \cdot \frac{a \cdot e^G}{1 + k \cdot a \cdot (1 - e^G)} \left[ 1 + k \cdot \frac{a \cdot e^G}{1 + k \cdot a \cdot (1 - e^G)}\right]

= \mu_{net} C(1 + kC)

(3.67)

Note that Equations (3.62)-(3.63) are used in the derivation. Substituting Equation (3.61) into Equations (3.59)-(3.60), we have:

\[
\frac{a(t - T(t, x = 0)) \cdot e^{G(t, x = 0)}}{1 + k \cdot a(t - T(t, x = 0)) \cdot (1 - e^{G(t, x = 0)})} = a(t).
\]

(3.68)

\[
\frac{a(-T(t = 0, x)) \cdot e^{G(t = 0, x)}}{1 + k \cdot a(-T(t = 0, x)) \cdot (1 - e^{G(t = 0, x)})} = b(x).
\]

(3.69)

Note that the relations of Equations (3.64)-(3.66) are used. Therefore, Equations (3.61)-(3.66) are the solutions to Equations (3.58)-(3.60).

2.2 Proof: Equations (3.61)-(3.66) are the unique solutions

Assuming there is another solution \( \psi \) satisfying Equation (3.58)

\[
\frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} = \mu_{net} \cdot \psi \cdot (1 + k \psi).
\]

(3.70)

Then, \( C + \psi \) should also satisfy Equation (3.58), which leads to:
\[
\frac{\partial (C + \psi)}{\partial t} + u \frac{\partial (C + \psi)}{\partial t} = \mu_{\text{net}} \cdot [1 + k(C + \psi)] \cdot (C + \psi)
\]
\[
= \mu_{\text{net}} \cdot (1 + kC) \cdot C + \mu_{\text{net}} \cdot (1 + k\psi) \cdot \psi + 2\mu_{\text{net}} \cdot C \cdot \psi
\]  

(3.71)

Since \( C \) and \( \psi \) are both solutions to Equation (3.58), this leads to:

\[
2 \cdot \mu_{\text{net}} \cdot C \cdot \psi = 0.
\]  

(3.72)

which implies that \( \psi \) must be zero. Therefore, Equations (3.61)-(3.66) are the unique solutions.
Chapter 4 Harmful Algal Bloom of *C. Plykrikoides* in the Lower Chesapeake Bay - the Observations and Numerical Experiments

Abstract

The observational analysis and numerical experiments were performed to investigate the algal bloom in the polyhaline of the Chesapeake Bay. The observed properties of *C. polykrikoides* bloom including its spatial distribution in the lower Chesapeake Bay and the temporal variation during 2012-2014 were first analyzed, and then the numerical experiments are conducted to investigate the bloom mechanism. This exploratory study is aimed to explain the broad distribution of *C. polykrikoides* blooms (not restricted to one location) in the lower Bay and the sudden disappearance of the bloom in 2014. In order to address these phenomena, a hypothesis is made regarding the origin of *C. polykrikoides* cysts. In this hypothesis, the cysts are considered to be originated from coastal ocean and their transport is under the influence of wind patterns and gravitational circulation. In this study, the coupled SCHISM+ICM model is applied for the entire Chesapeake Bay and its continental shelf. The hydrodynamics in the lower Chesapeake Bay was first analyzed regarding velocity distribution and the coastal upwelling. Then, a series of particle tracking experiments were conducted for investigating the physical transport of *C. polykrikoides* cysts under different conditions. Finally, water quality model ICM was used to simulate the algal blooms caused by *C. polykrikoides* in the lower Bay. The biological features of *C. polykrikoides* such as its capability of active vertical migration, uptake of organic nitrogen and temperature-dependent growth rate, and the transport of cysts during upwelling events are included in the modeling framework. The model can generate reasonable magnitude of the algal blooms in 2012, 2013 and simulate no algal bloom condition in 2014. Both data analysis and numerical modeling indicate that air temperature and wind patterns play important roles in controlling the development of the blooms. In summary, these exploratory experiments demonstrated that the algal blooms of *C. polykrikoides* can start with cysts transported from outside the Chesapeake Bay. The
new paradigm can explain the broad distribution of the *C. Polykrikoides* blooms in the lower Bay and the lacking of any blooms in 2014 due to the special wind patterns, temperature pattern, and the associated effects in this year.

4.1 Introduction

*Cochlodinium Polykrikoides* (*C. polykrikoides*) blooms are observed annually in the lower Chesapeake Bay. In this section, we will introduce the biological characteristics of *C. polykrikoides*, the information about *C. polykrikoides* blooms in the lower bay and the research progresses.

4.1.1 Characteristics of *C. polykrikoides*

*C. polykrikoides* is a dinoflagellate species and it blooms around the world. Figure 4-1 is a photo of *C. polykrikoides* in aggregation of several cells under microscope. Globally, *C. polykrikoides* bloom exhibits a rapid expansion in the past few decades. In Figure 4-2, the top panel shows the global distribution of *C. polykrikoides* bloom pre-1990 and the bottom panel shows the distribution after 1990. It indicates a rapid expansion of *C. polykrikoides* bloom over the last 20 years. The coastal regions affected by *C. Polykrikoides* include Korea, Japan, Philippines and Malaysia in Asia, Gulf of California, Long Island and Chesapeake Bay in the North America, parts of Europe, India and Persian Gulf. The bloom of *C. Polykrikoides* can cause severe impact towards aquaculture industry as it may cause mortalities for both wild, farmed fishes and shellfishes.

*C. polykrikoides* has some unique biological characteristics that enable it to bloom at various conditions. It can survive broad temperatures and salinity ranges. In east Asian, Kim et al., (2004) reported that *C. polykrikoides* can grow under temperature 10-30 °C and salinity 15-50 ppt, while the optimal growth happens around temperature of 25 °C and salinity of 34 ppt. In US East Soast, *C. polykrikoides* bloom can happen in salinity 19-30 ppt and temperature 27-29.5 °C (Mulholland et al., 2009; Kudela and Gobler 2012; Morse et al., 2013). Generally, *C. polykrikoides* prefers high temperature (>25 °C) and high salinity (25-40 ppt) environment. Figure 4-3 summaries the temperature and salinity ranges for *C. polykrikoides* blooms
happened around the world. Although *C. polykrikoides* can bloom very quickly, it actually has a small growth rate 0.3-0.9 day\(^{-1}\) (Yamatogi and Maruta 2002; Kim et al., 2004; Morse et al., 2011; Kudela and Gobler 2012; Morse et al., 2013; Fitzpatrick et al., 2014). Kim et al., (2004) reported a maximum growth rate of 0.41 day\(^{-1}\) in East Asian. Yamatogi and Maruta (2002) reported a larger growth rate of 0.90 day\(^{-1}\).

Due to the limited laboratory data, Kudela and Gobler (2012) mentioned that there is a fairly broad range for the maximum growth rate of *C. polykrikoides* (factor of 2). Another important characteristic of *C. polykrikoides* is that it has the capability of vertical migration. This feature provides this bloom species advantages in nutrient uptake and obtaining light. Additionally, it provides an adaptive strategy for *C. polykrikoides* to reduce predation by zooplankton (Jiang et al., 2010b; Jiang et al., 2010a). Park et al., (2001) reported a swimming speed of 3-4 m.h\(^{-1}\). Lim et al., (2014) mentioned that *C. polykrikoides* can swim at a speed of 1.4 mm.s\(^{-1}\) (over 100 m.day\(^{-1}\)). Overall, it is a fast-moving species. Moreover, *C. polykrikoides* can utilize organic nitrogen when inorganic nutrients are insufficient to support its growth (Mulholland et al., 2009). When ambient nutrients are abundant, it also exhibits a greater nutrient uptake rate and can store additional nutrients within its cell for later use. At certain life stage, *C. polykrikoides* will produce cysts which can then sink to sea bed. The *C. polykrikoides* cysts were also found in the sediment in the Chesapeake Bay (Seaborn 2008). These cysts can overwinter and survive the adverse conditions when ambient environment is not favorable. In addition, they can be transported along currents. With these biological features combined, *C. polykrikoides* appears to spread globally with an increasing trend of blooms. However, the factors that control the blooming of *C. polykrikoides* in different regions maybe different because they maybe genetical distinct (Gobler et al., 2008). For example, their biological features of *C. polykrikoides* in the Chesapeake Bay could be different from the ones in East Asian (Mulholland et al., 2009).
Figure 4-1. Photo of Cochlodinium Polykrikoides under microscope. Photo courtesy of Dr. Kim Reece. www.vims.edu/newsandeventstopstoriesarchives2012cochlo_bloom.php
Figure 4-2. Global distribution of *C. polykrikoides* blooms before 1990 (upper panel) and after 1990 (lower panel). Picture is from (Kudela and Gobler 2012).
4.1.2 Introduction to *C. polykrikoides* Blooms in the Chesapeake Bay

In the Chesapeake Bay, *C. polykrikoides* was identified in York River in 1960s (Mackiernan 1968). Since then, *C. polykrikoides* bloom happens annually in each summer (Mulholland et al., 2009; Morse et al., 2011). In 1992, an extensive *C. polykrikoides* bloom occurred in York River and this bloom spreads from York River to the lower Chesapeake Bay including the lower James River (Marshall 1994). After 1992, *C. polykrikoides* bloom appears in the lower James River every year including Lafayette and Elizabeth River (Mulholland et al., 2009). Figure 4-4 shows the distribution of *C. polykrikoides* blooms in the Chesapeake Bay in recent years (Todd Egertonk et al., 2014). It can be seen that *C. polykrikoides* bloom occurs frequently in the tributaries on the western bank of the Bay including Potomac River, Rappahannock River, York River and James River. Particularly, many blooms were found in the lower James River. In
addition, *C. polykrikoides* blooms can appear along the bay channel as well as along the eastern shore of the Bay. *C. polykrikoides* cysts are also identified in the sediment, which verified the existence of this bloom species in the Chesapeake Bay (Seaborn 2008). During blooming period, the cell concentration can exceed $10^4$ cells/ml. For example, in Elizabeth River, a *C. polykrikoides* bloom happened in 2007 has cell count of 28,120 cells/ml with chlorophyll-a concentration exceeding 300 µg/L (Morse et al., 2011). There are some theories to explain the *C. polykrikoides* blooming mechanism in the lower Chesapeake Bay. Morse et al., (2011) conjectured that Lafayette and Elizabeth Rivers may be initial grounds for *C. polykrikoides* blooms in 2007 and 2008. *C. polykrikoides* bloom develops first in the initial grounds and then is transported into James River through currents and tidal flushing. Mulholland et al., (2009) mentioned that there is a coincidence between the onset of *C. polykrikoides* bloom and the period of intense rainfall, which implies that the nutrient pulsing related to rainfall event may stimulate the growth of *C. polykrikoides*. Also, the bloom tends to happen in the summer when water temperature is above 25 °C in the period of calm wind (Morse et al., 2013).

However, the trigger mechanism of *C. polykrikoides* bloom is still not well understood. These theories mentioned above could not explain all of the *C. polykrikoides* bloom features in the lower Chesapeake Bay. For example, in 2008, there is also initiation of *C. polykrikoides* bloom in the mesohaline portion of the James River (Morse et al., 2011). Moreover, *C. polykrikoides* bloom has been found in York River before it began to appear in James River. The broad distribution of *C. polykrikoides* bloom in the lower Chesapeake Bay also suggests other mechanisms that may promote its spread.
4.2 Observation, and a revised hypothesis for *C. Polykrikoides* bloom dynamics

4.2.1 Observational Analysis

The characteristics of *C. polykrikoides* bloom including its spatial distribution in the lower Chesapeake Bay and the temporal variation during 2012-2014 are analyzed. On the spatial variation, the general distribution of *C. polykrikoides* bloom in the lower Bay is shown in Figure 4-4. Particularly in York River, Figure 4-5 shows the time series of chlorophyll at three stations from the river mouth to the middle part of the river. During the summer in 2012, the bloom (likely to be dominated by *C. polykrikoides*) in the
York River was observed to initiate first around the mouth of York River (Goodwin Island and Gloucester Point) and later in Clay Bank in the mid-River, as shown in Figure 4-5. This may suggest that the initiation of the bloom may start around the river mouth, probably under a potential influence from the lower Bay, likely through the York Spit Channel, a ship channel connected to the Bay mouth. This is different from the observation made by Morse et al., (2013) using 2007-2009 data, which states that the C. Polykrikoides bloom was first initiated in the Lafayette River and was then proliferated to the James River and lower Chesapeake Bay subsequently. If there is a unified mechanism for the development and proliferation of the C. Polykrikoides bloom in the lower Bay, could the transport of C. Polykrikoides cysts from the coastal ocean (e.g., transported into the Elizabeth and Lafayette Rivers from the Bay mouth, through the Norfolk and Thimble shoal Channels) can explain the phenomenon? On the temporal variation, the C. polykrikoides bloom has been observed continuously and persistently from 2005 to 2013. However, in 2014, there is no bloom observed in the lower Chesapeake Bay. Figure 4-6 shows the time series of chlorophyll concentration in 2012-2014 and the observational data are downloaded from VECOS (Virginia Estuarine and Coastal Observing System): [http://web2.vims.edu/vecos/Default.aspx](http://web2.vims.edu/vecos/Default.aspx). VECOS is a real-time observing system measuring salinity, temperature, DO, pH, chlorophyll, and turbidity by YSI sensor in 15-minute interval. The Station LAF001.63 is located at Lafayette River, as described in the right panel of Figure 4-6. It can be clearly seen that the 2012 bloom starts in late June and 2013 bloom starts in August and September, but there are very few bloom events happened in 2014. The vertical scale for chlorophyll concentration is plotted up to 200 µg/L in order that the bloom events are visible and distinguishable for all three years, but the actual value can exceed 200 µg/L. The observational data is further processed and Figure 4-7 shows the statistics for daily chlorophyll maximum at Station LAF001.63 in Lafayette River. The result displays the percentages of chlorophyll at different ranges from 2012 to 2014. The chlorophyll concentration in 2014 is relatively low, mostly below 25 µg/L, compared to the high chlorophyll concentrations in 2012 and 2013 with much larger percentage of daily chlorophyll maximum exceeding 100 µg/L. If chlorophyll >100 µg/L is regarded as a proxy of bloom, blooms are rare in 2014 and are very frequent in 2012 and 2013. This
difference raises the question as to why bloom stops in 2014. Are there any factors or mechanisms that may have inhibited the bloom in 2014?

