

CLIMATE CHANGE AND ALGAL BLOOMS

By

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A DISSERTATION

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

Integrative Biology—Doctor of Philosophy

2017

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ABSTRACT

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Algal blooms are new emerging hazards that have had important social impacts in recent years.

However, it was not very clear whether future climate change causing warming waters and stronger storm events would exacerbate the algal bloom problem. The goal of this dissertation was to evaluate the sensitivity of algal biomass to climate change in the continental United States. Long-term large-scale observations of algal biomass in inland lakes are challenging, but are necessary to relate climate change to algal blooms. To get observations at this scale, this dissertation applied machine-learning algorithms including boosted regression trees (BRT) in remote sensing of chlorophyll-*a* with Landsat TM/ETM+. The results show that the BRT algorithm improved model accuracy by 15%, compared to traditional linear regression. The remote sensing model explained 46% of the total variance of the ground-measured chlorophyll-*a* in the first National Lake Assessment conducted by the US Environmental Protection Agency. That accuracy was ecologically meaningful to study climate change impacts on algal blooms.

Moreover, the BRT algorithm for chlorophyll-*a* would not have systematic bias that is introduced by sediments and colored dissolved organic matter, both of which might change concurrently with climate change and algal blooms. This dissertation shows that the existing atmospheric corrections for Landsat TM/ETM+ imagery might not be good enough to improve the remote sensing of chlorophyll-*a* in inland lakes. After deriving long-term algal biomass estimates from Landsat TM/ETM+, time series analysis was used to study the relations of climate change and algal biomass in four Missouri reservoirs. The results show that neither temperature nor precipitation was the only factor that controlled temporal variation of algal biomass. Different reservoirs, even different zones within the same reservoir, responded differently to temperature and precipitation changes. These findings were further tested in 1157 lakes

across the continental United States. The results show that mean annual algal biomass generally increased with annual temperature. Greater increase was found in lakes with more nutrients. Mean annual algal biomass generally decreased with annual total precipitation. In both the “low” and the “high” greenhouse-gas emission scenarios, mean annual algal biomass in lakes generally increased with climate change, and greater increases are predicted from the high emission scenario.

Keywords: climate change, algal bloom, remote sensing, machine learning

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ACKNOWLEDGEMENTS

I would like to express my sincere gratitude to my committee chair, Professor R. Jan Stevenson, who continually conveys the patience of a mentor, the intelligence of a discoverer, the integrity of a scientist, and the passion of a teacher. This dissertation is made possible by his persistent guidance.

I thank my committee members, Professor Jiaguo Qi, Professor David W. Hyndman, and Professor Stephen K. Hamilton, who helped me all the way from course selection to the proposal and completion of this dissertation. They are genuinely willing to help guide me to succeed in my career. I still remember the comment from Professor Hamilton during my comprehensive examination. He encouraged me not to give up pursuing a career in academia simply because that I was not fully comfortable in speaking English. It turns out that as he said, time would solve the problem. The feedbacks from the committee have greatly improved the quality of my dissertation. They polished my writing almost sentence by sentence, far exceeding my expectation.

Professor John R. Jones at University of Missouri kindly provided 28 years of reservoir data for my study. Professor Charles P. Hawkins at Utah State University shared his spatial data corresponding to the lakes sampled by the first National Lake Assessment. These data are the basis of part of my dissertation research, and I deeply appreciate their generosity. I thank Professor Bryan Pijanowski at Purdue University for providing land use projection data. I did not finally use the data in the dissertation, but his kindness is appreciated.

This research was funded by US Environmental Protection Agency (EPA) (Grant #: R835203). Thanks to the PI and co-PIs who spent a lot of time to pursue this funding and made it available to me. The group members in the project, including Dr. Nathan Moore, Dr. Sherry Martin, and Dr. Anthony Kendall, have offered useful comments on my dissertation research.

My friends Brad Peter, Dr. Linda Novitski, and Dr. Timothy Cefai improved the language in parts of this dissertation. Visiting scholar Tao Tang from China provided the idea of *gradient forest* in the atmospheric correction analysis. Di Liang at the Kellogg Biological Station inspired me on the watershed impacts of climate change. I am lucky to have a lot of great friends and colleagues who emotionally and intellectually supported me in this dissertation, and filled my life with beer, laughter, and joy. I cannot list them all here. Their help extended far beyond this dissertation.

Last but not the least, thanks to my father Jiatian Lin and my mother Wenfang Xie for their unconditional love.

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1 GENERAL INTRODUCTION

1.1 Algal blooms

1.1.1 Species

Algal blooms are abnormally large accumulations of algae in oceanic or fresh water. There are two commonly known kinds of harmful algal blooms: “red tides” and cyanobacteria blooms. Red tides are oceanic algal blooms, often dominated by a group of algae called Dinoflagellates. Harmful algal blooms in freshwater are usually dominated by blue-green algae (cyanobacteria). Dinoflagellates and planktonic cyanobacteria are microscopic algae. However, “green tides”—caused by green macroalgae (*Enteromorpha prolifera*, A.K.A. *Ulva prolifera*) — are newly emerging algal blooms such as those occurred in waters along China’s eastern coast. The largest green tide was reported in Qingdao, China in summer 2008, covering 1200 km² along the Qingdao coast, the location of the 2008 summer Olympic sailing regatta (Liu et al. 2009; Keesing et al. 2011). All the algal species that dominate in blooms are common species that only bloom in certain conditions (Van Dolah 2000; Roelke and Buyukates 2001).

1.1.2 Public health impacts

Some dominant algal species in blooms can release toxins that are linked to fish kills and seafood poisons (Falconer, Beresford, and Runnegar 1983). Some are nontoxic, but light-shading and the decay of algae can lead to depletion of oxygen that also kills fish, creating dead zones (Anderson, Glibert, and Burkholder 2002). Red tides and cyanobacteria blooms are usually toxicogenic, while green tides are not. Some other groups of algae, like euglenoids and marine diatoms, can also produce toxic blooms. Toxicogenic blooms may not always be toxic to animals or humans, depending on toxin concentration and consumer sensitivity. The same algal species can form a toxic or non-toxic bloom, depending on genetic strains and dominance/accumulation of the toxin producers. Algal toxins include neurotoxins, liver toxins, and contact irritant-dermal toxins (Carmichael 2001).

1.1.3 Economic and social impacts

Due to algal blooms, costs for toxin detection and treatment in drinking water have increased; fisheries resources are contaminated by algal toxins or even perish in dead zones; and beaches, rivers, and lakes are closed. The annual economic loss due to algal blooms in the United States was estimated as: \$37 million in public health, \$38 million in commercial fisheries, \$4 million in recreation and tourism, \$3 million in monitoring and management, and \$82 million in total per year in 1987-2000 (Hoagland and Scatasta 2006). In addition to direct economic loss, algal blooms can cause wider indirect social impacts such as litigation, legislation, political change, and related social movements. These indirect impacts are difficult to measure and usually not included in existing assessments, which mostly focus on economic costs (Lewitus et al. 2012). More and more public attention has been directed to the social impacts of algal blooms, especially after 2013 when the number of algal-bloom news stories started to increase (Figure 1-1). Several unprecedented events drew this public attention, showing that the water around us could be a hazard. For example, on August 2, 2014, about half a million of people in Toledo (Ohio, USA) were given notice that their tap water from Western Lake Erie might be toxic due to a harmful algal bloom of the cyanobacterium *Microcystis*. In summer 2015, unprecedented harmful algal blooms hit the U.S. West Coast, resulting in long-lasting closures of commercial and recreational fishing. In 2016, algal blooms in Florida (USA) caused a state of emergency in four counties. The Florida blooms started from an inland lake called Lake Okeechobee then stretched to the eastern and western coasts through rivers, shaping a big “Green Slime” across Florida.

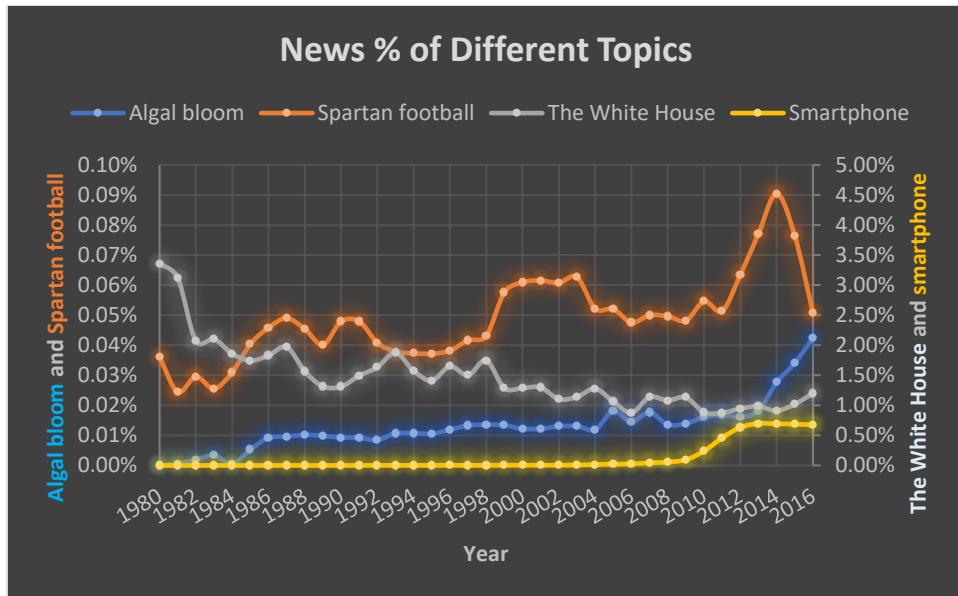


Figure 1-1 Time series of news in USA (1980-2016) that were related to algal bloom, Spartan football, the White House, and smartphone. News data were from the database NewsBank (<http://infoweb.newsbank.com>, accessed on Aug 30, 2016). The graph indicates an increasing trend of algal-bloom news. The other topics are used as references. News % = (news number of specific topic)/(total news count of each year).

1.1.4 Perceptions

Algal blooms are not a new phenomenon. They are part of nature, and have been recorded in the biblical and fossil records (Anderson 1997). What surprises us is the very recent proliferation of algal blooms (Anderson 1989). Algae usually grow faster in conditions of better light, enough nutrients, and suitable temperature. Any factor that creates a perfect combination of those conditions can trigger a bloom. For example, agricultural crop fertilization, more precipitation in spring, and long residence time of water were believed to cause the record-setting algal blooms in Lake Erie in 2011 (Michalak et al. 2013). In Taihu Lake (China), the main driver of algal blooms was identified as the nutrient loading (Huang et al. 2014). The triggers of algal blooms may vary lake by lake and the reasons behind the increase of occurrences remain debated (Sellner, Doucette, and Kirkpatrick 2003; Heisler et al. 2008).

The public blames mostly agriculture and extreme events to cause algal blooms as indicated by the news analysis of the NewsBank database (Figure 1-2). Climate change is also discussed by some scholars as a factor that is exacerbating the problem of algal blooms (Paerl and Huisman 2008), however this is debated in the scientific community (Reichwaldt and Ghadouani 2012; Lürling et al. 2013). More details about the relationships between climate change and algal blooms will be discussed in the following sections.