In order to answer the questions above, we first check the river discharge of James River and the record of precipitation in the lower Bay. In Figure 4-8, the upper panel shows the James River discharge from USGS gauge at Richmond for 2012, 2013, and 2014. The monthly river discharge is higher in 2013 and lower in 2012, and the river discharge in 2014 (in gray) is in between, not far from the long-term mean. The lower panel in Figure 4-8 shows the monthly precipitation from Norfolk International Airport in June, July, August, and September from 2012 to 2014. The precipitation in 2014 is lower in June and August, is higher in July and September. As we can see, the mean was slightly higher than the long-term average and the precipitation of this year became abnormally high only in September. Therefore, higher James River discharge or larger precipitation is not a good indication of *C. polykrikoides* bloom. Both factors cannot explain why *C. Polykrikoides* bloom disappears in 2014. In an attempt to find an answer to the question why 2014 is so different from 2012 and 2013 regarding *C. polykrikoides* blooms, we did an analysis about the distribution of the prevailing wind directions. The hourly wind data from Chesapeake Bay bridge tunnel in the past 15 years from 2000 to 2014 are analyzed. In Figure 4-9, wind components are shown for southwesterly wind (orange) and northwesterly wind (blue). As one can see, 2014 stands out as an abnormal year. The percentage of northeasterly wind in 2014 is one of the largest in the last past 15 years. At the same time, the percentage of southwesterly wind is the second lowest in 2014 (behind 2004). Since wind can affect the estuarine circulation (Valle-Levinson et al., 2001), coastal plume and upwelling (Shanks et al., 2002; Shanks et al., 2003), the air/water temperature, the surface wave and mixing regimes, it can potentially affect the environmental conditions for *C. polykrikoides* blooms. For example, there is often warm condition when southerly wind blows, which brings warm air from the south. On the other hand, northerly wind is usually associated with cool air, which cools the surface water. Figure 4-10 shows the air temperature in July, August and September from 2012 to 2014. The air temperature exceeding 28 °C is much more frequently in 2012 and 2013 than that in 2014. Because *C. polykrikoides* prefers warm
temperature and it usually blooms in the Chesapeake Bay when water temperature is constantly higher than 25 °C (Morse et al., 2013), it is thus understandable for the rare *C. polykrikoides* blooms in 2014 as the temperature is lower in this year. In contrast, the southwesterly wind is prevalent in the summer of 2012 and 2013 (in Figure 4-9) associated with higher temperature (Figure 4-10), and large *C. polykrikoides* blooms occur in these two years. To further see the correlation between chlorophyll concentration and wind condition, we plotted the distribution of daily chlorophyll maximum versus southwest-northeast wind component in Figure 4-11 (for each daily chlorophyll maximum value, it corresponds to wind averaged over the past 5 days). The tendency in 2012 and 2013 clearly shows that algal blooms (>100 µg/L) often occur during the period when southwesterly wind is prevailing. On the other hand, few algal blooms occur under northeasterly wind conditions. This demonstrates that the wind condition and the associated effects may be related to the environmental conditions for *C. polykrikoides* bloom.

Similar to other algal blooms, the onset of a *C. polykrikoides* bloom requires a suitable environmental condition of habitation (eg, suitable salinity and temperature) and sufficient nutrients to support the algal growth regardless locations. To the question why the southwesterly wind is more conducive to *C. polykrikoides* bloom than the northeasterly wind, the answer may be in three-fold:

1). In the western Atlantic Ocean, a heat wave with extreme high air temperature can occur when a high-pressure system originating from the Gulf of Mexico stays stationary off the US East Coast. The southwesterly winds associated with the high-pressure system can pump hot and humid air northeastward resulting in a high air temperature for much of the eastern US. In contrast, northwesterly wind usually brings cool air from the north. Since *C. polykrikoides* prefers high temperature, the southwesterly wind pattern meets the requirement of its biological requirement.

2). The southeasterly wind off the US East Coast also generates wind-induced transient upwelling, which has been documented off the Chesapeake Bay (Valle-Levinson et al., 2001; Austin and Lentz 2002; Wong and Valle-Levinson 2002; Clemente-Colon 2005). As an example, the continuous
measurements for the surface salinity and temperature in 20130701-20130930 at the mouth of the Chesapeake Bay (Figure 4-12) indicated several upwelling events associated with the southwesterly winds (not shown). It can be seen that the higher salinity and lower temperature occur simultaneously during upwelling event and the change can be up to 5 °C in temperature and 5 ppt in salinity. This maybe important because it can supply additional nutrients from the coastal ocean for *C. polykrikoides* during the summer when nutrients become scarce in the lower Bay.

3). The southwesterly wind around the Chesapeake Bay mouth can also reinforce the two-layer gravitational circulation in the lower Bay (Pritchard 1952; MacCready and Geyer 2010) by enhancing the surface outflow and bottom inflow (Reiss and McConaugha 1999; Anderson et al., 2012). The reinforced non-tidal current can reach to a speed that is efficient enough to transport algal cysts from costal ocean to the vast area in the lower Bay. This transport is even more efficient along the well-connected ship channel, which acts like super-highway for bottom current to transport cysts, nutrients and other vegetative cells. The numerical experiments of particle tracking shown later demonstrate that materials can be transported from the offshore into James River and Elizabeth River within 3-4 days under southwesterly wind conditions.

Based on the discussion above, there may be connection between southwesterly wind, the upwelling off the Chesapeake Bay mouth and the algal bloom inside the Bay. Thus, we raise a question whether there is a remote control on the onset of the *C. polykrikoides* bloom as a complement to the local control.
Figure 4-5. Chlorophyll measurements at three Continuously Monitoring Stations in York River in 2012: Clay Bank (upper panel), Gloucester Point (middle panel), and Goodwin Island (lower panel).
Figure 4-6. The chlorophyll measurement at Lafayette River in 2012-2014. There are large algal blooms in both 2012 and 2013, while there are very few algal bloom events happened in 2014. The vertical scale was up to 200 µg/L, but the actual values in 2012 and 2013 can exceed 200 µg/L.
Figure 4-7. Statistics for daily chlorophyll maximum in 2012, 2013 and 2014. The observational data are from Continuously Monitoring Station LAF001.61.
Figure 4-8. The upper panel shows the James river discharge from Richmond USGS gauge and the lower panel shows the monthly precipitation from Norfolk International Airport in 2012-2014 with long-term average from 1946 to 2014.
Figure 4-9. The distribution of wind directions in July and August from 2000 to 2014. The percentages of southwesterly wind (orange) and northeasterly wind (blue) are presented for each year.
Figure 4-10. The daily precipitation and air temperature from July 1 to August 30 in 2012-2014 for the lower Chesapeake Bay. The data are from Norfolk International Airport.
Figure 4-11. The distribution of daily chlorophyll maximum VS. southwest-northeast wind components at Station LAF001.63.
Figure 4-12. The time series of salinity and temperature at the water surface (left panels) from July 1st to September 15th in 2013. The blue arrows point to the periods when southwesterly prevailed (not shown). During these periods, it is signified by high salinity and low temperature, indicating upwelling events. The right panel shows the station location and description of the VECOS buoy.
4.2.2 A Revised Hypothesis about *C. polykrikoides* Blooms in the lower Chesapeake Bay

The current knowledge and hypothesis for explaining the initiation of the *C. polykrikoides* blooms in the lower Chesapeake Bay have been mainly drawn from the researches in the lower James River including Lafayette River and Elizabeth River. Below are some theories:

1) Mulholland et al., (2009) observed the coincidence between the onset of *C. polykrikoides* blooms and the period of rainfall events. The nutrients washed out from the watershed may stimulate the growth of *C. polykrikoides* that can also uptake various forms of nitrogen and organic nutrients.

2) Morse et al., (2011) pointed out that there may be initial sites in Lafayette and Elizabeth River for *C. polykrikoides* blooms.

3) Morse et al., (2013) mentioned that *C. polykrikoides* bloom tends to happen when water temperature is above 25 °C in the period of calm wind and neap tide.

The above studies about *C. polykrikoides* blooms focus on the local origin, but how the blooms in the entire lower Bay are connected are still not well understood. Are there any common mechanisms shared in different areas of the lower Bay that control the blooming of *C. polykrikoides* besides local controls? For precipitation, it seems to be a potential indicator of *C. polykrikoides* bloom, but the causal relationship is not established based on our data analysis in 2012-2014. Temperature (either water temperature or air temperature) seems to be a reasonable indicator as suggested by Figure 4-12 and (Morse et al., 2013). However, the inadequacy of the present knowledge about the initiation of *C. polykrikoides* blooms in the lower Chesapeake Bay is illustrated by the quote from (Morse et al., 2013): “the present study failed to determine a ‘smoking gun’ with regard to nutrient controls on bloom formation. The major implications of this study are that nutrient concentrations, while essential for the growth of algae, cannot be identified as a causative factor in determining when a bloom will form, and that there is no ‘smoking gun’ with regard to nutrient controls on bloom formation in a eutrophic estuarine environment.”
Based on the discussion above, the existing theories could not explain all the characteristics of *C. polykrikoides* blooms observed in Chesapeake Bay, in particular, the sudden disappearance of the algal bloom in 2014. It is plausible that the wind pattern (particularly the southwesterly wind) and the associated upwelling may play a role in contributing to the onset, development, and proliferation of *C. polykrikoides* blooms in the lower Chesapeake Bay basin. Thus, we proposed a revised hypothesis and tested it in numerical experiments:

*C. polykrikoides* cysts can be transported into the lower Chesapeake Bay from the inner continental shelf through the estuarine circulation, especially under southwesterly wind conditions, while high temperature combined with low wind condition could be the candidate as the trigger mechanism for *C. polykrikoides* blooms.

In essence, we attempt to answer the follow questions using numerical experiments:

1) Does the remote control exist (in addition to the local control) that is possible to initiate a *C. polykrikoides* bloom?

2) Can the Ekman transport and the upwelling induced by southwesterly wind be reasonably simulated by the numerical model?

3) Does the southwesterly wind promote the transport of *C. polykrikoides* cysts from offshore into the lower Chesapeake Bay?

4) What are the roles played by high air/water temperatures in the period of *C. polykrikoides* blooms?

5) Why *C. polykrikoides* blooms in 2012 and 2013, whereas it ceases to bloom in 2014? Can this phenomenon be simulated?

To address these questions, we will first set up a hydrodynamic model covering the entire Chesapeake Bay as well as the adjacent continental shelf. The model will be first used to investigate the estuarine transport and upwelling/downwelling phenomena under different wind conditions. Then, particles tracking experiments will be conducted to study the transport of *C. polykrikoides* cysts. Finally, we will adapt our
water quality model by assimilating the biological features of *C. polykrikoides* and use the new model to simulate the *C. polykrikoides* blooms in the lower Chesapeake Bay.
4.3 Model Description

In this part, we will first describe our model domain focusing on the model grid. Then, information about the initial conditions and boundary conditions will be given. The model inputs are critical in modeling the hydrodynamics as well as the ecosystem, and much effort was spent in preparing them by using various methods and incorporating various kinds of data resources. Our model has been set up separately for three years: 2012, 2013 and 2014. The first two years 2012 and 2013 are with strong *C. polykrikoides* blooms, while the year 2014 is a year with no blooms in contrast.

4.3.1 Model Grid

Chesapeake Bay is an estuary in the United States East Coast and is the largest estuary in this country. It is about 200 miles long and the width varies from 4 miles to over 30 miles. Figure 4-13 is our model grid. It has 27075 nodes and 41873 elements. The grid is of mixed triangles and quadrilaterals. Typically, quadrilateral elements are placed along the Bay channels to better simulate the flows. Triangular elements are used more generally. They are used to better fit the shorelines and smooth the transition zones. In addition, high resolution is placed along the channels because of their importance in directing the flows and determining the general circulation patterns. In order to accurately simulate the water circulation of the Chesapeake Bay, our model grid covers the entire Bay extending from the Susquehanna River in the north to the continental shelf 200-meter isobath. The model domain includes all the major rivers as well. It includes both York River and James River in the lower Chesapeake Bay where HAB usually blooms. These areas are also the focus of our study and high grid resolution is used to resolve the geomorphological features. The detail is shown is the zoom-in subplot in the lower left corner of Figure 4-13. The grid size ranges from 100 m to 1 km. Furthermore, the water quality calibration stations are shown in the subplot. These stations are also used for the temperature and salinity calibrations as well.

Figure 4-14 shows the bathymetry. The average depth in the Chesapeake Bay is about 7 meters, but the depth can be over 30 meters in the Bay channels. For both James River and York River in the lower
Chesapeake Bay, there is a channel connected to the main Bay. Around the Bay entrance, it is characterized by two deep channels. The North Channel is wider with a maximum depth of 14 meters and the north region is generally flat with depth smaller than 10 meters in most of the area. The south channel (Thimble shoal channel) is narrower with maximum depth of over 30 meters (Valle-Levinson et al., 2001). This channel is connected the James River. Our model domain includes the continental shelf adjacent to the Chesapeake Bay. It extends to the continental shelf break with 200-meter isobath and is about 100 km wide. The north boundary is near the Indian River Bay in Delaware, while the south boundary extends to Hatteras Island in North Carolina. In the broad continental shelf, the depth is about 30~40 meters with a very gentle slope.

The vertical grid is Localized Sigma Coordinates with Shaved Cells (LSC$^2$). The feature of this coordinate is detailed in Chapter 2 and in the literatures (Zhang et al., 2015; Zhang et al., 2016). Essentially, it allows varying vertical layers depending on the local depth.
Figure 4-13. Model grid for the Chesapeake Bay and the adjacent continental shelf. The zoom-in subplot in the lower left corner shows the lower Chesapeake Bay of our interest. The calibration stations for water quality model are shown in red dots.
Figure 4-14 The bathymetry of the Chesapeake Bay. In the continental shelf, the open boundary is aligned along the 200-meter isobath.
4.3.2 Initial Condition

For hydrodynamics, we first interpolate HYCOM data (Bleck et al., 2002) to continental shelf. HYCOM data provide 4 variables: water temperature, salinity, elevation, and velocity. For the initial conditions, we use only temperature and salinity information at the beginning to year, and the elevation is set mean sea level as a still water. This is not a problem because SCHISM model can adjust very quickly to a reasonable condition for elevation and velocity. Inside the Chesapeake Bay, the initial conditions of temperature and salinity have a considerable influence on the horizontal and vertical distribution of temperature and salinity in the model, which is in turn determines the stratification as well as the gravitational circulation. However, the HYCOM data have a very coarse resolution inside the Chesapeake Bay and it is insufficient to represent the three-dimensional structures of temperature and salinity. Therefore, we utilize the observational data of salinity and temperature from the Chesapeake Bay Program (Mallonee and Ley 2012) which has several dozens of gauge stations on the horizontal. Each station provides vertical profiles of measurements for both temperature and salinity. We interpolate these data in the entire Chesapeake Bay. In this way, the three-dimensional structures are well approximated. With the full set-up, we first run the hydrodynamic model for one year to let the model adjusts itself sufficiently in estuary. The final state of the model is then saved for a new initial condition. This extra step is aimed to further increase the model accuracy. Figure 4-15 shows an example for surface and bottom salinity distribution in the Chesapeake Bay. As we can see, there is a difference in the vertical with higher salinity in the bottom water.
After the initial condition of hydrodynamics is available, we will incorporate the information from water quality monitoring data. Here, we combine two kinds of data to generate an initial condition for the water quality model. In the continental shelf, we use the field measurement data from Ocean Acidification Data Stewardship (OADS) Project. The data are collected in the Gulf of Maine, Georges Bank, and Mid-Atlantic Bight from 11/03/2009 to 08/19/2016. For more information about this dataset, one can visit the NOAA website: https://www.nodc.noaa.gov/oceanacidification/data/0127524.xml, which provides measurements on ammonia, silicate, phosphate, nitrite+nitrate, dissolved oxygen and other variables. This dataset is also used for the boundary conditions of the water quality model. Inside the Chesapeake Bay, we use the Chesapeake Bay Program measurement data which have abundant information for most of the water quality variables: CHLA, POC, PON, DON, NH4, NO23, POP, DOP, Si, DO. Similar to method in generating the initial conditions of temperature and salinity, we use interpolation method to obtain the initial conditions for the water quality model inside in the Bay. For those variables whose observational data are not adequate for the interpolation in the entire Bay, we approximate their initial conditions by relating the concentrations to some known variables. For example, DOC is not known and we use relationship
DOC=0.5×POC to estimate its initial concentration. This should be acceptable for initial conditions since the model will adjust later based on our forcing data such as the watershed loading.

After the water quality model is run for multiple years when quasi-equilibrium state is reached, the final state will be saved for initial condition. This step is necessary. Not only it provides a better estimation for the initial condition of the water quality model, but also it allows the sediment to reach a quasi-steady state. A reasonable sediment condition is critical because the sediment nutrient fluxes can influence many ecosystem processes in the water column.

4.3.3 Boundary Condition

In the model, there are two types of boundaries: river boundary and open ocean boundary. The specification of river boundary is relatively simple. Usually, we specify the river discharge along with the concentrations of the water quality model variables. At present, the river boundary condition is implicitly included in the watershed loading which contains river flows and nutrients loadings. The details of watershed loading will be discussed later. In this section, we will focus on the second type of boundary in the open ocean.

The hydrodynamic boundary condition includes the information about elevation, velocity, temperature and salinity. For temperature and salinity, we interpolate the HYCOM data for the ocean boundary. The outcome is a time series of vertical profiles of temperature and salinity. For elevation and velocity, we separate the information from HYCOM data into tidal and subtidal signals. The reason is that HYCOM date do not provide tidal signal which is important for modeling the hydrodynamics inside the Bay. In order to obtain the tidal signal, we first run a barotropic model with a large domain (thanks to the help of Prof. Joseph Y. Zhang). Figure 4-16 shows the model grid that covers the entire Mid-Atlantic Bight. The elevation and velocity information from the barotropic model are then filtered for the tidal signals. On the other hand, the subtidal signal is obtained by filtering the high frequency component of HYCOM
signals. The final step is to combine the tidal and subtidal signals for both elevation and velocity. In this way, we can get the full hydrodynamic boundary condition in the open ocean.

The boundary conditions of the water quality model in the continental shelf need information for all the water quality variables. Here we use the OADS data. However, the measurements are very patchy and scatter in space and time (shown in the upper panel of Figure 4-17). In order to get more information in time and space, we clustered all available data into one year. Then, interpolation is performed along the dimensions of depth and time, and the results are shown in the lower panels of Figure 4-17. The outcome is used to specify our model boundary condition. The assumption is that the boundary condition is uniform in space. Although the measurements are patchy, we can still see the general features of nutrients in the open ocean. It shows that NO3, PO4 and Si have much higher concentrations in the deep water than in the surface layer. This is consistent with the scientific consensus about the distribution of dissolved inorganic nutrients in the ocean.
Figure 4-16. A large domain grid for a barotropic model which is used to generate tidal boundary conditions for the Chesapeake Bay model.
Figure 4-17. Ocean boundary conditions for water quality model. The upper panels show the measurements of nutrients and DO at different depths from 2009 to 2015. The middle panels show all the data clustered in one year. The lower panels are the interpolation results in time and in the vertical direction. Note, the unit is mg/L for all variables.
4.3.4 The Watershed Loading

Watershed nutrient loading is important to an ecosystem. Too much nutrient input may cause eutrophication problem and can lead to harmful algal bloom conditions. To some extent, the nutrient load also determines the capacity of phytoplankton growth in the system. Watershed loading to the Chesapeake Bay is provided by Environmental Protection Agency (EPA), Maryland. This loading includes information about many water quality variables: temperature, chlorophyll, total carbon, organic nitrogen and phosphorus, dissolved inorganic nitrogen and phosphorus species, silicate and dissolved oxygen. EPA have their own watershed model and they simulate nutrient loading to the Chesapeake Bay based on drainage basins (represented by watershed segments). In each watershed segment, the water discharge associated with nutrient loading are modeled. Besides, both point source nutrient loading (eg. waste water treatment plant) and nonpoint source loading are provided. Because our model does not differentiate them, we combine these two types of information into one single loading input file to SCHISM model. Figure 4-18 shows the average flow rates and nutrient loading for 2012, 2013, 2014. On average, the total average flow rate to the Chesapeake Bay is about 1922 m³/s with maximum flow rate 2061 m³/s in 2014. The average organic carbon loading to the Chesapeake Bay is about $1.675 \times 10^6$ Kg/day; the average nitrogen loading is about $3.014 \times 10^5$ Kg/day; and the average organic carbon loading is about $1.930 \times 10^4$ Kg/day. Overall, the nutrient loading increases from 2012 to 2014. Total nitrogen increases around 39% from 2012 to 2014, while total phosphorus increases 42%. It is interesting that 2014 has the highest loading input among these three years, but almost no *C. polykrikoides* blooms are observed in this year. Therefore, the amount of nutrient loading is not a determinant factor for algal blooms in the lower Chesapeake Bay.

One technical issue in preparing the nutrient input files is how to distribute the nutrient loading from watershed into model domain. The easiest way is to put nutrient loading in some fixed grid points of element. Each point receives nutrient loading from the nearby watersheds. However, this method needs much manual input and is tedious, which cannot well represent the real situation on how nutrient is brought into estuary either. Therefore, we developed an automatic method in distributing nutrient loading by
mapping each watershed loading to certain model grids based on the drainage system and proximity between watershed and model grid. The related information about drainage basins is also provided by EPA. Figure 4-19 is an example on how watershed loading is partitioned in the James River. For a certain watershed (a polygon with a certain color), its nutrient loading as well as the water discharge are assigned to the nearby boundary elements of model grid. This method is tested and working well in our model.

Watershed loading provided by EPA includes the water discharge from both point sources and nonpoint sources. It also implicitly includes the river discharges. This means that our water quality model does not need to be specified with river boundary conditions. Rather, we can include the information on the river boundaries in our watershed loading inputs. The inputs include volume rate of water discharge and nutrient concentrations for all the water quality model variables. In this way, river boundary condition is prescribed implicitly in our model for both hydrodynamics and water quality. In contrast, in the past, the model must explicitly declare the river boundaries and specified the boundary values of all variables. Figure 4-20 is a comparison of flow rates between from watershed loading and from USGS gauge data. It shows that they are consistent in general, but the watershed loading has more temporal variabilities.
Figure 4-18. The annual mean watershed loading for watershed flow, total organic carbon (TOC), total nitrogen (TN) and total phosphorus (TP) to the Chesapeake Bay in 2012, 2013 and 2014.

Figure 4-19. A snapshot of the watershed loading distribution from watershed to model grid. Each polygon with a color represents an individual watershed and each triangle/quadrilateral represent a boundary element of model grid.
Figure 4-20. The comparison of river flow rates between from watershed loading and from USGS gauge data for seven major rivers in the Chesapeake Bay.

4.3.5 Atmospheric forcing

The atmospheric forcing includes wind, solar radiation, air temperature, precipitation rate and other atmospheric properties. Similar to the model simulation for Back River study in Chapter 2, we adopt the same method to prepare with atmospheric forcing. We use hybrid winds by blending NARR wind dataset and NDLC dataset, while use NARR data for other parameters.
4.4 Hydrodynamic Modeling Results

In this section, we present the results of hydrodynamic calibration. The calibration is done for 2012, 2013, and 2014 separately. Figure 4-21 shows the calibration stations for elevation and velocity. We selected 12 elevation stations inside the Chesapeake Bay. These stations spread from the upper Bay Station ‘Baltimore’ to Station ‘Chesapeake Bay Bridge Tunnel’ near the Bay entrance. There are four velocity calibration stations in the lower Bay that are used to verify the velocity field of the model.