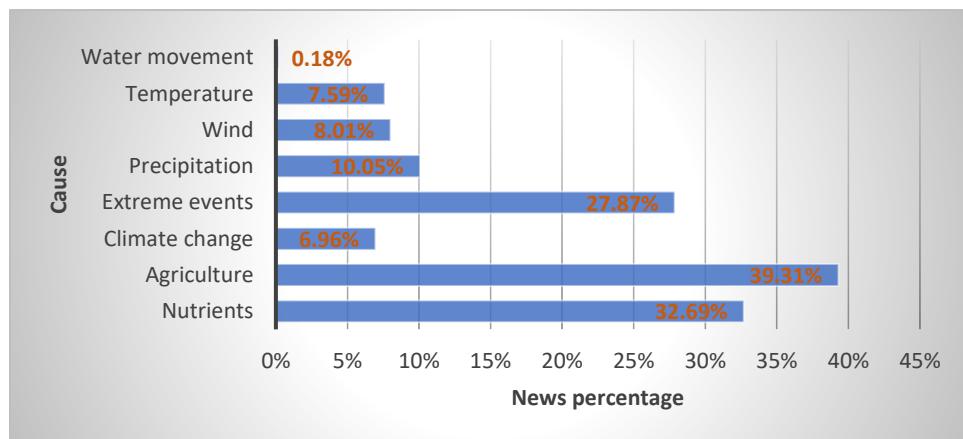


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1.2 Climate change

Climate change is predicted to manifest variably in different regions (IPCC 2014). According to the National Climate Assessment (Melillo, Richmond, and Yohe 2014), the US average temperature has increased 0.7-1 °C since 1895. Annual U.S. temperature is predicted to rise by 2-3 °C (the “low” emission scenarios, RCP 4.5) or 3-6 °C (the “high” emission scenarios, RCP 8.5) by the end of this (21st) century, compared to the level at the beginning of this century. Average US precipitation has increased in general

since industrialization, but some areas have increased more and some areas have decreased. Annual precipitation is predicted to increase in the northern US, but decrease in the southwest with climate change. Precipitation is predicted to change more in winter and spring than in summer and fall. The frequency and intensity of extreme precipitation events is predicted to increase in all areas of US. Droughts—indicated by the number of consecutive dry days—are predicted to increase over much of US.

1.3 Climate change impacts on algal blooms

The proliferation of algal blooms has triggered significant public attention and scientific investigation. However, the interactions between climate change and algal biomass occur in and are regulated by complex watershed systems. Therefore, the outcomes of algal abundance responding to climate change may vary greatly among individual lakes depending on other factors including watershed vegetation, watershed topography, soils, lake morphology and hydrology, internal nutrient sources, and food web interactions (Blenckner 2005). Paerl et al. (2008) argued that algal blooms, especially harmful cyanobacteria blooms, will increase with climate change based on some case studies (Paerl and Huisman 2008; Paerl and Huisman 2009; Paerl and Paul 2012). However, the evidence is not strong enough to represent a majority of lakes and the argument is more a hypothesis. For example, the Paerl and Huisman (2008) paper was published under the “perspective” category (not a research paper) in the journal Science. However, their theory (hereafter referred as “the Paerl theory”) is very popular and widely accepted in the scientific community (687 citations as of Feb 7, 2017, Figure 1-3). I randomly analyzed 44 of those publications that cited the Paerl and Huisman 2008 paper, 49% of them cited the Paerl theory with high confidence without using words like “predict”, “expect”, and “maybe” to imply the uncertainty of prediction. Only 32% of them cited the theory using words that indicated uncertainty.

In the Paerl theory, algal blooms increase with climate change mainly based on the following reasons:

- (1) Algal abundance may increase and surface-dwelling cyanobacteria may out-compete other species

when atmospheric CO₂ increases with climate change; (2) Algal abundance may increase and warm-adapted cyanobacteria may out-compete other species when temperature increases with climate change; (3) Algal abundance may increase and N-fixing cyanobacteria may out-compete other species when precipitation gets more variable with climate change, including more extreme events; (4) Other changes in water pH, water viscosity, water salinity, and lake stratification may also contribute to increased cyanobacteria blooms (Figure 1-4).

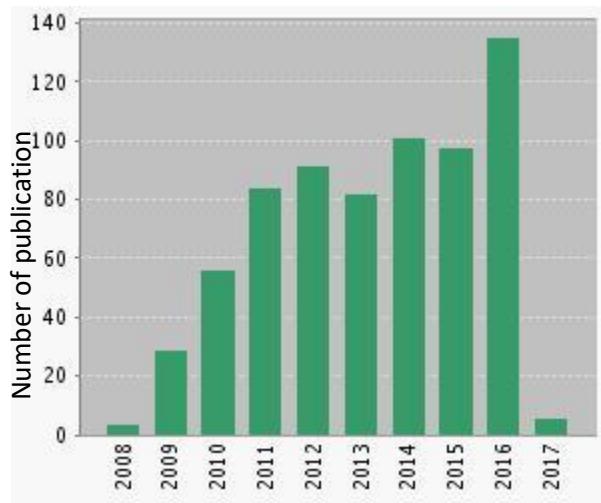


Figure 1-3 The number of publications (y-axis) that cite Paerl and Huisman (2008) changes over years (x-axis). Publications are those in the Web of Science Core Collection (<http://www.webofknowledge.com>) as of February 7, 2017. Total publication number = 687.

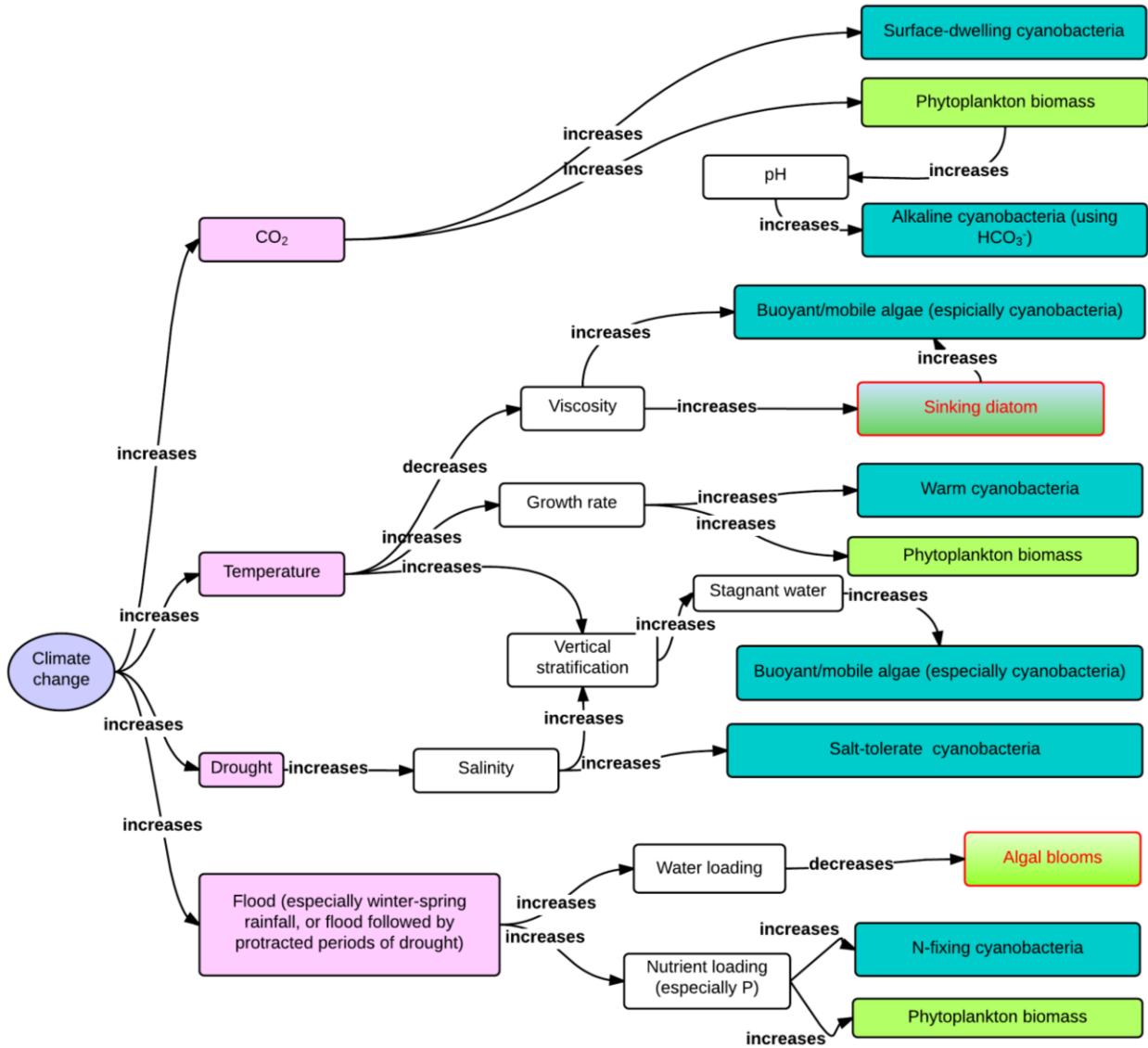


Figure 1-4 Possible pathways of climate change impacts on algal blooms. Summarized from Paerl and Huisman (2008). The red frame indicates a decrease of algal abundance due to climate change.

1.3.1 Temperature

Accumulated literature has cast doubt on the Paerl theory. After a more thorough literature review, Lürling et al. (2013) found that the optimal temperature for cyanobacteria species ($N = 62$) was not significantly higher than for green algal species ($N = 67$). Moreover, they found that the cyanobacteria growth rate at optimal temperatures was not significantly higher than that of green algae at their

optimal growth temperatures. They argued that higher growth rate due to higher temperature was not a major theoretical explanation for more harmful algal blooms in a warming climate. My preliminary analyses of the first National Lake Assessment data set (USEPA 2007) also indicated a weak relationship between lake surface temperature and algal biomass above about 20 °C (Figure 1-5), and that blue-green algae (cyanobacteria) did not necessarily dominate the algal community at high lake surface temperature, even when the nitrogen was limited favoring nitrogen-fixing species in cyanobacteria (Figure 1-6).

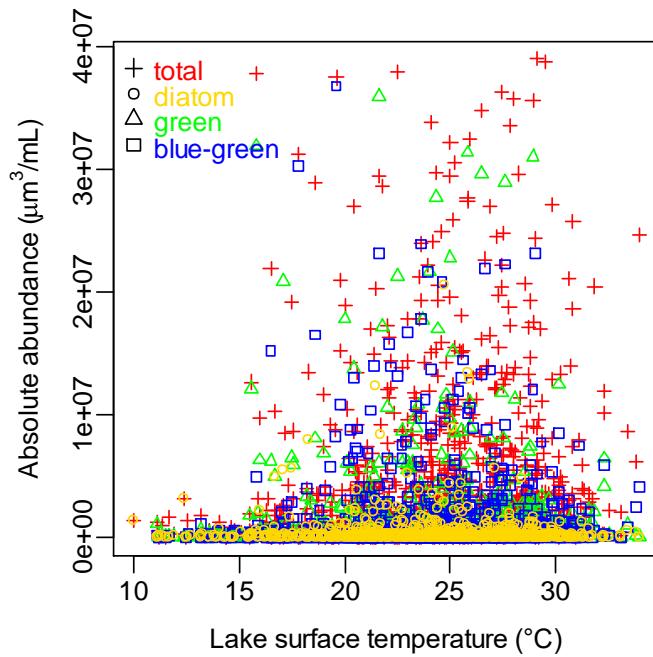


Figure 1-5 Absolute abundance (bio-volume) of algal divisions as a function of lake surface temperature.

Data source: U.S. EPA National Lake Assessment, 2007 (<http://www.usepa.gov>, accessed on Jan 20, 2014). Lake number = 1157. Figure indicates that algal abundance did not necessarily increase with temperature in the normal US summer range of about 20-30 °C. There might be other factors other than lake temperature controlling algal abundance.

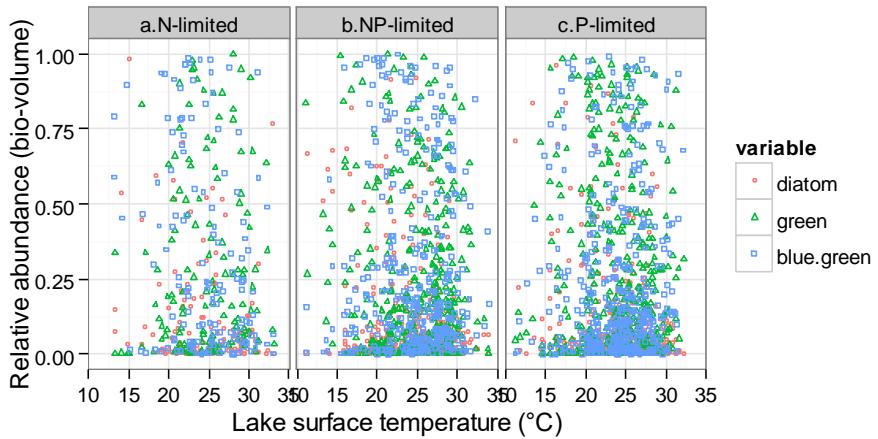


Figure 1-6 Relative abundance of algal divisions as a function of lake surface temperature and nutrient structure. Data source: U.S. EPA National Lake Assessment, 2007 (<http://www.epa.gov>, accessed on Jan 20, 2014). Nutrient limitation is defined by the molar ratio of total nitrogen (TN) to total phosphorus (TP): (a) N-limited, $TN:TP < 20$, (b) P-limited, $TN:TP > 50$, and (c) NP-co-limited, $20 \leq TN:TP \leq 50$ (Guildford and Hecky 2000). Figure indicates that when the lake surface temperature was high ($> 25^{\circ}\text{C}$), blue-green algae did not always dominate the algal community even when nitrogen was limiting relative to phosphorus.

1.3.2 Precipitation

Extreme precipitation events can carry more sediments and nutrients into lakes than other less intense events (McDiffett et al. 1989; Coser 1989). However, algal abundance may not change after extreme precipitation events due to a mismatch between nutrient availability and light availability (Minor, Forsman, and Guildford 2014). Precipitation events may dilute algal abundance in reservoirs and estuaries where algal accumulation is limited by flushing at short water residence times (Harris and Baxter 1996; Bouvy et al. 2003; Paerl et al. 2014). When precipitation frequency is high, the events may rinse nutrients from soils resulting in a decrease of algal abundance in rivers and lakes, showing an inverted relationship between total annual precipitation and algal abundance (Olson and Hawkins 2013;

Stevenson, Zalack, and Wolin 2013). Reichwaldt and Ghadouani (2012) reviewed literature on a wide range of lakes and commented that the Paerl theory is too simple for complex lake systems that respond to precipitation differently.

1.3.3 Watershed effects

Temperature and precipitation may change not only in-lake processes, such as algal growth and stratification, but also watershed processes, such as vegetation and soil properties (Davidson and Janssens 2006). For example, vegetation cover is predicted to increase with temperature in wet areas but decrease in dry areas (Breshears et al. 2005; Kardol et al. 2010). Watershed vegetation change may also affect nutrient availability in lakes (Kalbitz et al. 2000). The increase in evapotranspiration due to increasing temperature may neutralize the increase of precipitation (Chang, Evans, and Easterling 2001). When temperature and precipitation increase, more bioactive phosphorus may be released from soil to lakes due to more active bacterial activity, stronger ammonia nitrification, and lower soil pH (Stark and Firestone 1995; Post et al. 1982). The Paerl theory did not account for these watershed processes. Scholars are debating how climate change would affect soil properties such as soil organic matter (Davidson and Janssens 2006), and it is under-researched how climate change would affect algal abundance indirectly through changes in vegetation and soil properties.

1.4 Remote sensing of algal blooms

Algal abundance may change greatly over time and place even in the same lake, especially during periods of algal blooms (Yacobi et al., 1995). It is costly to use traditional ground methods to measure algal abundance for a period sufficiently long that it can be related to climate change. Remote sensors onboard satellites have routinely measured earth surface for decades. For example, eight satellites have been launched to continually observe the earth in the Landsat Missions since 1972. The newest one, Landsat 8, was launched in 2013, and Landsat 9 is planned to launched in 2020 (<https://landsat.usgs.gov>, accessed on Feb 8, 2017).

1.4.1 The theory of remote sensing

Chlorophyll- α is a common photosynthetic pigment of phytoplankton and its concentration is often used as a proxy of algal biomass. Remote sensing of algal abundance basically entails developing a relationship between remote sensing of reflectance from water surfaces and the chlorophyll- α concentration.

There are generally three steps to derive to chlorophyll- α concentration from the raw on-sensor digital number (DN) (Figure 1-7). Step 1, on-sensor DN values are converted to top of atmosphere reflectance (TOA) after geometric and radiometric corrections. Step 2, TOA is converted to surface reflectance (SR) after atmospheric corrections. Step 3, SR is related to chlorophyll- α using bio-optical models.

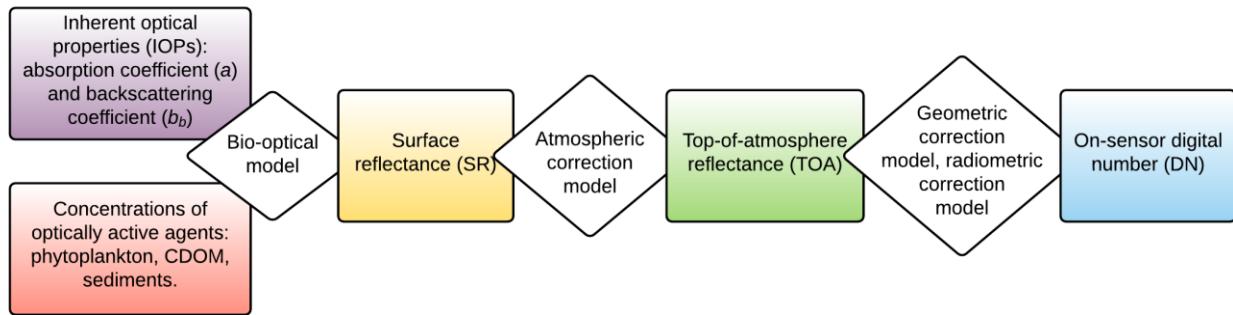


Figure 1-7 Analytical models to relate remote sensing signals to water constituents.

The bio-optical models are based on the relationship between SR and the inherit optical properties (IOPs) of water, *i.e.*, absorption coefficient $a(\lambda)$ and backscatter coefficient $b_b(\lambda)$:

$$SR(\lambda) = f\left(\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}\right)$$

where λ is the wavelength and f is used to simplify the relationship (Gordon et al. 1988). Each IOP, $a(\lambda)$ or $b_b(\lambda)$, is a function of constituent concentrations, such as algal pigments, sediments, and CDOM (colored dissolved organic matter). For example, in Case I water in which suspended sediments and

CDOM are low enough to assume it is zero, $a(\lambda)$ can be related to chlorophyll- a concentration (C) using the specific absorption coefficient, a_c^* , of chlorophyll- a :

$$a(\lambda) = a_w + a_c^* C$$

where a_w is the absorption coefficient of water (Bricaud et al. 1981). For Case II water, $a(\lambda)$ is not only contributed by water and phytoplankton, but also other constituents including CDOM, sediments, mineral chemicals, and other organic debris.

1.4.2 Remote sensing algorithms

Generally, either empirical or analytical approaches are used to derive chlorophyll- a concentration using remote sensing imagery. The analytical approach uses process-based models that include bio-optical models and atmospheric radiative transfer models to calculate chlorophyll- a or other water constituents from remotely sensed data (e.g., Dekker, Vos, and Peters 2002; Le et al. 2009). The empirical approach uses statistical regression techniques to directly relate remote sensing data to chlorophyll- a based on an experimental set of remote sensing and chlorophyll- a measurements (e.g., Brezonik, Menken, and Bauer 2005; Sudheer, Chaubey, and Garg 2006). Remote sensing data in the empirical approach could be the raw DN values with only geometric corrections, or SR with all corrections including radiometric and atmospheric corrections. The analytical approach is more complex than the empirical approach and requires the knowledge of IOPs. Both approaches rely on training data and field work, but the empirical approach usually measures fewer variables. The analytical approach has its physical limitation and it is sensitive to atmospheric corrections (Defoin-Platel and Chami 2007). Some studies also try to use semi-analytical approaches to simplify some processes in the analytical approach using empirical regressions in parts of the processes (e.g., Gitelson et al. 2008; Le et al. 2009). The analytical approach is expected to be more robust than the empirical approach, but in reality its transferability is as limited as the empirical approach because of the complexity of IOPs and the problematic atmospheric correction in turbid water

(see review of Matthews 2011). Therefore, chlorophyll- α algorithms for inland lakes are still constrained to a specific time and place. A new algorithm is required to relate climate change to historic remotely-sensed imagery in a large number of lakes.

1.5 Dissertation structure

In the ocean, harmful algal blooms were predicted to “become more frequent (limited evidence, medium agreement)” with future climate change (IPCC 2014). However, algal blooms in freshwater were not included in the climate change evaluation in that IPCC report, perhaps due to the lack of strong evidence of the climate change impacts. The overarching goal of this dissertation was to quantify the sensitivity of freshwater algal blooms to climate change. This study focused on inland lakes across the continental United States. I hypothesized that algal biomass in lakes increases with the higher temperatures that are predicted to occur by the climate models. I also hypothesized that more extreme precipitation events will amplify the temperature effects because more nutrients will be carried to the lakes by these events. Long-term whole-lake measurements of algal biomass in a large number of lakes were not available, so the analysis of climate effects on algal blooms was not possible with ground-measurements from water samples.

Given limitations in available data, this dissertation includes two steps to tackle these problems: Chapters 2 – 4 develop and test methods for remote sensing of algal blooms; and Chapters 5 – 6 analyze climate change impacts on algal biomass. Specifically, Chapter 2 introduces a machine-learning algorithm for remote sensing of algal blooms in inland lakes. Other color agents in water and atmospheric effects are two major classes of factors that affect the accuracy of inland-water remote sensing of algal biomass. Therefore, Chapter 3 evaluates the sensitivity of algorithms for remotely sensing chlorophyll- α (RS-Chl) to interference by sediments and CDOM (colored dissolved organic matter). Chapter 4 tests whether the existing atmospheric corrections in the standard USGS Landsat Surface Reflectance products have improved the algorithm performance. After developing the remote

sensing models and having the long-term whole-lake algal biomass data, Chapter 5 uses time series analysis to study the relationship between the climate change and algal biomass in four Missouri reservoirs. Chapter 6 uses the approach of space as substitution of time to evaluate climate change impacts on lakes across the continental United States. From Chapter 2 to Chapter 6, each chapter is prepared as an independent manuscript for peer-reviewed journals. Chapter 1 (this chapter) is a general introduction to the research topics, and it is not a thorough literature review. Chapter 7 (the last chapter) summarizes the findings and suggests some directions for future research. My dissertation findings fill an important gap in the assessment of how climate change will likely affect freshwater quality.

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2 MACHINE-LEARNING ALGORITHMS FOR CHLOROPHYLL-A MEASUREMENTS IN INLAND LAKES USING LANDSAT TM/ETM+

Abstract

Remote sensing of algae in inland lakes is challenging, and existing empirical models are limited to small areas and short application periods, where and when conditions of water and atmosphere are relatively the same. The goal of this study was to test algorithms that could be used to measure chlorophyll-*a* in lakes across USA using Landsat TM/ETM+ imagery. This study hypothesized that machine-learning algorithms (*i.e.*, boosted regression trees and random forest) could estimate chlorophyll-*a* concentrations from Landsat TM/ETM+ data when trained with ground-measured chlorophyll-*a* concentrations from the 2007 National Lake Assessment conducted by the US Environmental Protection Agency, predicting ecologically meaningful estimates of algal biomass for limnological studies. Results showed significant improvements in accuracy using the machine-learning algorithms, compared to traditional linear regressions. Specifically, the models using boosted regression trees and random forest could explain respectively 45.8% and 44.5% of chlorophyll-*a* variance. The model using multiple linear regression could only explain 39.8% of chlorophyll-*a* variance. Algal biomass maps derived from Landsat TM/ETM+ identified the spatial distributions and temporal duration of the 2009 algal bloom in Lake Erie. Compared to ground-measured algal biomass data, algal biomass measured by Landsat TM/ETM+ had a comparable accuracy in relation with lake total phosphorus concentrations. These findings enable long-term, large-scale, low-cost water quality observations for scientific research as well as environmental management.