4.4.1 Elevation Comparison

There are 3-year results for elevation. Here, we only show the results and analysis in 2012 and attach the results in 2013 and 2014 in the Appendix C for brevity. Figure 4-22 shows the comparison of subtidal elevation between model results (in red lines) and measurements (in blue lines). Overall, the modeled elevation matches the observation well at all stations. At the Station ‘Chesapeake Bay Bridge Tunnel’ around the Bay entrance, the range of subtidal elevation is below ±0.5m. It is evident that the elevation has an oscillation with period about 5-7 days. These quasi-weekly signals are well captured by the model, although sometimes the model underestimates the peaks. For example, there is a large elevation surge about 0.86 meter on October 28th, 2012 and the model successfully reproduces this event with a peak value about 0.67 meter. As we can see, the model performs well in the middle bay. In the upper bay, the general pattern from the model still matches the observation. However, the model seems to overpredict the elevation a little for Stations ‘Baltimore’ and ‘Tolchester Beach’. Though, the results are acceptable since the focus of our study is in the lower Bay. In order to evaluate the tidal components, we conduct a harmonic analysis and decompose the elevation data into tidal constituents. Figure 4-23 shows the amplitudes and phases of 5 major tidal constituents: O1, K1, M2, S2 and N2. The results are satisfactory in that model results are very close to observation for both amplitudes and phases. The major tidal constituent is M2 and its amplitude is about 0.4 meter in the lower Bay. The amplitude of M2 is smaller in the middle and upper bay with minimum about 0.13 meter in Station ‘Annapolis’. The amplitudes for the other 4 tidal constituents
are comparable, around 0.04-0.08 meter in the lower Bay. The tidal phases from the model also match well
the observation. From the lower panel of Figure 4-23, we can see that the progression of tide is obvious
with phase increasing from the lower Bay towards the upper Bay. Table 4-1 and Table 4-2 show the values
of amplitudes and phases along with the relative error of the model simulation. For the M2 amplitude, the
largest error is 38.48% at Station ‘Annapolis’, while the smallest error is achieved at station ‘kiptopeke’
with value 1.43%.

According to discussion above, our model elevation is well calibrated in 2012 for both subtidal and
tidal components. The results in 2013 and 2014 in the same format are attached in Appendix C from Figure
4-63 to Figure 4-66 and from Table 4-4 to Table 4-7.
Figure 4-21. Calibration stations for elevation and velocities.
Figure 4-22. The comparison of elevation between model and measurement in 2012. Tidal signal is filtered out and only subtidal signal is shown.
Figure 4-23. Water level comparison between model results (white bar) and measurements (black bar) for tidal constituents in 2012. Here we decompose the tidal signal of elevation into five constituents: O1, K1, M2, S2, and N2.
Table 4-1. Statistics for the amplitudes of tidal constituents in 2012. Both model results and measurements are shown for comparison.

<table>
<thead>
<tr>
<th>Station</th>
<th>Baltimore</th>
<th>Tolchester Beach</th>
<th>Annapolis</th>
<th>Cambridge</th>
<th>Solomons Island</th>
<th>Bishops Head</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1</td>
<td>0.0486</td>
<td>0.0448</td>
<td>7.81%</td>
<td>0.0483</td>
<td>0.0469</td>
<td>2.87%</td>
</tr>
<tr>
<td>K1</td>
<td>0.0581</td>
<td>0.0717</td>
<td>23.42%</td>
<td>0.06</td>
<td>0.076</td>
<td>26.80%</td>
</tr>
<tr>
<td>M2</td>
<td>0.1531</td>
<td>0.1657</td>
<td>8.22%</td>
<td>0.1688</td>
<td>0.1855</td>
<td>9.87%</td>
</tr>
<tr>
<td>S2</td>
<td>0.0229</td>
<td>0.0264</td>
<td>23.94%</td>
<td>0.0241</td>
<td>0.031</td>
<td>28.38%</td>
</tr>
<tr>
<td>N2</td>
<td>0.0324</td>
<td>0.0362</td>
<td>11.61%</td>
<td>0.0348</td>
<td>0.0405</td>
<td>16.41%</td>
</tr>
</tbody>
</table>

Table 4-2. Statistics for the phases of tidal constituents in 2012. Both model results and measurements are shown for comparison.

<table>
<thead>
<tr>
<th>Station</th>
<th>Lewisetta</th>
<th>Windmill Point</th>
<th>Yorktown</th>
<th>Kiptopeke</th>
<th>Swells Point</th>
<th>Ches. Bay Bridge Tunnel</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1</td>
<td>0.0152</td>
<td>0.0181</td>
<td>18.85%</td>
<td>0.0199</td>
<td>0.0187</td>
<td>6.06%</td>
</tr>
<tr>
<td>K1</td>
<td>0.0201</td>
<td>0.0321</td>
<td>59.96%</td>
<td>0.0278</td>
<td>0.0356</td>
<td>28.18%</td>
</tr>
<tr>
<td>M2</td>
<td>0.1839</td>
<td>0.1759</td>
<td>4.35%</td>
<td>0.1732</td>
<td>0.1765</td>
<td>1.92%</td>
</tr>
<tr>
<td>S2</td>
<td>0.0262</td>
<td>0.0297</td>
<td>13.32%</td>
<td>0.0302</td>
<td>0.0306</td>
<td>1.46%</td>
</tr>
<tr>
<td>N2</td>
<td>0.0372</td>
<td>0.0375</td>
<td>0.77%</td>
<td>0.0377</td>
<td>0.0392</td>
<td>3.99%</td>
</tr>
</tbody>
</table>
4.4.2 Velocity Comparison

There are four velocity calibration stations in the lower Bay: cb0102, cb0201, cb0402 and cb0601. ADCP measurements are available at these stations and the data are downloaded from NOAA website: https://www.co-ops.nos.noaa.gov/. At each station, a vertical profile of current speed is measured every 6 minutes with one-meter resolution in the vertical direction. Figure 4-24 shows the velocity comparison with observational data at Station cb0102. Velocities from the model result and observation are projected along the Bay channel direction. In the figure, the model result is instantaneous velocity and one-month result is shown. This is used to show that the model is capable of reproducing the 3D velocity filed. The velocity profile is plotted at depth from 3.52 meter in the near-surface to 20.52 meter in the bottom. In general, our model result matches the observation very well. For surface velocity, the amplitude and phase are both well captured by the model as well as some temporal variabilities. For example, in the first week of July (from July 1st to July 7th), the velocity amplitude is larger than that in the second week (from July 8th to 14th) and our model has reproduced this variation. In the vertical, the velocity magnitude decreases as deep increases. At depth of 19.52 meter, the velocity speed becomes relatively small where it is largely impacted by the bottom friction, our model simulation is still satisfactory in term of velocity amplitude and phase. In the bottom layer where depth equals 20.52 meters, both modeled and measured velocities approach zeros, which again validates the capability of the model in simulating the real situation. Furthermore, all velocity data in July 2012 are grouped into 4 categories: 0-5m, 5-10m, 10-15m and >15m and are plotted in Figure 4-25. The statistics are also shown in each subplot. In general, model skill for velocity is better in the surface layers than in the bottom layers. For surface layers (0-5m), it has a mean absolute error of 0.164 m/s and $R^2$ of 0.879, while it has a mean absolute error of 0.098 m/s and $R^2$ of 0.765 in the bottom layers (>15m).

In addition, results and statistics for the other three stations are shown in the Appendix C from Figure 4-67 to Figure 4-72. As we can see, these results are also satisfactory. It proves that the simulation of current velocity is accurate in the lower Bay.
4.4.3 Temperature and Salinity Comparison

Temperature and salinity are calibrated in the Chesapeake Bay and 11 stations in the lower bay are selected for comparison. There are 8 stations located in the main Bay (station names beginning with ‘CB’), 1 station in York River mouth (LE4.3) and 2 stations (LE5.4 and LE5.5) in James River mouth. Figure 4-26 shows the water temperature. The surface and bottom water temperatures are plotted along with observational data. As we can see, the model results match the observational data well. The water temperature is well simulated by the model, which captures the seasonal variation at every station. Note that there is a phase lag between bottom temperature and surface temperature. This is more evident during the spring and summer when the bottom temperature is constantly lower than the surface temperature, which is also captured by the model. Overall, the result is satisfactory.

Figure 4-27 shows the time series of the surface (green lines) and the bottom (red lines) salinities in the lower Chesapeake Bay. The salinity presents much temporal variabilities with a salinity range 10-25 ppt. Particularly, the modeled surface salinity changes very rapidly as it is the instantaneous output from the model with no filtering. The model captures the general patterns of salinity for both surface and bottom water, although it is overestimated at some stations. In estuarine, one important characteristics is the salinity stratification. Here, it is represented by the surface to bottom salinity difference shown in Figure 4-27. The salinity stratification is most prominent in the bay channel. For example, at station CB7.4, the bottom salinity is constantly higher than the surface salinity and the difference can be as large as 10 ppt. For all the main Bay stations, salinity stratification is well estimated by our model. In the river mouth, salinity stratification is also evident at Stations LE5.5-W and LE5.4 in James River mouth. The model overestimates the bottom salinity at Station LE5.5-W by several ppt, but the stratification pattern is clearly shown in the model result.
Figure 4-24. Velocity comparison at station cb0102 between model and observation in July 2012. At each depth, time series of Along Channel Velocity are shown for both ADCP measurements (blue line) and model result (red line).
Figure 4-25. Statistics for velocity at station cb0102 in 2012. Velocity data are grouped into four depth ranges: 0-5m (upper left), 5-10m (upper right), 10-15m (lower left) and >15m (lower right). In each subplot, three statistical numbers are shown: $R^2$, Mean Absolute Error (MAE) and Standard Deviation (STD).
Figure 4-26. Temperature comparison for 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) water temperatures are displayed with observation points (black dot).
Figure 4-27. Salinity comparison for 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) water salinities are displayed with observation points (black dot).
4.4.4 Upwelling off the Chesapeake Bay

Upwelling can happen in the coastal region off the Chesapeake Bay under southwesterly (SW) wind condition. At the same time, the SW wind also drops the water level at the mouth and increases the two-way flow exchange between bay and ocean by enhancing the near-surface outflows and bottom inflows (Valle-Levinson et al., 2001). One aspect of our hypothesis is that *C. polykrikoides* cysts could be transported into the Bay from the coastal ocean. This transport has two characteristics. First, cysts in the coastal ocean lies in the bottom water. This makes sense because cysts are deposited in the sediment and sediment resuspension may release them back to the water column. Second, cysts are transported within the bottom inflow current. Since SW wind can induce coastal upwelling and increase bottom inflows, it is plausible that cysts transported into the lower Bay can also be enhanced. To simulate the mechanism, it is necessary to see whether the model can reproduce the upwelling phenomenon.

In this part, we present the modeled temperature in the horizontal and in the vertical with focus on the upwelling and downwelling phenomena under different wind conditions. Figure 4-28 and Figure 4-29 show sea surface temperature (SST) for two periods in 2012: 1st period (from 2012-06-05 to 2012-06-20) and 2nd period (from 2012-07-15 to 2012-07-30). In each subfigure, daily averaged SST is compared with G1SST observation. For more information about G1SST, one can find more information on this website: https://podaac.jpl.nasa.gov/dataset/JPL_ourocean-L4UHfnd-GLOB-G1SST. Along with model result, time series of wind from 3 costal National Data Buoy Center (NDBC) stations are shown for the wind condition during each day. There are two major features for temperature. The first is that temperature is higher around the south boundary of our model, while it is lower in the north. The second is that the temperature inside Chesapeake Bay seems higher than the adjacent coastal ocean. We can see that the model captures these features well as compared with G1SST observation. Along the coastline, a general pattern we can see from Figure 4-28 and Figure 4-29 is that temperature changes with wind patterns. Under northeasterly wind (NE) wind, the surface water becomes cold. For example, NE wind blows in the period from 2012-06-14 to 2012-06-17 and the temperature decreases in the coastal ocean as shown in both model
and G1SST observation in Figure 4-28. By examining the patterns carefully, we can see that the NE wind pushes the surface water to the southern coast, which causes the downwelling of the nearshore water. On the other hand, SW wind condition induces upwelling. From 2012-07-15 to 2012-07-20, we can see that SW wind blows continuously as shown by the wind time series in Figure 4-29. During this period, the cool water emerges along the coastline outside of the Chesapeake Bay. This is evident along the southern coastline and less evident along the northern coastline. However, on July 19th and July 20th, 2012, we can see cool water appears in the broad regions along both coastlines, probably due to the persistent upwelling under SW wind. The upwelling phenomenon can also be identified in G1SST observation as well on July 19th and July 20th, but it is not as evident as in the model.

In order to see how wind influences upwelling and downwelling around the Chesapeake Bay mouth, we choose three transects near the Chesapeake Bay mouth as shown in Figure 4-30. The 1st and 3rd transects are perpendicular to the southern and northern coastlines, while the 2nd transect are from the coastal ocean to the Bay mouth. For each transect, its vertical temperature profile is shown in Figure 4-31, Figure 4-32 and Figure 4-33, respectively. In each figure, the daily average temperature in July is plotted for the corresponding transect. The x-axis is the distance to the shore in Figure 4-31 and in Figure 4-33, while it represents the distance to the Bay mouth in Figure 4-32. In addition, the corresponding time series of wind conditions at three separate NDBC stations (44009, chlv2 and 44014) are also shown during each day. In the upwelling period from 2012-07-15 to 2012-07-20 when SW wind blows, we can see that cold water slides towards the coastline along the sea bottom in Figure 4-31. At the same time, the surface isothermal lines curve up towards the ocean because cold water is upwelling along the coastline and pushing the surface warmer water parcels towards the ocean. The same variation can also be seen in Figure 4-33 in the northern part of coastal region. On the other hand, NE wind causes the opposite variations. For example, NE wind blows from 2012-07-10 to 2012-07-13 with strongest NE wind on July 11th and July 12th, and downwelling of costal water can be seen in both Figure 4-31 and in Figure 4-33. The variation is well represented by the downward movement of isothermal lines along the coastline. Therefore, SW/NE wind could induce
upwelling/downwelling around Chesapeake Bay mouth. Also, we noticed that the response of upwelling/downwelling to the wind is very quick and the time lag should be less than one day. For the 2nd transect, there is no coastline boundary at the end of transect. The upwelling/downwelling feature is less evident on the surface isothermal lines. However, the movement of bottom cold water under different wind condition is clearly seen in Figure 4-32. For example, in the SW wind period from 2012-07-15 to 2012-07-20, the progression of bottom water towards the mouth can be identified, which suggests that SW wind may enhance the bottom inflow current. On the other hand, the movement of bottom water is more evident in the NE wind period form 2012-07-10 to 2012-07-13. When NE wind blows, the bottom water slides down towards the ocean along the slope. In summary, all these variations of temperature patterns in Figure 4-32 are consistent with the upwelling/downwelling shown in Figure 4-31 and Figure 4-33. Basically, SW wind can induce bottom water movement towards the coastline or the Bay mouth (enhancing the bottom current), while NE wind has the opposite effect. The implication is that SW wind can advect bottom algal cysts towards the Bay mouth, while the bottom current can facilitate the cysts transport into the Bay.
Figure 4-28. Sea Surface Temperature comparison between model and G1SST observation from 2012-06-05 to 2012-06-20. In each subplot, model result is shown in the left with G1SST observation in the right. In addition, time series of wind from three coastal NDBC stations (44009, chlv2 and 44014) are shown along with the model result during each day.
Figure 4-29. Sea Surface Temperature comparison between model and G1SST observation from 2012-07-15 to 2012-07-30. In each subplot, model result is shown in the left with G1SST observation in the right. In addition, time series of wind from three coastal NDBC stations (44009, chlv2 and 44014) are shown along with the model result during each day.
Figure 4-30. Three transects are selected to show the vertical profiles of temperature.
Figure 4-31. Temperature profile along the 1st transect shown in Figure 4-30. The result is shown from 2012-07-01 to 2012-07-30 with wind time series at three NDBC stations (44009, chlv2 and 44014) in the lower left corner of each subplot.
Figure 4-32. Temperature profile along the 2nd transect shown in Figure 4-30. The result is shown from 2012-07-01 to 2012-07-30 with wind time series at three NDBC stations (44009, chlv2 and 44014) in the lower left corner of each subplot.
Figure 4-33. Temperature profile along the 3rd transect shown in Figure 4-30. The result is shown from 2012-07-01 to 2012-07-30 with wind time series at three separate NDBC stations (44009, chlv2 and 44014) in the lower left corner of each subplot.
4.5 Particle Tracking Simulation

In this section, we will introduce particle tracking experiments conducted in the lower Chesapeake Bay. Particles released at Bay mouth are used to simulate the transport of *C. polykrikodes* cysts and we will study how they are transported in the lower Bay under two wind conditions: SW wind and NE wind.

4.5.1 Results Under SW and NE Wind Conditions

In order to see the flow patterns under different wind conditions, we plot out the residual velocity in the lower Chesapeake Bay. Figure 4-34 and Figure 4-35 show the distribution of residual velocities at three depths: surface, 6-meter and 10-meter. In Figure 4-34, the mean velocity is computed based on the velocity results from 2012-07-15 to 2012-07-20 when SW wind blows. In Figure 4-35, the mean velocity is computed based on the velocity results from 2012-06-14 to 2012-06-19 when NE wind blows. Because the magnitude of surface residual velocities is much larger than these of the velocities at 6-meter and 10-meter depths, we use a smaller vector scale for the surface velocities in both Figure 4-34 and Figure 4-35. Under SW wind condition, the surface outflow is very strong as shown in the left panel of Figure 4-34. The SW wind pushes the surface water out from the James River and York River. Then, the surface water flows out of Bay and goes into the coastal ocean. However, at the middle and bottom depths, the residual flow presents a very different pattern when SW wind blows. Around the Bay mouth, inflow appears in the southern corner at lower depths and the inflow is strongest along the Bay channel. Because of the shallow depth in the northern part of Bay mouth, wind effect is dominant and no major inflow appears. Only limited inflow can be seen around the upper corner of Bay mouth where the depth becomes deeper (see Figure 4-14). Inside the Bay, we can see that the mean flow at lower depths generally follows the channels where one channel leads to James River and another channel leads to York River. In summary, under SW wind condition, strong surface outflow is accompanied with inflows at middle and lower depths. Under NE wind condition, we can see that the surface water is pushed by the winds into the Bay from the northern coastal ocean shown in Figure 4-35. However, the mean flow turns left outside of James River mouth after entering the lower Bay. Then, the mean flow goes out from the southern corner at the bay mouth. At 6-meter and
10-meter depths, this outflow is clearly seen. In addition, we can see the outflow outside the James River and York River. There is some surface inflow inside the James River and York River, but it is not evident. Therefore, around the bay mouth, it seems that the two-layer exchange flow is weakened under NE wind condition. However, along the bay channel towards the middle bay, the two-layer exchange flow seems enhanced because the channel direction is from the south to the north.

Based on the flow patterns described above, the easiest way for coastal algal cysts in the bottom water to enter the Bay is under SW wind condition. Figure 4-36 shows a particle tracking experiment under SW wind conditions. Particles are released on 2012-07-14 around the Bay mouth and in the areas with large depth. Also, particles are released in the near-bottom water. The distribution of the released particles is displayed for the following 11 days. In addition, the wind time series on each day is shown during each day. As we can see, SW wind blows in the first week and particles are transported into the Bay very quickly. Particles begin to enter James River after 3 days of particle releasing. After one week, many particles begin to enter the lower James River. However, it takes more time for particles to enter the York River. After one week of particle releasing, some particles get close to the mouth of York River and begin to enter the river on 2012-07-25. It is also interesting to notice that the ship channels act like high speed conduit for particle transport. This is due to the strong bottom current inside the channel. This experiment verifies our prediction that algal cysts can be transported into the James River and the York River along with the bottom currents under SW wind conditions. In contrast, we did an experiment by releasing particles in the water surface around the Bay mouth under SW wind conditions. Figure 4-37 is the result. It is obvious that particles are flushed out very rapidly instead of being transported into the Bay.

In order to see whether particles can be transported into the Bay under NE wind conditions, similar experiments are conducted by releasing particles in the near-bottom and near-surface on 2012-06-15 when NE wind blows. The results are shown in Figure 4-38 and Figure 4-39. In the first week with NE winds, most of particles are actually transported out of the Bay and into the coastal ocean no matter whether they are released in the near-surface or near-bottom. Only some particles enter the Bay when released in the
near-bottom through the channel to the York River. When NE wind stops and SW wind blows after 2012-06-20, some particles begin to move close the river mouths. However, there are still no particles entering the York River and very few particles entering the James River by the end of 2012-06-26.

As shown in Figure 4-11, algal blooms tend to happen when SW wind blows, but fewer blooms happen under NE wind conditions. Our particle tracking experiments show that *C. polykrikoides* cysts can be from the coastal ocean. Under SW wind conditions, it is easier for *C. polykrikoides* cysts to enter the lower bay compared to under NE wind conditions, which can partially explain why *C. polykrikoides* blooms tends to happen under SW wind conditions in the lower Bay. It shows that the most efficient way for *C. polykrikoides* cysts entering the Bay is to be transported along with the bottom current under SW wind conditions. On the other hand, NE wind condition does not favor the transport.
Figure 4-34. Residual velocity under SW wind condition in the lower Bay at three depths: 0m, 6m and 10 m.

Figure 4-35. Residual velocity under NE wind condition in the lower Bay at three depths: 0m, 6m and 10 m.
Figure 4-36. Particle tracking experiment from 2012-07-08 to 2012-07-25 with particles released under SW wind condition. Particles are released at Bay mouth in the near-bottom.
Figure 4-37. Particle tracking experiment from 2012-07-08 to 2012-07-25 with particles released under SW wind condition. Particles are released at Bay mouth in the near-surface.
Figure 4-38. Particle tracking experiment from 2012-06-19 to 2012-06-26 with particles released under NE wind condition. Particles are released at Bay mouth in the near-bottom.
Figure 4-39. Particle tracking experiment from 2012-06-19 to 2012-06-26 with particles released under NE wind condition. Particles are released at Bay mouth in the near-surface.
4.5.2 Some Statistics for Particle Tracking Simulation

Figure 4-40 shows the vertical profiles of current velocity and particles transport. As we can see the mean velocity in the near-surface is oceanward with the largest velocity about 6.5 cm/s. The actual outward surface velocity should be larger. It is interesting that the direction of mean velocity reverses at the depth around 6-meter and remains reversed all the way to the bottom. The largest landward velocity occurs at the depth about 11 meters with maximum velocity of 11.8 cm/s. In order to see how particles are transported in the vertical, an experiment is done by releasing particles at various depths with one-meter interval in the vertical at the Bay mouth. The left panel of Figure 4-40 shows the number of particles that can enter the James River after one week of releasing. Overall, the distribution is very consistent with the distribution of mean current speed and maximum number of particles can enter the James River when they are released around at the depth with maximum landward current speed.

Because algal cysts are present in the sediment and can be resuspended into the bottom water constantly, they can be constantly transported into the Bay. It is meaningful to see the temporal variation of algal cysts transport. Here, we do an experiment by releasing particles continuously at the Bay mouth from July to August and count the number of particles that enter the Elizabeth River after one week of particle releasing. Figure 4-41 shows the results for 2012. The upper panel is SW-NE wind component by low-pass filtering the time series of SW-NE wind. Similarly, the middle panel is low-pass filtered current speed at middle depth along the channel direction. The lower panel shows the statistics of particles that entered the Elizabeth River. Overall, a general consistence can be observed that the dominance of SW wind is accompanied with the dominance of landward currents and the pulses of particles entering the Elizabeth River. For example, from July 15th to July 21st in 2012, there is an apparent SW wind component. Then, a period of landward currents is observed with current speed above 0.1 m/s. On the other hand, NE wind is usually associated with small landward current speed or even oceanward current and the transport of particles into the Bay is largely depressed. The same experiments are done for 2013 and 2014 respectively and the results are attached in Appendix C in Figure 4-73 and Figure 4-74. The general conclusion drawn
from the result in 2012 also holds for 2013 and 2014. Table 4-3 shows the statistics for the number of particles that enter Elizabeth River for 2012, 2013 and 2014. We can see that most particles are transported into the Elizabeth River in 2012 and the fewest happen in 2014. Particularly, in the period from July 16 to August 15, particles that entered the Elizabeth River in 2014 are substantially less than the ones in 2012 and 2013. Again, this difference may partially explain why bloom disappeared in the lower Chesapeake Bay in 2014.

Table 4-3. Number of Particles that enter the Elizabeth River

<table>
<thead>
<tr>
<th>period</th>
<th>2012</th>
<th>2013</th>
<th>2014</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jul. 1-15</td>
<td>70</td>
<td>166</td>
<td>251</td>
</tr>
<tr>
<td>Jul. 16-31</td>
<td>484</td>
<td>274</td>
<td>148</td>
</tr>
<tr>
<td>Aug. 1-15</td>
<td>280</td>
<td>260</td>
<td>105</td>
</tr>
<tr>
<td>Aug. 16-31</td>
<td>51</td>
<td>67</td>
<td>74</td>
</tr>
<tr>
<td>Total</td>
<td>885</td>
<td>767</td>
<td>578</td>
</tr>
</tbody>
</table>
Figure 4-40. The left diagram shows the profile of mean velocity along the bay channel. The velocity data are from ADCP observation at station cb0102. The right diagram shows the number of particles that enter James River one week after the particles are released. In this experiment, particles are released in the near-bottom water at the Chesapeake Bay mouth.
Figure 4-41. The upper diagram is the time series of wind component along SW-NE direction in 2012. The wind observation data is from NDBC station cbbv2 with the high frequency signals filtered out. The middle diagram is the along channel current speed in 2012. The current data is from NOAA current station cb0102 with the high frequency signals filtered out. The lower diagram is the number of particles that enter the Elizabeth River from July 1st to August 31st, 2012. The number of particles is counted one week after the particles are released. In the experiment, the particles are continuously released in the near-bottom at the Chesapeake Bay mouth.
4.6 Water Quality simulation

In this section, we try to simulate the *C. polykrikoides* bloom in the lower Chesapeake Bay using our water quality model ICM coupled on SCHISM. The model has three phytoplankton species: diatom, green algae and cyanobacteria. Among them, cyanobacteria is a freshwater species. For more information, one can refer to Chapter 2 for detailed description about this model. Since the lower Chesapeake Bay belongs to polyhaline region, cyanobacteria should not be the dominant phytoplankton species. Therefore, we modified its biological behaviors in our model to simulate *C. polykrikoides*.