Keywords: phytoplankton, Landsat, chlorophyll-*a*, boosted regression trees, decision trees, surface reflectance, remote sensing

Highlights

- Machine-learning algorithms are more accurate than traditional algorithms for estimation of chlorophyll- α concentrations from Landsat satellite observations.
- Landsat chlorophyll- α information can be used to identify algal bloom events.
- Landsat chlorophyll- α are correlated as well as ground-measured chlorophyll- α to phosphorus concentrations.

2.1 Introduction

2.1.1 Long-term large-scale measurement of algal biomass is needed

Algal blooms, especially involving toxic or otherwise harmful taxa, can cause severe problems for natural systems and human society (Hudnell, 2010). Droughts, heat waves, and floods have been predicted to increase with climate change (IPCC, 2014). Extreme floods, especially those after droughts, can introduce nutrients into downstream water bodies, creating conditions conducive to algal blooms (Paerl and Huisman, 2008). Long-term and large-scale observations of algae are needed to study the relationship between climate change and algal blooms. However, long-term field samples are usually limited to a small number of lakes, while large-scale surveys are limited to short periods. Remote sensing is a potential tool for global, long-term, and low-cost measurements of algal blooms. The overarching goal of this study was to develop and test a tool that can be used to produce long-term large-scale data of algal blooms from the large library of existing remote sensing images.

2.1.2 Remote sensing of algae in inland water bodies is challenging

Oceanic color products, including chlorophyll- α (Chl) concentration, are measured by remote sensors and have been available for public use for about two decades (<http://oceancolor.gsfc.nasa.gov/>, accessed on Sep 8, 2015). However, remote sensing of Chl in inland lakes is problematic because of the more variable optical characteristics, and particularly the presence of inorganic turbidity, and there is no

standard product available. Principal problems with Chl remote sensing in inland water bodies include the following: (1) Traditional atmospheric correction methods for oceanic clear water (Case I water) cannot be used in turbid water (Case II water) because suspended sediments violate the assumption of zero remote sensing reflectance at infrared wavelengths (Gilerson et al., 2010); (2) Relative atmospheric corrections such as dark-object subtraction are good for small areas where atmospheric conditions are similar to reference objects (Chavez Jr., 1996). For a large area over a long time, it is hard to pick reference objects that are assumed to have constant relationships with atmospheric effects; (3) Analytical algorithms are theoretically able to discriminate Chl from sediments and CDOM (colored dissolved organic matters), but they require inherent optical properties (IOPs) of water constituents, which change over time and place and are usually unknown without measuring them at a particular time and place (Dekker et al., 1997); (4) Semi-analytical algorithms indirectly estimate IPOs using reflectance relations between bands or band ratios and their accuracies are also limited by the atmospheric corrections (Carder et al., 1999); (5) Inland lakes require high spatial resolution because they are small, but sensors with high spatial resolution often have low spectral resolution – indicated by band number and width – which limit algorithm development. For example, algorithms based on red and infrared bands, such as the fluorescence line high (FLH) method, have shown promising results in turbid water with less impact of sediments and lake bottoms than traditional algorithms using blue and green bands (Gower et al., 2005, 2004) However, the FLH algorithm requires at least two bands within the wavelength range of fluorescence curve so FLH can be calculated. That requirement can be met by using MERIS (MEdium Resolution Imaging Spectrometer) and MODIS (Moderate Resolution Imaging Spectroradiometer), but they have spatial resolutions of 0.25 - 1.2 km which may be too coarse for inland lakes. Thematic Mapper (TM) and Enhanced Thematic Mapper Plus (ETM+) onboard Landsat have good spatial resolution (30 m), but they have only one red band and one near infrared band, which are not sufficient for the FLH algorithm.

Due to these limitations, no remote sensing algorithm has been developed and successfully used for large-scale study of inland lakes, such as all lakes of the continental United States or a decades-long history of remote sensing images. Most algorithms in turbid waters are empirical (see review by Matthews, 2011). Empirical algorithms utilize statistical relationships between remote sensing reflectance and concentration of water constituents. For a small area, such as one lake, model R^2 could be as high as 0.8 even if model input data are raw digital numbers of Landsat without radiometric and atmospheric corrections (Brezonik et al., 2005; Brivio et al., 2001; Carpenter and Carpenter, 1983; Dona et al., 2014; Rodríguez et al., 2014). However, these models are generally not transferable to new locations and periods. For example, models were suggested to be developed by zones in an area as large as Minnesota (USA) (Olmanson et al., 2008).

2.1.3 Objective and research questions

With accumulated data collected over time, machine-learning algorithms have received more and more attention in the age of big data (Olden et al., 2008). Machine-learning algorithms can reveal hidden patterns in large or complex data to enable better predictions. Machine-learning algorithms include decision tree learning, artificial neural networks (ANN), support vector machines, Bayesian networks, and genetic algorithms. For remote sensing of turbid water, better performance have been reported using machine-learning algorithms such as ANN (Sudheer et al., 2006) and genetic algorithms (Chen et al., 2008) compared to traditional linear regressions. However, the algorithms were only tested in individual lakes, and the performance has not been tested across large areas and long periods.

The objective of this study was to find a reliable and practical algorithm for long-term (decadal) and large-scale (continental) observation of algal biomass in inland lakes with Landsat TM/ETM+. We hypothesized that machine-learning algorithms would be able to improve algal biomass estimation from remote sensors compared to multiple linear regression (MLR) as well as non-linear general additive models (GAM). To test this hypothesis, two of the most commonly used and mature machine-learning

algorithms were chosen for testing: boosted regression trees (BRT) and random forest (RF). BRT builds trees consecutively, with later trees built to reduce errors of the former tree. Trees in RF are built in parallel. Each tree is built to explain a random subset of the sample with a random subset of independent variables. RF was of special interest because the algorithm had a built-in function in Google Earth Engine that could be used to efficiently process remote sensing imageries. Most empirical Landsat models are based on MLR. GAM was included to test whether non-linear algorithms could improve algorithm performance without using machine-learning algorithms. Our study was designed to answer two specific questions:

- Are machine-learning algorithms—BRT and RF—better than MLR and GAM for remote sensing of algal biomass in a large number of lakes using Landsat TM/ETM+?
- Is the accuracy of the machine-learning algorithms ecologically meaningful for lake assessments?

2.2 Methodology

2.2.1 Model comparison

2.2.1.1 Model data

2.2.1.1.1 Ground-measured water quality data

Ground-measured water quality data were obtained from the first National Lake Assessment (NLA) in 2007 (<http://water.epa.gov>, accessed on Jan 20, 2015). The NLA dataset included 1252 water samples from 1157 lakes, *i.e.*, 8% of lakes were revisited. Samples were collected during May to October of 2007. Lakes were selected randomly for the NLA with the intent that the sample of lakes would represent all inland lakes in the continental United States. Lakes also met the criteria that they had areas greater than 10 acres (0.004 km^2) and depths greater than 1 m (Figure 2-1). Measurements included chlorophyll-*a* (Chl) and total phosphorus (TP).



Figure 2-1 Chlorophyll-*a* (Chl) concentration in the first National Lake Assessment sample sites.

2.2.1.1.2 Remote sensing data

This study used Landsat Land Surface Reflectance products (<http://landsat.usgs.gov>, accessed on Apr 4, 2015), generated from the Landsat Ecosystem Disturbance Adaptive Processing System, where the MODIS land surface architecture was used to remove atmospheric effects (Masek et al., 2006). More specifically, the 6S (Second Simulation of a Satellite Signal in the Solar Spectrum) atmospheric correction model (Kotchenova et al., 2006; Vermote et al., 1997) was run to generate a look-up table accounting for the atmosphere pressure, water vapor, ozone, and geometrical conditions. Aerosol optical thickness was estimated using the dark dense vegetation method (Kaufman et al., 1997). The data were downloaded from the on-demand ESPA Data Access Interface (<http://espa.cr.usgs.gov>, accessed on Apr 3, 2015). The products were “provisional” and under evaluation at the time of downloading (April 3, 2015).

Ideally, we would have satellite images with the same dates and times as ground measurements. However, the Landsat revisit period was 16 days, so the odds of having an image on the same date as the ground sampling was low, even if cloudy pixels were not excluded. The study in Minnesota lakes showed that water clarity correlated the most with TM reflectance on the same day, but the correlation between water clarity in TM reflectance only decreased slightly when comparing measurements separated by one day ($R^2 = 0.86$) and seven days ($R^2 = 0.72$) (Kloiber et al., 2002). Similar results were found in Wisconsin: the correlation between water clarity in TM reflectance only slightly decreased from $R^2 = 0.82$ (1-3 day separation) to $R^2 = 0.75$ (4-7 day separation) (Chipman et al., 2004). In this study, to ensure as many data pairs of ground and satellite data as possible, we picked both TM and ETM+ images that were close to but not separated by more than 8 days before or after the ground sampling dates.

Mean values of multiple pixels could remove some signal noise and improve image signal-to-noise ratio (Kloiber et al., 2002; Ma and Dai, 2005). Therefore, we used a 3-by-3-pixel window from TM/ETM+ images surrounding the sample site to calculate a mean pixel value for bands and band ratios. Each location was checked to make sure all pixels in the 3-by-3-pixel window were pure pixels of water. If a sampling point was too close to the shoreline, its location was slightly adjusted with distances less than 100 m so the corresponding image pixels were water. Gaps due to the scan line corrector failure on ETM+ were excluded.

2.2.1.1.3 Data screening

Image pixels with surface reflectance (SR) < 0 were excluded as abnormal values. Image pixels with SR $> 15\%$ indicated cloud cover and were excluded. Image pixels with Band 2 $<$ Band 4 were excluded to remove pixels of land and cloud shadows on water. Surface reflectance of water is normally less than 15% and with band 2 $>$ band 4, even for waters with very high Chl and sediment concentration (Han, 1997; Rundquist et al., 1996). This image screening procedure, *i.e.*, removing pixels with SR < 0 , or SR $> 15\%$, or Band 2 $<$ Band 4, was able to remove land, cloud, and most cloud shadow pixels.

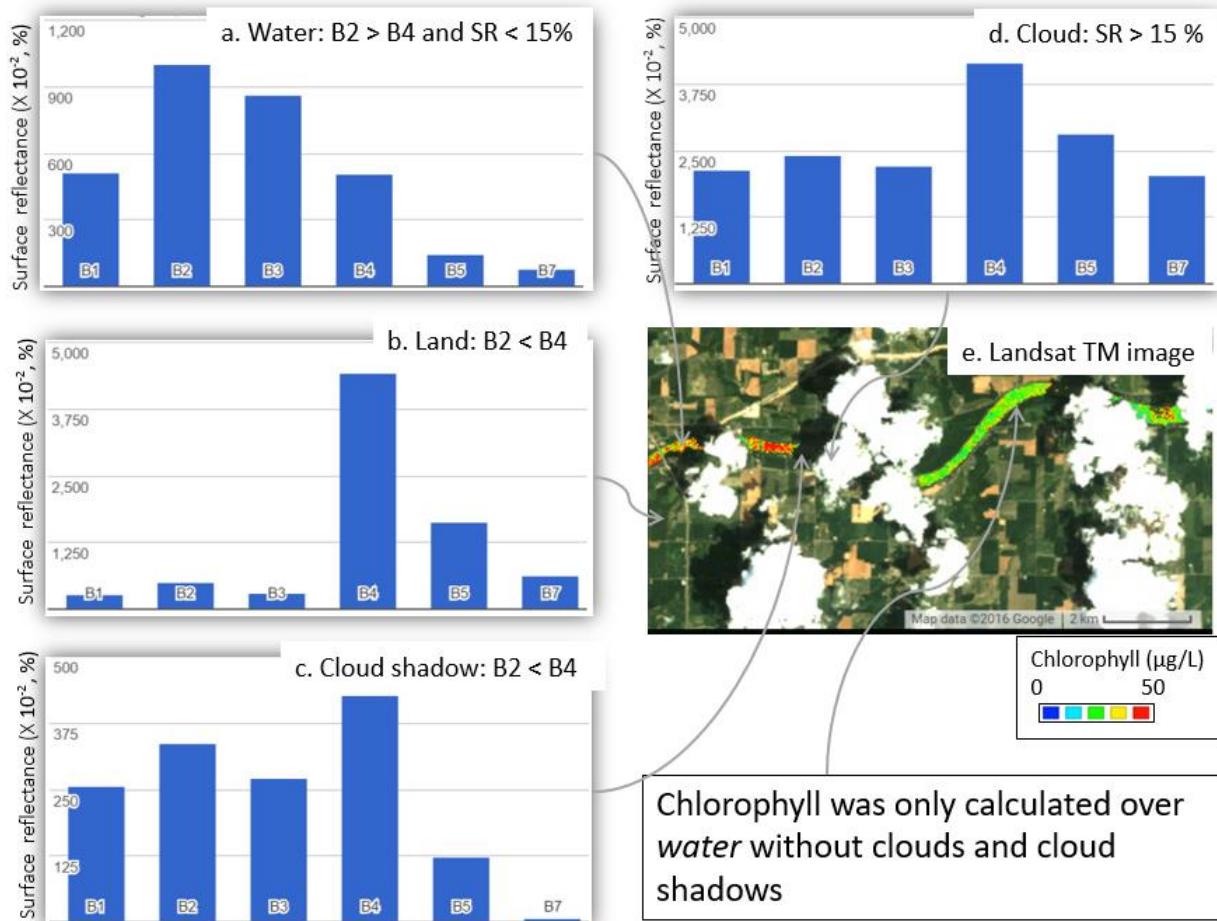


Figure 2-2 Chlorophyll-*a* (Chl) concentration of Maumee River (part) in Ohio (USA) as an example of data screening results. Band reflectance (B1-B5, and B7) of (a) water, (b) land, (c) cloud shadow, and (d) cloud, whose locations are indicated on (e). (e) Chl map overlaid on Landsat 5 Surface Reflectance (SR) image.

For demonstration purpose, Figure 2-2 shows the reflectance characters of water, land, cloud shadow, and cloud in a Landsat TM image over Maumee Rive (OH, USA). After applying the screening criteria, Chl was only calculated over water without clouds and cloud shadows. To avoid pseudo-replication, only one visit of revisited lakes was kept for the model development. After data screening, we had paired satellite and ground measurements in 483 lakes covered with 383 Landsat images. Chl ground measurements in the final dataset ranged from 0.07 to 349.2 $\mu\text{g/L}$, with the mean = 22.2 $\mu\text{g/L}$.

2.2.1.2 Model performance comparison

Models were developed with four different algorithms, *i.e.*, multiple linear regression (MLR), general additive models (GAM), boosted regression trees (BRT), and random forest (RF). Precision of model performance was characterized by 10-fold cross validation. Specifically, the dataset was split into 10 lake groups. In each cross-validation step, one of the lake groups (1/10 of the data) was withheld for validation and the other nine lake groups (9/10 of the data) were used for model calibration. This cross-validation step was repeated nine times with each of the other nine lake groups withheld from model calibration at separate times. This provided independence between the datasets used for model calibration and model testing. Model performance was characterized by the Nash–Sutcliffe model efficiency coefficient (NSE).

$$\text{NSE} = 1 - \frac{\sum_1^i (y_i - \hat{y}_i)^2}{\sum_1^i (y_i - \bar{y})^2}$$

- y_i is measured value
- \hat{y}_i is modelled value
- \bar{y} is mean of y_i

The likelihood that performance of two models was the same was determined by using a paired sample *t*-test. Specifically, each algorithm had 10 NSEs from validations of the 10 sample groups in the 10-fold validation. NSEs of two algorithms were compared by pairing the NSEs for the same validation lake group and calculating a pairwise *t*-test.

2.2.1.3 Model development

In the literature, Chl model variable combinations include: (1) a single band or single band ratio (Ma and Dai, 2005); (2) one band combined with one band ratio (Brezonik et al., 2005); and (3) all bands (Keiner and Yan, 1998). We tested all possible variable combinations with the algorithms and found that models

with all bands and band ratios had performances greater than or equal to the models with fewer variables. For example, if band ratios were removed from the BRT and RF model, leaving only bands, the model performance of BRT decreased from NSE = 0.458 (se = 0.047) to NSE = 0.408 (se = 0.042), and the model performance of RF decreased from NSE = 0.455 (se = 0.024) to NSE = 0.404 (se = 0.032). Variable reduction tests were carried out and we found that redundant variables did not decrease the model's predictive performance (Figure 2-3). Therefore, all models used all bands and band ratios as independent variables (21 independent variables). The thermal band (Band 6) was not included to avoid temperature information in the Chl measurement, thereby avoiding auto-correlation in future studies of relationships between climate and algal blooms.

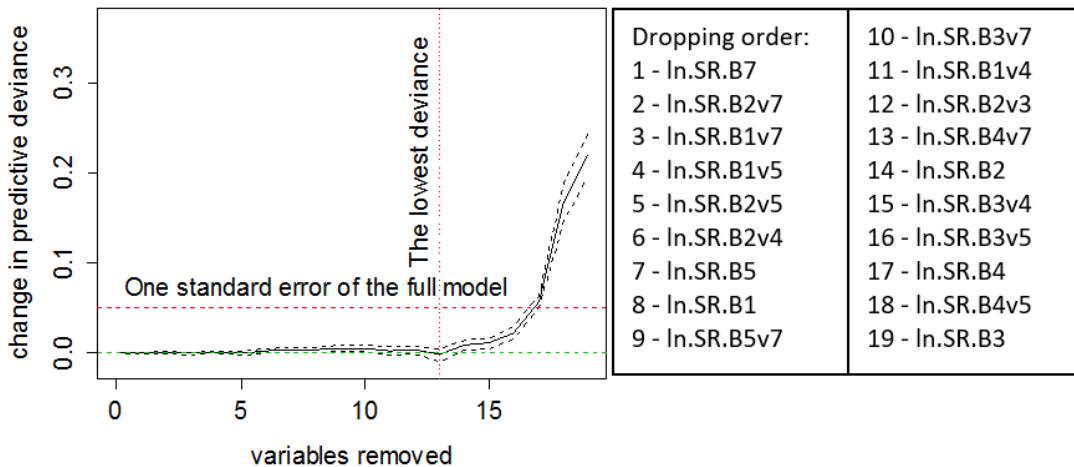


Figure 2-3 Variable reduction test for the BRT algorithm. Variable ln.SR.B7 reads log-transformed surface reflectance of Band 7. B2v7 reads the ratio of Band 2 vs. Band 7. Dropping order was based on relative importance of variables. The two most important variables, *i.e.*, ln.SR.B1v3 and ln.SR.B1v2, were always included in the model.

The function “*lm*” in R was utilized for MLR calibration, and the function “*predict*” in R was utilized for the MLR model prediction. The R packages for the other algorithms were: “*mgcv*” (Wood, 2001) for GAM, “*gbm*” (Friedman, 2001) for BRT, and “*randomForest*” (Liaw and Wiener, 2002) for RF.

2.2.2 Evaluation of model applications

2.2.2.1 Algal bloom detection

Landsat observations have an almost global coverage and potentially provide information about algal blooms, such as occurrence time, place, area, and duration. An algal bloom event occurred in Lake Erie around September 4, 2009, indicated by ground measurements and the aircraft and satellite imageries from NOAA – Great Lakes Environmental Research Laboratory (NOAA-GLERL, <https://www.glerl.noaa.gov>, accessed on February 22, 2017). RF was applied in Google Earth Engine servers (Gorelick, 2012) to calculate Chl of Western Lake Erie in 2009 and verify if the algorithm could identify the algal bloom event around September 4, 2009. RF was trained by the “*ee.Classifier.randomForest*” function in the Google Earth Engine servers. Chl was predicted from surface reflectance of Landsat TM 5 images (ImageCollection ID in Google Earth Engine = "LEDAPS/LT5_L1T_SR"). Chl was calculated by the “*classify*” function in the Google Earth Engine servers.

2.2.2.2 Validation by relation with total phosphorus

Total phosphorus (TP) is associated with anthropogenic activities (e.g., fertilization), and has a causal relationship with algal biomass in lakes (Stow and Cha, 2013). We hypothesized that (1) remotely sensed Chl (RS-Chl) is sufficiently accurate and ecologically meaningful if its correlation with TP is as strong as the correlation between ground-measured Chl (ground-Chl) and TP. Landsat TM/ETM+ provides multiple measures of the same lake over a long time, and we further hypothesized that (2) the average RS-Chl over a period as long as a summer would correlate with TP better than one-time estimates of RS-Chl since average algal biomass is better estimated by multiple measures.

Revisited lake samples were used to test if average algal biomass is better estimated by multiple measures by comparing correlations between ground-Chl and TP when using average ground-Chl of

repeated measurements from the same lake versus using one measurement of ground-Chl. Remote sensing images were basically the same as those in the model comparison, except that duplicated measurements were not excluded so some lakes might have multiple RS-Chl measures. For a period of eight days before/after a NLA sample date, Landsat TM and ETM+ together could measure a lake as many as five times. Multiple RS-Chl measurements were used to test if the average of multiple RS-Chl measures had a higher correlation with TP than singular RS-Chl measures did. BRT was used for the RS-Chl calculation.

2.3 Results

2.3.1 Algorithm comparison

Algorithm predictive capabilities in descending order of performance were: BRT ($\text{NSE} = 0.458$, $\text{se} = 0.047$) > RF ($\text{NSE} = 0.445$, $\text{se} = 0.051$) > GAM ($\text{NSE} = 0.401$, $\text{se} = 0.065$) > MLR ($\text{NSE} = 0.398$, $\text{se} = 0.045$). The non-linear algorithm GAM was almost the same as the linear algorithm MLR ($t\text{-test } p = 0.906$). BRT was significantly better than MLR ($t\text{-test } p = 0.004$) or GAM ($t\text{-test } p = 0.038$). RF was slightly but not significantly worse than BRT ($t\text{-test } p = 0.136$). RF was significantly better than MLR ($t\text{-test } p = 0.020$), and very likely better than GAM ($t\text{-test } p = 0.067$). Overall, the machine-learning algorithms (*i.e.*, BRT and RF) showed better performances than the other algorithms (*i.e.*, GAM and MLR) (Table 2-1, Figure 2-4).

All models explained less than 50% of the variance in Chl (ground-measured). Data screening removed some abnormal image pixels and slightly but not significantly ($t\text{-test } p > 0.05$) improved model performances for all algorithms. For example, NSE for BRT and MLR increased by 0.057 and 0.063, respectively, as the result of data screening.

Table 2-1 Model performance differences indicated by p values of paired t -tests.

	GAM (NSE = 0.401, se = 0.065)	BRT (NSE = 0.458, se = 0.047)	RF (NSE = 0.445, se = 0.051)
MLR (NSE = 0.398, se = 0.045)	0.906	0.004	0.020
GAM (NSE = 0.401, se = 0.065)		0.038	0.067
BRT (NSE = 0.458, se = 0.047)			0.136

Table notes: NSE is from 10-fold cross validation. MLR = multiple linear regression; GAM = general additive models; BRT = boosted regression trees; RF = random forest. Bold font indicates $p < 0.05$.