4.6.1 Incorporating the Features of *C. polykrikoides*

One important feature of *C. polykrikoides* is that it can uptake organic nitrogen, which provides it advantage at growth in the competition with other phytoplankton species. In order to simulate these characteristics, we allow *C. polykrikoides* to uptake dissolved organic nitrogen when inorganic nitrogen is depleted. In the water quality model, we add a parameter: organic nitrogen preference $P_{DON}$, to achieve this purpose (Shen et al., 2016a). Below are the expressions related to this parameter.

\[ P_{DON} = 1 - P_{DIN} \]  
\[ P_{DIN} = \frac{DIN \cdot DON}{(KHN_c + DIN)(KHN_c + DON)} + \frac{DIN \cdot KHN_c}{(DIN + DON)(KHN_c + DON)} \]  
\[ P_{NH4} = P_{DIN} \cdot PN_c \]  
\[ P_{NO3} = P_{DIN} \cdot (1 - PN_c) \]  
\[ PN_c = \frac{NH4 \cdot NO3}{(KHN_c + NH4)(KHN_c + NO3)} + \frac{NH4 \cdot KHN_c}{(NH4 + NO3)(KHN_c + NO3)} \]

where

- $P_{DON}$: preference for dissolved organic nitrogen ($0 \leq P_{DON} \leq 1$)
- $P_{DIN}$: preference for dissolved inorganic nitrogen ($0 \leq P_{DIN} \leq 1$)
- $P_{NH4}$: preference for ammonia nitrogen ($0 \leq P_{NH4} \leq 1$)
- $P_{NO3}$: preference for nitrite-nitrate nitrogen ($0 \leq P_{NO3} \leq 1$)
- $PN_c$: preference for ammonia nitrogen to nitrite-nitrate nitrogen ($0 \leq PN_c \leq 1$)
- $DIN$: dissolved inorganic nitrogen (mg[N]/L) and $DIN = NH4 + NO3$
**DON**: dissolved organic nitrogen (mg[N]/L)

**KHN_c**: half saturation constant for nitrogen uptake for *C. polykrikoides* (mg[N]/L)

Another important feature of *C. polykrikoides* is its swimming capability. It means that it can vertically migrate to obtain the optimal light condition during the daytime. During the nighttime, it can migrate downward to the places where the nutrient concentration maybe higher and the salinity is more favorable for its living. Park et al., (2001) reported a swimming speed of 3-4 m.h\(^{-1}\). Lim et al., (2014) mentioned that *C. polykrikoides* can swim at a speed of 1.4 mm.s\(^{-1}\) (over 100 m.day\(^{-1}\)). These speeds mean that *C. polykrikoides* can swim very fast compared with the depth inside the lower Bay. In the model, we use a smaller speed than the literature values and assume that *C. polykrikoides* has a swimming speed of 12 m/day (0.5 m.h\(^{-1}\)) and it begins to swim up at 6 am and begins to swim down after 6 pm.

Based on the past researches, *C. polykrikoides* has a small growth rate compared to other phytoplankton species which have growth rates normally larger than 1-2 day\(^{-1}\) in our water quality model. Kim et al., (2004) reported a growth rate about 0.4 day\(^{-1}\) for *C. polykrikoides* in Asian regions. However, in Atlantic regions, the growth rates are generally larger and can be as large as 0.9 day\(^{-1}\) (Yamatogi and Maruta 2002; Kudela and Gobler 2012; Fitzpatrick et al., 2014). Here, we apply a growth rate of 0.6 day\(^{-1}\) to *C. polykrikoides* in our model.

In addition, *C. polykrikoides* prefers high temperature and it usually blooms in the Chesapeake Bay when temperature is higher than 25 °C (Morse et al., 2013). Figure 4-42 shows the time series of chlorophyll concentration at Station LAF001.63 in the summer of 2012 and 2013. The air and water temperatures are superposed in the figure. As we can see, there is coincidence between temperature and chlorophyll concentration. For example, in the period from 2013-08-06 to 2013-09-20, high temperatures above 30 °C are often associated with high chlorophyll concentration. Therefore, it is very likely that high temperature plays a role in influencing the growth of phytoplankton. Also, Morse et al., (2013) mentioned that blooms tend to happen during the period of calm wind. On the other hand, there is a big uncertainty related to the growth rate of *C. polykrikoides*. Kudela and Gobler (2012) mentioned that the range for maximal growth rate can be fairly broad (factor of 2) for *C. polykrikoides*. By taking all these factors into our consideration,
we added a modulating function onto the growth rate of *C. polykrikoides* to represent the high temperature and low wind effect. The modulating function has a form:

\[
f(T) = \min \left( 1 + \alpha \cdot \frac{T_{\text{water}} - 25}{U_{\text{wind}}^2}, 2.0 \right)
\]

(4.6)

where \(T_{\text{water}}\) is the water temperature, \(T_{\text{wind}}\) is daily averaged wind speed, and \(\alpha\) is a coefficient to normalize. In this way, the high temperature effect on the growth rate of *C. polykrikoides* can be represented in our model. On the other hand, when wind speed is small, a thin thermal boundary layer may form which is suitable for *C. polykrikoides* to grow and accumulate. Figure 4-43 is an example showing the value of the modulating function during the period from June 2012 to September 2012.

In order to test our hypothesis, we place a *C. polykrikoides* cysts bed just outside of Chesapeake Bay mouth (Figure 4-44). In each year from 2012 to 2014, cysts are continuously released in this region from June. Also, we adopt a varying cyst concentration by relating it to upwelling index which is based on Ekman’s theory of mass transport due to wind stress. From June to October, the average cyst concentration in 2012 is 3.0 mg[C. polykrikoides]/L.

With the model adjustment above, we run our model separately for 2012, 2013, and 2014. The running speed varies on very different HPC clusters. In Hurricane cluster of Sciclone system, the College of William and Mary, it normally takes about 4 days to finish one-year simulation.
Figure 4-42. Time series of water temperature (black dashed lines) and air temperatures (black solid line) at Station LAF001.63 in the James River as well as the chlorophyll time series (red lines). Observations from July to September in 2012 (upper panel) and 2013 (lower panel) are shown.

Figure 4-43. Temperature modulating function on *C. polykrikoides* from June to September 2012.
Figure 4-44. Cyst bed (red region) for *C. polykrikoides*. From the June in each year, *C. polykrikoides* cysts are continuously released in the cyst beds.
4.6.2 Model Calibration

The calibration of the water quality model is done in the lower Chesapeake Bay. Eleven water quality monitoring stations (shown in Figure 4-13) are selected for comparison. In order to show the model performance, we include all the model results for the major variables. For simplicity, only five of them are presented in this section, while the rest of the results are attached in the Appendix C.

Figure 4-45 is the comparison for chlorophyll-a between model and observation. In this figure, model results from 2012 and 2014 are presented along with all the observational chlorophyll-a data available in the period. Generally, the model result has an evident seasonal variation that chlorophyll-a is high in summer and low in the winter. However, the model underestimates the spring blooms at many stations. Given that the focus of our study is about the *C. polykrikoides* blooms in the summer, this result is acceptable. Also, we can see that the concentration of bottom chlorophyll-a is comparable to the observation, but the surface chlorophyll-a concentration is usually overestimated along with much temporal variabilities.

Figure 4-46 shows the result for dissolved oxygen. Overall, the result is satisfactory. The model result matches the observational mean very well. Also, the model captures the seasonal variation of dissolved oxygen for all the three years and for both surface and bottom. In addition, the surface to bottom difference of dissolved oxygen is reproduced by the model. For stations that are in the north, there are some underestimation of surface dissolved oxygen and overestimation of bottom oxygen. For stations close to James River, the model performs better in matching the observation data as the surface to bottom difference is small.

From Figure 4-47 to Figure 4-49, total nutrient concentrations for nitrogen, phosphorus and silica are shown. The total nitrogen concentration is fairly constant with small seasonal and inter-annual variations. This feature is captured by our model, although there is overestimation for the surface concentrations at some northern stations. In the lower Bay close to James River and York River, the model result behaves well in term of mean concentration for both surface and bottom total nitrogen. However, the
model result overestimates the total phosphorus for most stations, especially for the stations in the north. In the lower Bay close the bay mouth, the model performance for total phosphorus improves and the discrepancy between model and observation is reduced. The comparison for total silica between model and observation is satisfactory. The model captures the mean concentration as well as the seasonal trends in each year. Overall, the calibration for total nutrients is acceptable except some small flaws.

The calibration for carbon species are shown in Figure 4-75 and Figure 4-76 in Appendix C. From Figure 4-77 to Figure 4-83, nutrient species for nitrogen and phosphorus are shown. For carbon species, model result match the observation and the mean is captured well for all the 3 years. For nitrogen, model results for particulate organic nitrogen, dissolved organic nitrogen, ammonia nitrogen and nitrite-nitrate nitrogen are presented. The model captures the mean concentration for all nitrogen species except that there is overestimation for ammonia and nitrate in the spring. It is hard for the model to capture the seasonal variation, but some variations are shown in the model result. For example, there is an evident seasonal variation of ammonia at Station LE4.3 and the model performs well in reproducing the changes. For phosphorus, model results for particulate organic phosphorus, dissolved organic phosphorus and phosphate are shown. In general, the model performs well in capturing the mean, but there is much errors associated with the results. In summary, there is discrepancy between model and observation in term of short-term variabilities. However, the model does well in capturing the mean variations. Given that there is a large uncertainty with the watershed loading and the complexity of biogeochemical processes in the water column, the calibration of nutrient species in our model is acceptable and the model is capable of capturing the general features for both nitrogen and phosphorus.
Figure 4-45. Calibration results for chlorophyll-a at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) chlorophyll-a are displayed with observation (black dot).
Figure 4-46. Calibration results for dissolved oxygen at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) dissolved oxygen are displayed with observation (black dot).
Figure 4-47. Calibration results for total nitrogen at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) total nitrogen are displayed with observation (black dot).
Figure 4-48. Calibration results for total phosphorus at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) total phosphorus are displayed with observation (black dot).
Figure 4-49. Calibration results for total silica at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) total silica are displayed with observation (black dot).
4.6.3 Simulation of *C. Polykrikoides* Blooms

This section focuses on the simulation of *C. polykrikodes* blooms. The purpose of this simulation is to verify our hypothesis that *C. polykrikodes* blooms are related to cyst transport, wind conditions and the unique biological features of *C. polykrikodes*. We want to investigate whether the model can reproduce the phenomenon about the *C. polykrikoides* blooms observed in the lower Chesapeake Bay. Particularly, many intense *C. polykrikodes* blooms were observed in 2012 and 2013, while almost none was observed in 2014. One major difference in 2014 from other years is that NE wind blows more frequently and SW is less frequent in this year as shown in Figure 4-9. We want to see whether this can account for the disappearance of *C. polykrikoides* blooms in 2014. At present, it is impossible to strictly compare the chlorophyll-a concentration from the model with the observational data because the model specification is still too simple to account for all the factors that are responsible for *C. polykrikoides* blooms. Therefore, we choose six diagnostic stations in the lower Chesapeake Bay to study the blooms. The six stations are shown in Figure 4-53. Among them, two (L1 and L2) are in Lafayette River; two (J1 and J2) are in lower James River and two (Y1 and Y2) are around York River mouth.
Figure 4-50. Stations selected to show C. polykrikodes blooms. There are two stations (L1 and L2) located in the Lafayette River, two stations (J1 and J2) located in James River, and two stations (Y1 and Y2) located in York River.

Figure 4-51 and Figure 4-52 are the time series of chlorophyll in James River in 2012 and 2013. The upper panel shows the observational data from Marshall and Egerton (2013). They are weekly measurements in James River covering the mesohaline and polyhaline of James River, Elizabeth River and Lafayette River. The lower panel is modeling result for daily chlorophyll maximum at 4 diagnostic stations in James River and Lafayette River. Results are shown only from July to September because C. polykrikoides blooms often appears in this period. After September, temperature drops and algal blooms crash rapidly. For all these results, large chlorophyll-a concentration is mainly attributed to the high concentration of C. polykrikoides. Other phytoplankton species (diatom and green algae) are only partially responsible for the total chlorophyll-a concentration. Figure 4-51 and Figure 4-52 describe the overall
variation of the *C. polykrikoides* blooms in the James River in 2012 and 2013 based on observational data and model. They are not strict station to station comparisons. However, we can see that *C. polykrikoides* blooms in James River are successfully reproduced by the model. The bloom magnitude from the model is comparable to the observed. In addition, the observation and model are consistent in that algal blooms appear mainly from July to September. The chlorophyll concentration is relatively small at the beginning of July and toward the end of September. Another feature is that the algal bloom in 2013 starts later than the bloom in 2012, which is also reflected by the model. For the modeling results, the algal bloom in 2013 last longer and are still present in the middle September. As we can see, it is not practical to directly compare model result with the observational data. First, the sampling of the observational data is sparse in time, which may miss some big blooms. Second, our model configuration is too simple to include all the factors that are responsible for algal bloom variabilities. Third, the locations of the model output are not consistent with the locations of the observational data. Even though, the model behavior is reasonable in term of catching the bloom timing and bloom magnitude.