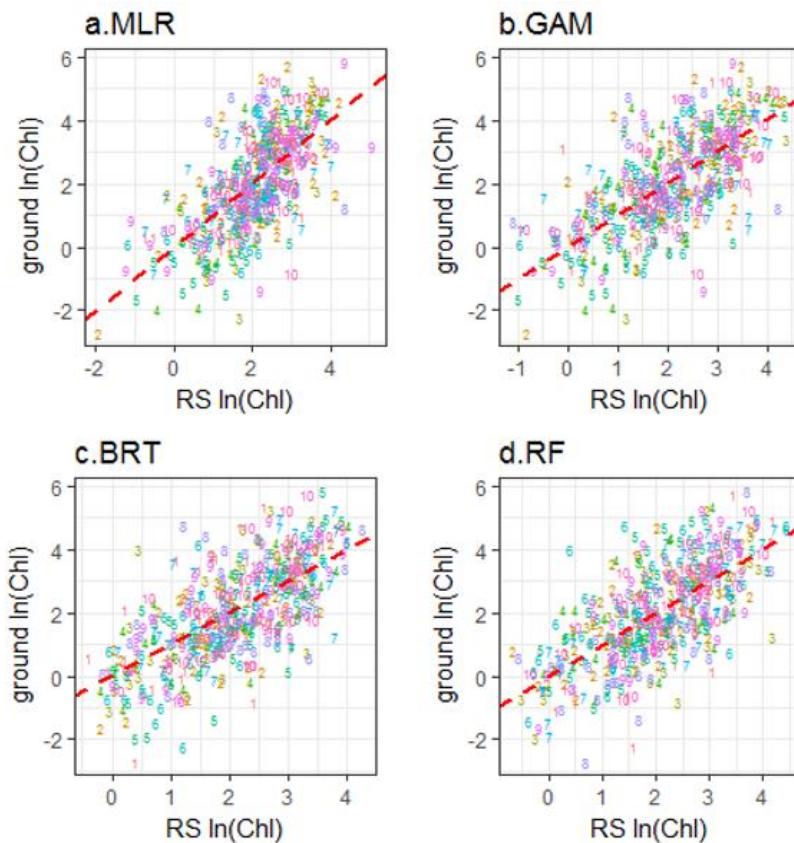


Figure 2-4 Scatter plot of ground-measured chlorophyll- a (ground Chl, $\mu\text{g/L}$) and remotely sensed chlorophyll- a (RS Chl, $\mu\text{g/L}$) in 10-fold cross validation. Algorithms include (a) multiple linear regression (MLR), (b) general additive models (GAM), (c) boosted regression trees (BRT), and (d) random forest (RF). Results of each fold in 10-fold validation are coded with numbers. Dashed lines are the 1:1 ratio lines.

2.3.2 Performance for algal bloom identification

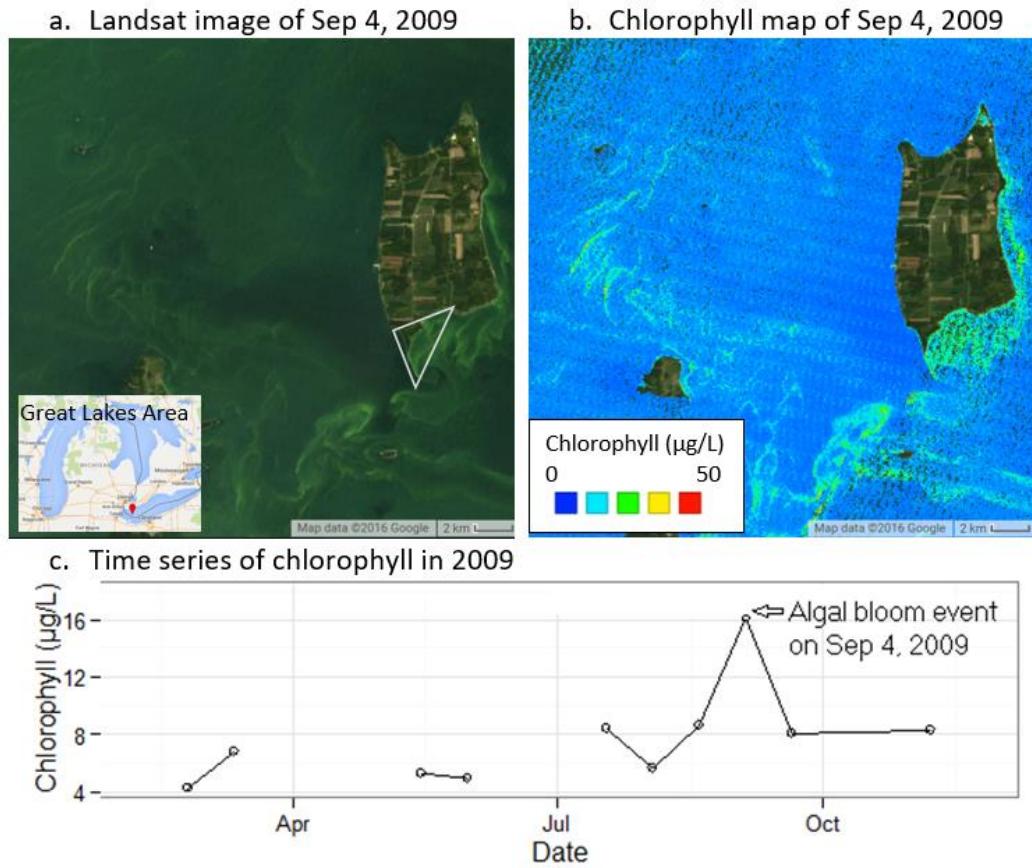


Figure 2-5 Example of an algal bloom event around Pelee Island in Lake Erie on September 4, 2009. (a) Landsat 5 TM image of the bloom area. The island location is indicated by the red dot on the bottom left map. (b) Chlorophyll- α concentrations estimated from Landsat-5 TM data using the random forest (RF) algorithm. (c) The bloom is indicated by the time series of mean chlorophyll- α over the south shore of the island (*i.e.*, the triangle area indicated in a) predicted using the RF algorithm.

The Chl maps produced with the RF algorithm applied with Google Earth Engine and Landsat TM data identified algal bloom spatial patterns and temporal duration around Pelee Island in Lake Erie on September 4, 2009. Specifically, the spatial patterns in Chl observed by the true-color Landsat image (Figure 2-5 a) were very similar to the patterns produced with the RF algorithm applied with Google

Earth Engine (Figure 2-5 b). The time series of Chl nearby southern Pelee Island showed that Chl peaked on the same date of the observed bloom date that was reported by NOAA-GLERL (Figure 2-5 c).

2.3.3 Relation with total phosphorus

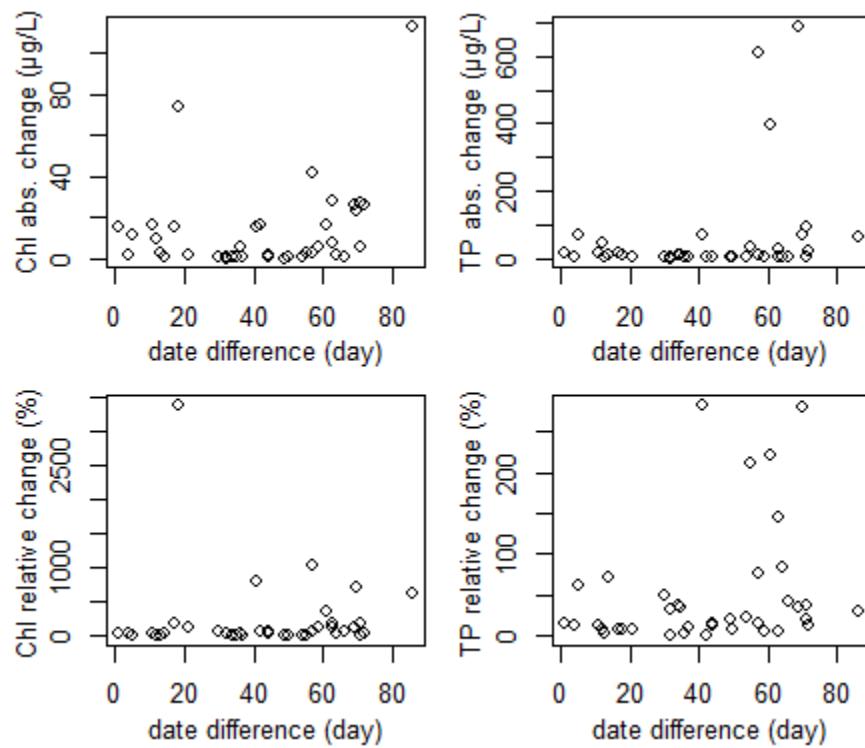


Figure 2-6 Change of Chlorophyll- α (Chl) and total phosphorus (TP) between two samplings of a subset of lakes in the first National Lake Assessment, 2007. Each point represents one lake ($N = 36$). For the first measurements, median Chl = 42.2 $\mu\text{g}/\text{L}$, median TP = 20.0 $\mu\text{g}/\text{L}$. Let x_1 = the first measurement, and x_2 = the second measurement, then abs. change = absolute $(x_1 - x_2)$, and relative change (%) = (abs. change) / x_1 .

In the lakes sampled more than once during the National Lake Assessment survey, both ground-measured Chl and ground-measured total phosphorus (TP) concentrations varied greatly between visits (Figure 2-6). Specifically, the second measurements of Chl in three months could differ from the first

measurements by as much as 10 folds. TP was less variable than Chl over time. The second measurements of TP in three months differed from the first measurements by no more than three folds.

Both one-time RS-Chl and one-time ground-Chl had strong correlations with TP: the Pearson r between RS-Chl and TP and between ground-Chl and TP was 0.723 and 0.608, respectively. Multiple Chl measurements increased the Chl-TP correlations for both methods of Chl measurement (*i.e.*, RS-Chl and ground-Chl). Specifically, average ground-Chl from two visits had a stronger correlation with TP ($r = 0.804$) than ground-Chl from only one visit ($r = 0.723$). Average RS-Chl from one, two, and three visits had correlations with TP of 0.655, 0.715, and 0.734, respectively. The correlation of average RS-Chl from three remote sensing measurements ($r = 0.734$) was as high as one-time ground-Chl ($r = 0.723$) (Table 2-2).

Table 2-2 Correlation coefficient (Pearson r) between ground-measured total phosphorus (TP) and chlorophyll- a (Chl) measured on ground as well as by remote sensing (RS). “Rev. N ” is the number of revisit times of Chl measurement for each lake. Chl for each lake is the average value of revisited measurements when Rev. $N > 1$. The measurement times (“Meas. N ”) used in each average Chl are indicated in the first column. For a lake that was revisited four times (Rev. $N = 4$), Chl could be averaged from one, two, three, or four measurements (*i.e.*, Meas. $N = 1, 2, 3$, or 4).

Meas. N	Ground-measured Chl		RS-measured Chl			
	Rev. $N = 1$; 790 lakes	Rev. $N = 2$; 39 lakes	Rev. $N = 1$; 90 lakes	Rev. $N = 2$; 394 lakes	Rev. $N = 3$; 121 lakes	Rev. $N = 4$; 26 lakes
1	0.723	0.723	0.608	0.599	0.655	0.547
2		0.804		0.669	0.715	0.585
3					0.734	0.605
4						0.620

2.4 Discussion

2.4.1 Are machine-learning algorithms our best choice?

Different bands and/or band ratios of Landsat TM/ETM+ have been recommended for RS-Chl models in different studies (*e.g.*, Carpenter and Carpenter, 1983; Kloiber et al., 2002; Papoutsas et al., 2014; Rodríguez et al., 2014). The variety of selections of bands and/or band ratios reflects a variety of possible relationships between Chl and remote sensing signals (hereafter referred as Chl-RS relationship). Many factors have been known to affect this relationship, including atmospheric interference, wind, sediments, CDOM (colored dissolved organic matter), and species composition of algae. Empirical algorithms in the literature usually only work in specific areas and times with relatively constant conditions. For instance, after trying all band/band ratio combinations, Ma and Dai (2005) suggested a linear model with Band 3 was the best in Taihu Lake, China, with NSE = 0.551. However, when the same model was applied in the National Lake Assessment (NLA) dataset, the 10-fold cross validation NSE was only 0.164, which was the result after new model coefficients were fit by the NLA dataset. For another example, Brezonik et al (2005) suggested a “band + band ratio” combination as predictors and found that “Band 3 + Band 1/3” was the best to predict ln(Chl) (reported calibration NSE = 0.89, $N = 15$ within one Landsat scene) after trying all variable combinations including the best model of Ma and Dai. Validation NSE for this algorithm with the NLA dataset was only 0.240. These examples indicate a variable Chl-RS relationship over time and place, thus those relationships are not transferable.

To account for regional and temporal variation in factors affecting the Chl-RS relationship, we could build separate models for different regions, lake types, and weather conditions. However, decision-tree algorithms, such as BRT and RF, have the potential to split data into stratified groups and thereby satisfy the need for higher predictive performance and consistency with one model. For instance, CDOM absorption mostly occurs in visual wavelengths, so the signal combination of algae and sediments can be estimated with red and infrared wavelengths resulting in a minor CDOM effect (Gilerson et al., 2010).

After the discrimination of Chl from CDOM, Chl can further be discriminated from sediments since band ratios can partly remove sediment interference in a Chl signal (Han, 1997). This stage-by-stage model modification process is similar to decision tree processes in BRT and RF, which fully consider interactions between predictors with multiple classification trees. Therefore, BRT and RF may be able to discriminate Chl from sediments and CDOM and improve Chl estimation accuracy. Our results indicate that machine-learning algorithms (*i.e.*, BRT and RF) provide higher accuracy than the traditional linear algorithm MLR or the non-linear algorithm GAM, although further research is required to confirm the discrimination capability of BRT and RF. The improvement of machine-learning algorithms might be the result of: (1) decision trees might have better corrected the Chl-RS relationship by accounting for interactions between optical agents in water; and/or (2) machine-learning algorithms have found hidden rules in the Chl-RS relationship that we may not know yet. GAM was not significantly better than MLR, indicating that model performance did not improve by simply replacing a linear algorithm with a non-linear algorithm. Our results indicated that the machine-learning algorithms, which were non-linear, better address complex interactions among variables than simple non-linear algorithms like GAM.

To estimate Chl in turbid lakes over a large temporal and spatial scales, machine-learning algorithms may be the best tools that we have to date. Interactions between optical agents are usually tested in laboratories, which may not apply to complex realities. For example, Han (1997) found the Chl-RS relationship was independent of suspended sediments. However, the size or color of sediments was the same in the experiment. In reality, sediment size and color varies substantially, and we probably cannot correct Chl estimates for sediment interference when using simple MLR. It is unrealistic to build a traditional MLR model for a large spatial and/or temporal scale due to almost infinite combinations of atmospheric and water optical conditions.

On the other hand, more Chl data have been collected from many sources and are available for use in future model testing and updates, and this could improve the models. For example, after the first

National Lake Assessment (NLA) in 2007, the 2nd NLA was carried out in 2012, providing more validation and re-training data for machine learning. Machine-learning together with increasing data for training may be easier than developing “clever” analytical bio-optical algorithms (*e.g.*, Maritorena et al., 2002).

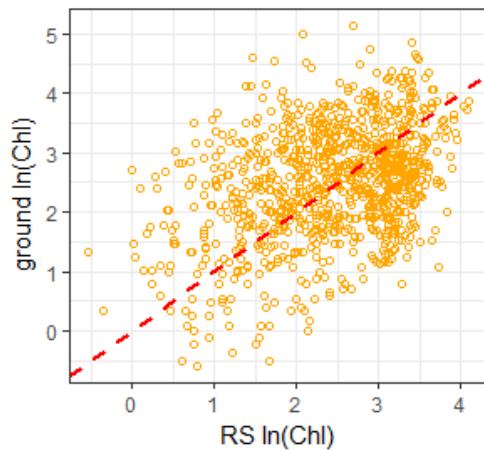


Figure 2-7 Cross-dataset validation of the chlorophyll-*a* (Chl, $\mu\text{g/L}$) random forest model. The random forest model was trained by the dataset of the first National Lake Assessment, then validated by the dataset of 24 years (1989-2012) and 39 reservoirs in Missouri, USA. Validation NSE = -0.137, indicating a model failure. Dashed line is the 1:1 ratio line.

Machine-learning algorithms learn from data, so data quality is critical. Data from different sources may not be comparable. For lake Chl, there are two commonly used sampling methods: (1) an integrated sample of constant depth, such as 0.25-0.5 m, and (2) an integrated sample over one-Secchi depth, which varies with lake turbidity. The first NLA collected integrated samples of the surface to the Secchi disk depth. We found that the RF model trained by the NLA data performed poorly (NSE = -0.137) compared to cross-validation with NLA data, when predicting the Chl in 39 Missouri (USA) reservoirs, which were sampled during 1989-2012 (23 years) with constant depth with near-surface samples (Figure 2-7). Mean depth of the NLA samples was 1.59 m ($\sigma = 0.02 \text{ m}$), which was different from the range of

Missouri sample depths (0.25-0.5 m). Including sampling methods in future algorithms could account for these factors when training machine-learning algorithms.

2.4.2 Error sources

The best algorithm, *i.e.*, BRT, only had NSE of 0.458 ($se = 0.047$), indicating half of Chl variance was not explained by the model. The model errors could be from (1) phytoplankton spatial and temporal heterogeneity, (2) image quality, and (3) other lake conditions, which are discussed in detail in the following sections.

2.4.2.1 Phytoplankton spatial and temporal heterogeneity

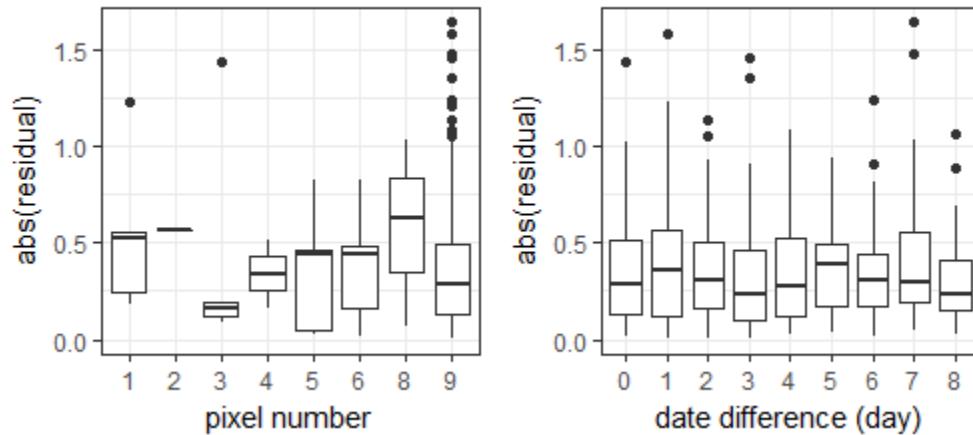


Figure 2-8 The absolute residual of the random forest model did not change with the pixel numbers less than 9 or day difference less than 8 between the ground measure dates and remote sensing dates.

There were spatial differences between the location of the 3-by-3 image pixel windows and the points of ground measurements. Moreover, there were 0-8 days of differences in timing between satellite and ground measurements. Over areas with high Chl concentration, high spatial and temporal variation is expected, especially during algal bloom periods (Yacobi et al., 1995). However, further analyses of our data did not show model errors increased with smaller pixel numbers less than 9 in the 3-by-3 image

pixel window or with longer day differences between satellite and ground measurements, indicating the small spatial and temporal deviation in phytoplankton was a minor source of error in the models (Figure 2-8).

2.4.2.2 Image quality

Other important error sources could arise from atmospheric interference, considering the heterogeneity of the atmosphere across 383 images that we used in the NLA models, as well as from specular reflectance off water surfaces. Without atmospheric effects and specular reflectance, remote sensing signals are strongly correlated with Chl even when other color producing agents exist (Wiangwang, 2006). However, for high altitude (*i.e.*, satellite borne) sensors subject to atmospheric effects, water-leaving radiance only accounts for a small part (~10%) of the total at-sensor radiance (Hu et al., 2001). Even though atmospheric corrections had been applied in the data we used, the correction accuracy might not be good enough for weak water signals. The errors of atmospheric correction for land surface reflectance were about ± 0.006 standard deviation of blue and red bands (Kaufman et al., 1997), thus it was less than 5% of reflectance from land objects. However, that standard deviation of ± 0.006 accounted for about 14.6% and 15.4% of the average surface reflectance in Bands 1 and 3, respectively, for the NLA lakes, which have substantially lower reflectance than land objects. Atmospheric correction for water applications is still an unsolved problem (Kutser, 2012; Ritchie et al., 1990; Torbick et al., 2013).

Specular reflectance, which is strongly related to wind speed, potentially produces errors that have a magnitude similar to Chl values themselves in the ocean waters (Gordon, 1997). In the United States, average terrestrial wind speed is around 4-9 m/s (US Department of Energy, <http://apps2.eere.energy.gov>, accessed on Aug 8, 2015). Wind speeds about 8-9 m/s can produce error of ± 0.002 in reflectance (Gordon, 1997). That was about 4.9-13.3% (different among bands) of the

average surface reflectance for the Landsat bands applied for the NLA lakes. Specular reflectance increases according to a power function (power = 3.52) of wind speed (m/s) (Gordon and Wang, 1994; Koepke, 1984). Therefore, specular reflectance might be another reason that no significant improvement was seen in atmospherically corrected data compared to TOA (Kutser, 2012; Ritchie et al., 1990; Torbick et al., 2013). Specular reflection can be estimated by wind speed above water and then included in algorithms, but wind speed is not available for most inland lakes.

Some errors might be related to radiometric calibrations. On Chl maps of lakes, we often found abnormal stripes (Figure 2-9). Chl concentration differences between neighbor stripes could be as high as 10 µg/L. Those stripes might be caused by detector-to-detector mis-calibration or scan-to-scan mis-calibration. Striping effects are corrected in Landsat 7 products but not Landsat 5.

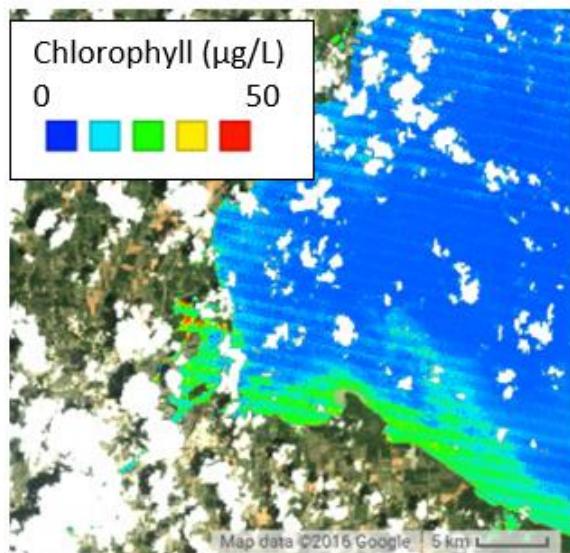


Figure 2-9 Landsat TM abnormal stripes on chlorophyll map of Maumee Bay (USA). Landsat image ID = "LT50200312009199GNC02". The chlorophyll map was overlaid on the Landsat image. White areas are clouds.

2.4.2.3 Lake condition

Bottom effects, floating scum, aquatic macrophytes, suspended sediments, colored dissolved organic matter (CDOM), or phytoplankton compositional variability may also introduce large uncertainty in the models (Menken et al., 2006; Quibell, 1991). All these factors can change the leaving-water radiance. Some impacts, such as the lake bottom, floating scum, and aquatic macrophytes, may be hard to discriminate with Chl algorithms, so it is better to detect them and remove those pixels (Ackleson and Klemas, 1987; Matthews et al., 2012). Our data screening process removed some areas covered by scum and macrophytes, since they showed land reflectance traits. Some impacts such as sediments and CDOM might have been minimized by the machine-learning algorithms as we discussed above, but further research is required.