Figure 4-53 shows the chlorophyll-a time series from the water quality model simulation in the Lafayette River. Surface chlorophyll-a at stations L1 and L2 is presented for 2012, 2013 and 2014. In each subfigure of Figure 4-53, we plotted out the daily maximum (red lines), daily mean (blue lines) and daily minimum (black lines). As we can see, large *C. polykrikoides* blooms appear in 2012. The chlorophyll-a concentration is high at both Station L1 and L2. The bloom in this year starts in early July and the daily maximum in the middle August can approach 300 µg/L. It is noted that daily minimum at L1 is much higher than that at L2. The daily minimum at L1 can maintain above 100 µg/L for most of the time, while the daily minimum at L2 is maintained around 50 µg/L in the whole summer. This is probably due to that station L2 is closer to Elizabeth River and is influenced more by the tidal flushing. In addition, the vertical migration of *C. polykrikoides* can also account for the large daily chlorophyll-a variation because the depth at L2 is larger than the depth at L1. In 2013, *C. polykrikoides* blooms are also shown in the model results. However, in this year, large blooms appear only at station L1, while bloom intensity at station L2 is much weakened.
In 2014, the C. polykrikoides blooms are terminated for the entire lower Chesapeake Bay except there are background perturbations for chlorophyll-a concentration at station L1. In Lafayette River, it seems that chlorophyll-a is generally higher at L1 than at L2.

Figure 4-54 is the chlorophyll-a time series at James River Stations J1 and J2 with the same format to Figure 4-53. It shows that algal blooms happen in 2012 at both stations. The daily maximum of chlorophyll-a concentration can exceed 100 µg/L. At station J1 and J2, large daily chlorophyll-a variation is presented and the daily minimum is around 20 µg/L for most of the time. Consistent with the blooms in Lafayette River, the algal blooms in lower James River start in July and last until middle September, but the bloom intensity is much weaker. For 2013 and 2014, however, no C. polykrikoides blooms appear in the model. The result in 2014 is consistent with the observational chlorophyll-a data, but the model result in 2013 needs more investigation.

Figure 4-55 is the chlorophyll-a time series at York River stations Y1 and Y2. Overall, the model results are similar to the results in James River. The model reproduced the algal blooms in 2012 as well as the disappearance of algal bloom in 2014. However, it fails to simulate any C. polykrikoides blooms in York River in 2013.

Overall, our simulation is able to reproduce 2012 bloom phenomenon observed in the Lower Chesapeake Bay as well as no bloom condition in 2014. For 2013, our simulation captures C. polykrikoides blooms only in Lafayette River, but fails to capture any blooms in lower James River and York River. It becomes clear to us that the ecology of C. polykrikoides bloom in the Chesapeake Bay entails a delicate balance between physical and biological processes, and both factors much work in unison for a bloom to occur. The present knowledge of the HAB ecology and its interaction with the coastal dynamics is not sufficient for us to develop a deterministic predictive tool yet. Despite that, the model results do show some success that the current model configuration can enable C. polykrikoides to bloom in the lower Chesapeake Bay. Thus, with needed improvement, it can serve as a working-progress tool to further study the C.
polykrikoides blooming dynamics particularly for 2013 condition. More observational data linking summer environmental conditions to the lower Bay blooms are also needed to verify the model.

Figure 4-51. Time series of chlorophyll in 2012 in James River. The upper panel is observational data form (Marshall and Egerton 2013) and the lower panel is model result at four diagnostic stations in James River. Note this figure is a general comparison for the overall chlorophyll variation in James, not a station to station time series comparison.
Figure 4-52. Time series of chlorophyll in 2013 in James River. The upper panel is observational data form (Marshall and Egerton 2013) and the lower panel is model result at four diagnostic stations in James River. Note this figure is a general comparison for the overall chlorophyll variation in James, not a station to station time series comparison.
Figure 4-53. Time series of chlorophyll-a at Lafayette River Stations from July to September. The left panels are for 2012, the middle panels are for 2013, and the right panels are for 2014.
Figure 4-54. Time series of chlorophyll-a at James River Stations from July to September. The left panels are for 2012, the middle panels are for 2013, and the right panels are for 2014.
Figure 4-55. Time series of chlorophyll-a at York River Stations from July to September. The left panels are for 2012, the middle panels are for 2013, and the right panels are for 2014.
As mentioned above, it is not practical to directly compare modeled chlorophyll-a with observational data. However, it is worth looking at the time series of the high frequency of chlorophyll-a concentration caused by *C. polykrikoides*. Figure 4-56 shows the time series of chlorophyll-a from the model (lower panel) at Station L2 along with the chlorophyll-a observation (upper panel) at Station LAF001.63 which is close to station L2. It shows that algal blooms happen mainly in July and early August. The model generally captures the timing of blooms. The observational data shows that the algal bloom crashes after middle August and the chlorophyll-a stays low in September. Our model also shows a quick drop of chlorophyll-a concentration in the late August, but it is higher than the observed. This rapid decrease of chlorophyll-a is probably related to the temperature drop in the later August. On the hand other, both model and observational data present many high frequency variabilities and a larger daily variation seems to be associated with the observational data. Figure 4-57 is a zoom-in picture for the time series from July 21st to July 30th in Figure 4-56. The model and observation are consistent in term of chlorophyll-a magnitude and the general patterns of daily variations. From the model result, we can clearly see the diel and semi-diel signals. Overall, the results from Figure 4-56 and Figure 4-57 indicate that our model can simulate the behaviors of *C. polykrikoides* as the model successfully reproduces the general patterns of observed chlorophyll-a.

Figure 4-58 and Figure 4-59 show the spatial distribution of surface chlorophyll-a simulated by the water quality model in the lower Bay. Two snapshots of surface chlorophyll-a are taken on July 15th and August 14th in 2012. On July 15th, the surface chlorophyll-a is slightly higher in lower James River and around York River mouth than in other areas. High chlorophyll-a concentration appears only inside Lafayette River suggesting the algal blooms there. On August 14th, large patches of algal blooms are observed in many places, especially in the James River. No bloom, however, appears in the York River. This reinforces the notion that the bloom conditions are the results of a delicate balance between the physical and biological processes.
Figure 4-56. Time series of chlorophyll-a at station L2 in Lafayette Rive from July to September in 2012. The upper plot is observation and the lower is model result.
Figure 4-57. Time series of chlorophyll-a at station L2 in Lafayette Rive from July 21st to July 31st in 2012. The upper plot is observation and the lower is model result.
Figure 4-58. Spatial distribution of surface chlorophyll-a on July 15th, 2012 in the lower Chesapeake Bay.

Figure 4-59. Spatial distribution of surface chlorophyll-a on August 14th, 2012 in the lower Chesapeake Bay.
4.7 Discussion

Chesapeake Bay is a typical partially mixed estuary with a strong two-layer gravitational circulation (Pritchard 1952; MacCready and Geyer 2010). The fresh water from the Susquehanna and Potomac Rivers accounts for the major buoyance and forms a surface layer of outflow, while the salty water from the ocean has a greater density and forms a bottom layer of inflow. This transport associated with the gravitational circulation has important implication on the ecosystem of tributaries in the lower Bay (Kuo and Neilson 1987; Kuo et al., 1991). In the lower James River, an tidal induced eddy system develops around Newport News points and there exists an strong upriver bottom transport (Shen et al., 1999; Shen and Kuo 1999).

At the same time, winds in the Chesapeake Bay and coastal zones have been recognized as an important factor that affects the estuarine circulation (Wang 1979a; Wang 1979b). It can influence the water circulation, modify the vertical mixing, affect the distribution of nutrients and thus must have an impact on the summer algal blooms (Weisberg et al., 2009). In the mid-Atlantic Bight, wind direction is also an important indicator for the distribution of surface water temperature: namely, northerly wind normally brings cool air, while the southerly wind brings hot air, resulting in the cooler or warmer temperature on the surface of the water. In addition, the wind is the main driver for inducing the upwelling/downwelling in the coastal ocean (Valle-Levinson et al., 2001; Wong and Valle-Levinson 2002; Valle-Levinson 2010). When NE wind blows, the water tends to pile up at the lower Bay as the result of Ekman effect from coastal ocean and local wind effect inside the bay. This will favor downwelling. In contrast, SW wind will favor upwelling. Also, SW wind can enhance the bottom landward current as discussed above.

Based on the particle tracking experiments under different wind conditions, SW wind is the most favorable condition for the transport of algal cysts from coastal ocean into the bay. The most efficient way in transporting cysts at the bottom is through the bottom inflow current. The bottom current speed is largest along the shipping channels, which also guides the fast transport of phytoplankton cysts. Seabornd (2008) reported that there are many types of algal cysts in the sediment in the Chesapeake Bay. Among them, *C. polykrikoides* is one of the major species. According to the upwelling patterns shown before, SW wind can
bring cysts toward the Chesapeake Bay mouth along with the bottom water. The particle tracking experiments prove that these cysts can then be transported into the lower Bay such as James River and York River. In this way, it partially explains why *C. polykrikoides* was widely spread in the lower Bay. Also, it explains why the *C. polykrikoides* blooms can happen inside both James River and York River. At the same time, this theory can partially explain why there are many *C. polykrikoides* blooms in 2012 and 2013, but almost none in 2014. This increase in 2012 and 2013, SW wind is more frequent and is favoring transport of *C. polykrikoides* cysts. In contrast, SW wind is less frequent and NE wind is dominant in 2014, which is not favoring the transport of *C. polykrikoides* cysts. Figure 4-60 is a sensitivity test representing an extreme case when there are no *C. polykrikoides* cysts in the coastal ocean, there are no cysts transported into James River from coastal ocean and no *C. polykrikoides* bloom occurs. Thus, chlorophyll-a concentration was low compared to the high chlorophyll-a concentration in the base case.

Furthermore, the water quality model simulation captured the general feature of *C. polykrikoides* bloom in the lower Chesapeake Bay. The model shows that *C. polykrikoides* can bloom in the lower James River, especially in Lafayette River, and around the York River mouth. The persistent and intense *C. polyrikoides* blooms in 2012 are well simulated, but the model underestimated some of the blooms in James River and York River in 2013. In addition, the model successfully captured the disappearance of *C. polykrikoides* blooms in 2014. These modeling results again verify our hypothesis about the origin of *C. polykrikoides* cysts from the coastal ocean. On the other hand, the model also shows that the biological features of *C. polykrikoides* are important. In our model, the chlorophyll-a can exceed 300 µg/L because *C. polykrikoides* can uptake organic nitrogen to support its growth. Otherwise, the depletion of dissolved inorganic nitrogen will limit its growth. At the same time, the swimming capability of *C. polykrikoides* allows it to obtain optimal growth easily. As a result, it outcompetes diatom and green algae in our model.

In order to model the *C. polykrikoides* blooms, it is necessary to take all these factors into consideration. Lastly, temperature plays a role in regulating the onset of *C. polykrikoides* bloom. The correlation between temperature and chlorophyll-a is clearly shown in Figure 4-42 and we adopt a modulating function of
Equation (4.6) to simulate this effect. Figure 4-61 shows a result of chlorophyll-a concentration in Lafayette River when this modulating function is taken off from the growth rate of *C. polykrikoides*. As we can see, the chlorophyll-a concentration is heavily reduced compared with the base case. As can be seen from Figure 4-42 and Figure 4-56, chlorophyll-a concentration was observed very high in Lafayette River in 2012. The modeling result without modulating function obviously underestimate the observation, whereas the base case with modulating function obtains a reasonable chlorophyll-a concentration. In order to study the effect of nutrient, Figure 4-62 shows a sensitivity test when the watershed loading in Elizabeth River is turned off. As a result, the chlorophyll-a was kept low all the summer. In this case, the growth of *C. polykrikoides* is controlled by the supply of nutrients.

![Daily CHLA Maximum at Station L2](Image)

Figure 4-60. Sensitivity test if no cyst are released in the coastal ocean. The base is shown in black line and the result with no cysts released is shown in red line.
Figure 4-61. Sensitivity test without temperature modulating function. The base is shown in black line and the result without temperature modulating function is shown in red line.

Figure 4-62. Sensitivity test if nutrient loading in Elizabeth River is turned off. The base is shown in black line and the result without nutrient loading is shown in red line.
4.8 Summary

In this study, the data analysis and numerical modeling experiments were conducted to investigate the harmful algal bloom of *C. polykrikoides* in the polyhaline of the Chesapeake Bay. The characteristics of *C. polykrikoides* bloom including its spatial distribution in the lower Chesapeake Bay and the temporal variation during 2012-2014 were first analyzed. In York River, it was observed that the *C. polykrikoides* bloom generally first started around the mouth of York River. We also observed that *C. polykrikoides* bloom suddenly disappeared in 2014, after continued bloom in each summer from 2005-2013, highlighting certain environmental factors may inhibit the bloom to occur. The James River discharge and precipitation in 2014 were examined and ruled out the causes. It was found, however, that the wind pattern in 2014 stood out in the record covering from 2000 to 2014 in that it has highest percentage of northeasterly wind and second lowest percentage southwesterly wind. Based on above observation, it is hypothesized that *C. polykrikoides* cysts are originated from the coastal ocean and are transported under the influence of wind, coastal upwelling and estuarine circulation. The southwesterly wind in particular has an important influence on its transport by increasing the bottom inflow, which facilitates the movement of cysts into the bay, especially into the James River. In the study, a SCHISM and ICM model was applied for the entire Chesapeake Bay and the adjacent continental shelf. The hydrodynamics in the lower Chesapeake Bay is first analyzed regarding velocity distribution and the coastal upwelling. Then, a series of particle tracking experiments were conducted by investigating the physical transport of *C. polykrikoides* cysts under different conditions. Finally, water quality model ICM is used to simulate the algal blooms caused by *C. polykrikoides* in the lower Bay. The biological features of *C. polykrikoides* such as its capability of active vertical migration, uptake of organic nitrogen and temperature-dependent growth rate, and the transport of cysts during upwelling events are all included in the modeling framework. The model can generate reasonable magnitude of the algal blooms in 2012, 2013 and simulate the no algal bloom condition in 2014. Both data analysis and numerical modeling indicate that air temperature and wind patterns play important roles in controlling the development of the blooms.
The numerical experiments suggest that the algal bloom of *C. polykrikoides* may start with cysts transported from outside of the Chesapeake Bay and initiate in many places where the nutrient supply and residence time are favorable to the algal growth inside the Bay. This new paradigm provides a mechanism for explaining the broad distribution of the *C. Polykrikoides* blooms in the lower Bay and also explain the sudden disappearance of algal bloom in 2014, which is due to the more frequent northeasterly wind, lower air temperature, and fewer upwelling events as a result of less frequent southwesterly wind.
Appendix D: Additional figures and Tables for Chapter 4
Figure 4-63. Elevation comparison between model and measurement in 2013. The tidal signal is filtered out and only subtidal signal is shown.
Figure 4-64. Elevation comparison between model and measurement in 2014. The tidal signal is filtered out and only subtidal signal is shown.
Figure 4-65. Water level comparison between model results (white bar) and measurements (black bar) for tidal constituents in 2013. Here we decompose the tidal signal of elevation into five constituents: O1, K1, M2, S2, and N2.
Figure 4-66. Water level comparison between model results (white bar) and measurements (black bar) for tidal constituents in 2014. Here we decompose the tidal signal of elevation into five constituents: O1, K1, M2, S2, and N2.
Table 4-4. Statistics for the amplitude of tidal constituents in 2013. Both model results and measurements are shown for comparison.

<table>
<thead>
<tr>
<th>Station</th>
<th>Baltimore</th>
<th>Tolchester Beach</th>
<th>Annapolis</th>
<th>Cambridge</th>
<th>Solomons Island</th>
<th>Bishops Head</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1</td>
<td>0.0463</td>
<td>0.0433</td>
<td>5.84%</td>
<td>0.0455</td>
<td>0.0445</td>
<td>2.27%</td>
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<tr>
<td>K1</td>
<td>0.0583</td>
<td>0.0675</td>
<td>15.75%</td>
<td>0.0601</td>
<td>0.0723</td>
<td>20.29%</td>
</tr>
<tr>
<td>M2</td>
<td>0.1534</td>
<td>0.1664</td>
<td>8.42%</td>
<td>0.1687</td>
<td>0.1857</td>
<td>10.09%</td>
</tr>
<tr>
<td>S2</td>
<td>0.0224</td>
<td>0.0278</td>
<td>24.44%</td>
<td>0.0238</td>
<td>0.0305</td>
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</tr>
<tr>
<td>N2</td>
<td>0.0314</td>
<td>0.0354</td>
<td>12.78%</td>
<td>0.0337</td>
<td>0.0391</td>
<td>15.84%</td>
</tr>
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</table>

Table 4-5. Statistics for the amplitude of tidal constituents in 2014. Both model results and measurements are shown for comparison.

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<th>Tolchester Beach</th>
<th>Annapolis</th>
<th>Cambridge</th>
<th>Solomons Island</th>
<th>Bishops Head</th>
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<tbody>
<tr>
<td>O1</td>
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<td>11.94%</td>
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<tr>
<td>K1</td>
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<td>0.0728</td>
<td>20.13%</td>
<td>0.0619</td>
<td>0.0769</td>
<td>24.33%</td>
</tr>
<tr>
<td>M2</td>
<td>0.1547</td>
<td>0.1681</td>
<td>8.69%</td>
<td>0.1698</td>
<td>0.1878</td>
<td>10.61%</td>
</tr>
<tr>
<td>S2</td>
<td>0.0213</td>
<td>0.0273</td>
<td>28.06%</td>
<td>0.0218</td>
<td>0.0291</td>
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<td>16.53%</td>
<td>0.0344</td>
<td>0.0412</td>
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Table 4-6. Statistics for the phase of tidal constituents in 2013. Both model results and measurements are shown for comparison.

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<th>Baltimore</th>
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<th>Annapolis</th>
<th>Cambridge</th>
<th>Solomons Island</th>
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<tbody>
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<td>Tidal Const.</td>
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<td>Model</td>
<td>Obs</td>
<td>Model</td>
<td>Obs</td>
<td>Model</td>
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<tr>
<td>O1</td>
<td>125.1</td>
<td>124.3</td>
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<td>121</td>
<td>-3.1</td>
</tr>
<tr>
<td>K1</td>
<td>351.5</td>
<td>346.6</td>
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<td>-7.2</td>
</tr>
<tr>
<td>M2</td>
<td>66.2</td>
<td>73.5</td>
<td>7.2</td>
<td>76.6</td>
<td>72.7</td>
<td>-3.9</td>
</tr>
<tr>
<td>S2</td>
<td>9.3</td>
<td>11.2</td>
<td>1.8</td>
<td>11.8</td>
<td>11.5</td>
<td>-0.3</td>
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<tr>
<td>N2</td>
<td>296.4</td>
<td>305.4</td>
<td>8.5</td>
<td>304.1</td>
<td>303.4</td>
<td>-0.7</td>
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Table 4-7. Statistics for the phase of tidal constituents in 2014. Both model results and measurements are shown for comparison.

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<th>Windmill Point</th>
<th>Yorktown</th>
<th>Ki科普ke</th>
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<th>Ches. Bay Bridge Tunnel</th>
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<td>Model</td>
<td>Obs</td>
<td>Model</td>
<td>Obs</td>
<td>Model</td>
</tr>
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<td>48.1</td>
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<td>361</td>
<td>7</td>
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<tr>
<td>K1</td>
<td>202.1</td>
<td>251.1</td>
<td>-11</td>
<td>209.9</td>
<td>206.6</td>
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<tr>
<td>M2</td>
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<td>7</td>
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<td>194.8</td>
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<td>125.8</td>
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<td>67.4</td>
<td>70.4</td>
<td>2.9</td>
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<table>
<thead>
<tr>
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<th>Windmill Point</th>
<th>Yorktown</th>
<th>Swells Point</th>
<th>Ches. Bay Bridge Tunnel</th>
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<td>Tidal Const.</td>
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<td>Model</td>
<td>Obs</td>
<td>Model</td>
<td>Obs</td>
</tr>
<tr>
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<td>2.3</td>
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<tr>
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Figure 4-67. Velocity comparison at station cb0201 between model and observation in July 2012. At each depth, time series of Along Channel Velocity are shown for both ADCP measurements (blue line) and model velocity (red line).
Figure 4-68. Velocity comparison at station cb0402 between model and observation in July 2012. At each depth, time series of Along Channel Velocity are shown for both ADCP measurements (blue line) and model velocity (red line).
Figure 4-69. Velocity comparison at station cb0601 between model and observation in July 2012. At each depth, time series of Along Channel Velocity are shown for both ADCP measurements (blue line) and model velocity (red line).
Figure 4-70. Statistics for velocity at station cb0201 in 2012. Velocity data are grouped into four depth ranges: 0-5m (upper left), 5-10m (upper right), and 10-15m (lower left). In each subplot, three statistical numbers are shown: $R^2$, Mean Absolute Error (MAE) and Standard Deviation (STD).

Figure 4-71. Statistics for velocity at station cb0402 in 2012. Velocity data are grouped into four depth ranges: 0-5m (upper left), 5-10m (upper right), 10-15m (lower left) and >15m (lower right). In each subplot, three statistical numbers are shown: $R^2$, Mean Absolute Error (MAE) and Standard Deviation (STD).
Figure 4-72. Statistics for velocity at station cb0601 in 2012. Velocity data are grouped into four depth ranges: 0-5m (upper left), 5-10m (upper right), 10-15m (lower left) and >15m (lower right). In each subplot, three statistical numbers are shown: $R^2$, Mean Absolute Error (MAE) and Standard Deviation (STD).
Figure 4-73. The upper diagram is the time series of wind component along SW-NE direction in 2013. The wind observation data is from NDBC station cbbv2 with the high frequency signals filtered out. The middle diagram is the along channel current speed in 2012. The current data is from NOAA current station cb0102 with the high frequency signals filtered out. The lower diagram is the number of particles that enter the Elizabeth River from July 1st to August 31st, 2013. The number of particles is counted one week after the particles are released. In the experiment, the particles are continuously released in the near-bottom at Chesapeake Bay mouth.
Figure 4-74. The upper diagram is the time series of wind component along SW-NE direction in 2014. The wind observation data is from NDBC station cbbv2 with the high frequency signals filtered out. The middle diagram is the along channel current speed in 2012. The current data is from NOAA current station cb0102 with the high frequency signals filtered out. The lower diagram is the number of particles that enter the Elizabeth River from July 1st to August 31st, 2014. The number of particles is counted one week after the particles are released. In the experiment, the particles are continuously released in the near-bottom at Chesapeake Bay mouth.
Figure 4-75. Calibration results for particulate carbon at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) particulate carbon are displayed with observation points (black dot).
Figure 4-76. Calibration results for dissolved organic carbon at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) dissolved organic carbon are displayed with observation points (black dot).
Figure 4-77. Calibration results for particulate organic nitrogen at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) particulate organic nitrogen are displayed with observation points (black dot).
Figure 4-78. Calibration results for dissolved organic nitrogen at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) dissolved organic nitrogen are displayed with observation points (black dot).
Figure 4-79. Calibration results for ammonia at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) ammonia are displayed with observation points (black dot).
Figure 4-80. Calibration results for nitrite-nitrate at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) nitrite-nitrate are displayed with observation points (black dot).
Figure 4-81. Calibration results for particulate organic phosphorus at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) particulate organic phosphorus are displayed with observation points (black dot).
Figure 4-82. Calibration results for dissolved organic phosphorus at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) dissolved organic phosphorus are displayed with observation points (black dot).
Figure 4-83. Calibration results for phosphate at 11 stations (shown in Figure 4-13) in the lower Chesapeake Bay. The surface (green line) and bottom (red line) phosphate are displayed with observation points (black dot).
**Chapter 5 Future Work**

In this study, we have investigated the algal blooms in the oligohaline and polyhaline regions of the Chesapeake Bay. Various methods are used to identify the blooming mechanisms in different areas. Overall, algal blooms are influenced by many factors including seeds, nutrients, physical transport, light, temperature and the biological features of bloom species. In Back River, we prove that nutrient (phosphorus) plays a key role in regulating the blooms. Furthermore, the theoretical study in Chapter 3 shows the importance of physical transport and origin of seeds (boundary condition). In the lower Chesapeake Bay, the *C. polykrikoides* blooms maybe attributed to the combination of biological features of *C. polykrikoides* and the transport of cysts under the influence of gravitational circulation and wind patterns.

However, the present work is far from covering all the factors that are responsible for the algal blooms in the Bay. Particularly, the experimental study in the lower Chesapeake Bay is an over-simplified diagnostic case and is far from complete. There are still many scientific and modeling questions that are needed to be considered in our future work.

1) Is it possible to apply the pH related positive feedback mechanism in other regions of the Chesapeake Bay to explain the local blooms? For example, in the Corcica River in the upper Bay, the chlorophyll concentration can be 500 μg/L and it is not explained yet.

2) In our study, the application of pH model focuses on the Back River. Can it be used for the entire Bay to explain the pH variation, such as the lower pH values in the bottom in the summer times?

3) The solution to Equation (3.1) can represent the key processes of phytoplankton in a well-mixed tidal freshwater river system. Can it be applied in other tidal freshwater river systems beside James River? Can it be applied in river system beyond tidal influence?
4) For the *C. polykrikoides* blooms in the lower Bay, only cysts from the coastal ocean are considered in our model. Is there a local source of the *C. polykrikoides* cysts? What is the role of the local source for algal blooms?

5) In this study, the progression of the *C. polykrikoides* blooms in the lower Bay is not well-investigated. There is a need to give out a detailed description of blooming progression.

6) In Chesapeake Bay, other phytoplankton species can also induce heavy blooms in the summer besides the *C. polykrikoides*. Is it possible to take them into our numerical model as well?

All these questions are important and need further investigation. They are, however, beyond the scope of the current work. I hope to continue working on them in my future endeavor to enrich our understanding about the algal bloom dynamics in the Chesapeake Bay.
References


Marshall, H. G. and T. A. Egerton (2013). "Assessing seasonal relationships between chlorophyll a concentrations to phytoplankton composition, biomass, and abundance, emphasizing the bloom producing algae (HAB and others) within the James, Elizabeth, and Lafayette rivers in Virginia."


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