2.4.3 Are machine-learning algorithms good enough?

“Good” is a comparative judgement based on a specific application. Our results illustrated: (1) remote sensing of Chl successfully identified algal bloom areas in Lake Erie; (2) the variation of the algal bloom over time was identified; and (3) remotely sensed Chl was related to TP almost as well as ground measured Chl, and was as good as was ground measured chlorophyll if multiple remote sensing Chl measures were used. Therefore, remote sensing Chl is good enough for applications such as:

- Quantifying the extent of algal blooms within specific lakes.
- Monitoring lakes and identifying lakes with high algal biomass to prioritize lakes for management.
- Providing a low cost and efficient tool for environmental management, *e.g.*, monitoring restoration of lakes with remotely sensed Chl before and after management plans are implemented.

- Studying algal bloom mechanisms by building time series of algal biomass in one or more lakes using historical remote sensing data and then linking measured algal biomass with environmental factors.

Moreover, Chl is not the only water quality variable that can be measured by remote sensing. Our study in Missouri reservoirs showed that CDOM as well as sediments can be estimated by BRT models with even higher confidence than Chl (Lin et al. unpublished data). Therefore, remotely sensed Chl along with sediments and CDOM are valuable data for limnological studies, especially for those on large spatial and temporal scales.

2.5 Conclusion

Machine-learning algorithms (*i.e.*, BRT and RF) were better than a traditional linear algorithm MLR for remote sensing of Chl in inland lakes across the continental United States. The improvement in algorithm performance was more likely from the automation of stage-by-stage learning and accounting for complex interactions among variables than from the non-linear character of the machine-learning algorithms. No matter how intelligent the algorithm was, remote sensing of inland lakes was still limited by both training data quality and image quality. Nonetheless, remotely sensed Chl based on machine-learning algorithms and Landsat TM/ETM+ was good enough for algal bloom detection and could be a valuable measurement for environmental monitoring and management.

Acknowledgement

This report was made possible through support of the Environmental Protection Agency (EPA), USA (Grant no. R835203). The opinions expressed herein are those of the authors and do not necessarily reflect the views of the US EPA or the US Government.

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3 EFFECTS OF SEDIMENTS AND COLORED DISSOLVED ORGANIC MATTER ON REMOTE SENSING OF CHLOROPHYLL-A USING LANDSAT TM/ETM+ OVER TURBID WATERS

Abstract

In turbid inland waters, remote sensing of chlorophyll- α is challenging because waters commonly contain inorganic suspended sediments (*i.e.*, non-volatile suspended solids, NVSS) and colored dissolved organic matter (CDOM). The effects of NVSS and CDOM on empirical models for chlorophyll- α using remote sensing imagery in inland waters have not been determined on a broad spatial and temporal scale. This study was conducted to evaluate these effects with a long-term (1989-2012) dataset that included chlorophyll- α , NVSS, and CDOM for 39 reservoirs across Missouri (USA). Model comparison indicated that the machine-learning algorithm BRT (boosted regression trees, validation $R^2 = 0.350$) was better than a traditional linear regression (validation $R^2 = 0.214$) for chlorophyll- α measurement using Landsat TM/ETM+ imagery. Minimal BRT model residuals could be explained by sediments or CDOM, and the residual trends were different from the theoretical trends related to sediments and CDOM. The results indicate that the BRT model had small systematic bias but the bias was not likely caused by sediments or CDOM.

Keywords: turbid water, biomass; water quality, phytoplankton, remote sensing

Highlights

- The BRT machine-learning algorithm provided more accurate chlorophyll- α estimates than MLR based on Landsat.
- The BRT model had systematic bias but this was not likely caused by sediments nor by dissolved organic matter.

3.1 Introduction

3.1.1 Remote sensing of chlorophyll- α in inland lakes

Lake algal biomass assessments using traditional field-based sampling methods are challenging due to the high spatial and temporal variation of phytoplankton, especially during bloom periods (Yacobi, Gitelson, and Mayo 1995). Remote sensing has been used increasingly to map algal biomass at a higher frequency, over a wider geographic coverage, and with a lower cost than traditional field measurements (Sellner, Doucette, and Kirkpatrick 2003). Many operational ocean color sensors and algorithms have been developed since 1970's (see review Blondeau-Patissier et al. 2014). However, in turbid inland waters, sediments and CDOM not only interfere with the characteristic chlorophyll- α spectral signal, but they also make atmospheric correction complicated. Atmospheric effects can be estimated for Case I water (*i.e.*, clear water with a minor sediment effect) assuming the water-leaving radiance is zero at infrared wavelengths (Gordon 1997). In turbid waters, the radiance from sediments violates the zero-infrared assumption and has caused great concern for using satellites to measure chlorophyll- α concentrations.

Landsat data are most often used in inland lakes for its relatively high spatial resolution and 16-day revisit time compared to other images. Even though the atmospheric correction problem remains unsolved for turbid waters, Landsat data have been tested over inland waters with fairly good correlations (with r around 0.7) between chlorophyll- α and remote sensing bands and band ratios when applied over relatively homogeneous areas (*e.g.*, Ritchie, Cooper, and Schiebe 1990). However, these relationships are not consistently good when considering multiple lakes, or lakes over a long duration, in which lake conditions vary, especially their sediment concentrations varie (Sváb et al. 2005). Suspended sediments and CDOM are therefore a major concern as interferences in the remote sensing of chlorophyll- α in inland lakes

3.1.2 Sediment effects

Adding sediments to algae-laden water causes water reflectance to increase (Figure 3-1). Since reflectance increases proportionally with suspended sediments in algae-laden water, Han et al. (1994) suggested the ratio between red and near-infrared red (NIR) could be used as an chlorophyll-*a* index. They found that the red/NIR ratio was totally independent of suspended sediments. Therefore, it is possible to use TM/ETM+ Band 4 (NIR)/Band 3 (red) to estimate chlorophyll-*a* concentrations with minor sediment interference. However, the relationship between reflectance and sediment concentration changes with particle size of sediment, particle constituents such as organic carbon, and even the concentration of the chlorophyll-*a* (Karabulut and Ceylan 2005). The study of Han et al. (1994) was carried out in a lab using a spectroradiometer and one source of sediments. The reliability of the NIR/red method in multiple lakes over a long time is unknown.

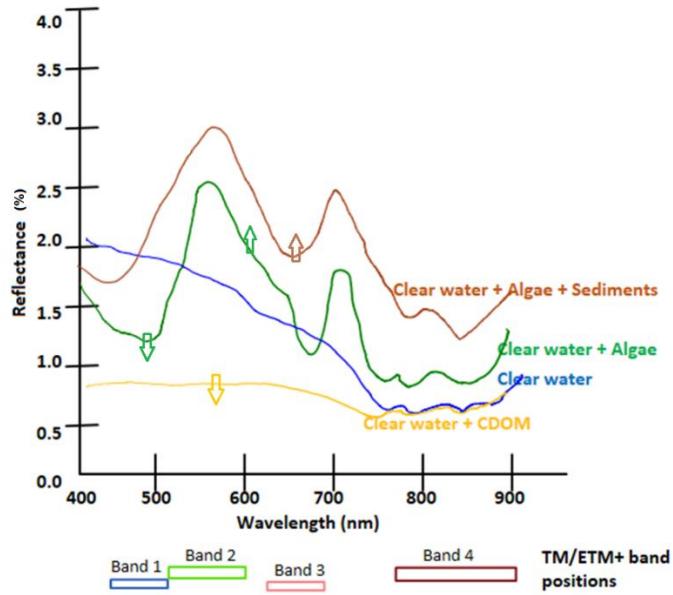


Figure 3-1 Schematic diagram of water reflectance affected by algae, sediments, and CDOM (colored dissolved organic matter). Arrows indicate the expected change in the curve when concentrations of corresponding substances increase (after Carder et al. 1989; Han 1997).

3.1.3 CDOM effects

CDOM is produced by degradation of phytoplankton, especially during periods of algal blooms, and of organic matter of terrestrial and wetland origin (Zhao et al. 2009). CDOM absorption is high in the blue spectral region, and decreases exponentially with wavelength, reaching almost zero absorption at the infrared spectral region (Figure 3-1). The CDOM spectrum has no unique characteristics, like multiple peaks and lows, which can be used for developing satellite algorithms for measuring CDOM. With the interference of chlorophyll- α and sediments, remote sensing estimates of CDOM is even harder (Menken, Brezonik, and Bauer 2006). The magnitude of CDOM effects in the visual spectral region can be as high as moderate chlorophyll- α concentrations in the ocean (Bricaud et al. 1981). Gilerson et al. (2010) found that the red/NIR algorithm for MERIS images was not very sensitive to CDOM absorption in water with CDOM absorption coefficients ranging within $0\text{--}5 \text{ m}^{-1}$. However, in freshwater, the CDOM absorption coefficient is usually around 30 m^{-1} , which is much higher than in open ocean waters ($< 0.1 \text{ m}^{-1}$), so the interference effect of CDOM on chlorophyll- α estimates with remote sensing in freshwater is expected to be stronger than oceanic waters (Brezonik, Menken, and Bauer 2005). CDOM impacts on chlorophyll- α estimates with remote sensing however have not been tested extensively over a large region, over a long time, and in turbid water with both high concentrations of sediments and CDOM.

3.1.4 Landsat chlorophyll-a algorithms

In inland turbid waters, empirical algorithms such as linear regression, are more commonly used than analytical or semi-analytical algorithms in chlorophyll- α estimation due to complexity of intrinsic optical properties (IOPs), which are the basis for analytical or semi-analytical models (e.g., Kloiber et al. 2002; Brezonik, Menken, and Bauer 2005; Kabbara et al. 2008; Dona et al. 2014; Rodríguez et al. 2014). Both Landsat bands and band ratios have been used as independent variables in previous studies (e.g., Carpenter and Carpenter 1983; Brivio, Giardino, and Zilioli 2001; Olmanson, Bauer, and Brezonik 2008; Papoutsas et al. 2014). More complex empirical algorithms have also been used, including: linear mixture

modelling using an algorithm called noise fraction transformation to enhance image quality when applying spectral end members as variables (Tyler et al. 2006); and the spectral decomposition approach using decomposition coefficients of optically active substitutes (*i.e.*, phytoplankton, sediments, and CDOM) as independent regression variables (Oyama et al. 2007). For optical complications in turbid waters, using advanced machine-learning algorithms, *i.e.*, artificial neural networks (ANN) and genetic algorithms, has provided better performance than conventional linear regression (Sudheer, Chaubey, and Garg 2006; Chen et al. 2008). A growing literature in ecology has shown stronger performance by boosted regression trees (BRT) than linear regression or non-linear models such as GAM (general additive models) when developing empirical models because BRT can account for complex interactions among variables (Elith et al. 2006; Moisen et al. 2006). Machine-learning algorithms such as BRT could be valuable for discriminating chlorophyll- α from sediments and CDOM by accounting for their interactions on reflectance in different bands and band ratios of Landsat imagery.

3.1.5 Objective

To our knowledge, no study has quantified the effects of sediments and CDOM on chlorophyll- α estimates using Landsat images in inland lakes considering effects of both sediments and CDOM. Discriminating chlorophyll- α from sediments and CDOM is important for studying phytoplankton ecology because sediments and CDOM often co-vary with storm events, runoff, nutrient loading, and algal blooms (Zhang et al. 2009; Paerl and Paul 2012). The objective of this study was to quantify the effects of sediment and CDOM on chlorophyll- α estimates using Landsat TM/ETM+ data. A Missouri reservoir dataset provided a unique opportunity to assess these effects. The dataset has measurements of chlorophyll- α , suspended sediments, and CDOM from water samples that were collected three or four times per year over a long period (1989-2012, 24 years) and for 39 Missouri reservoirs. First, a remote sensing model for chlorophyll- α using Landsat TM/ETM+ imagery was built with a BRT algorithm, and then model residuals were related to sediments and CDOM to quantify their effects on chlorophyll- α .

estimates. The magnitudes of sediment and CDOM effects were indicated by the range and significance of their relationships to model residuals.

3.2 Methodology

3.2.1 Data

3.2.1.1 In-situ data

Data for this analysis were from 39 Missouri reservoirs (Figure 3-2) that were sampled from May to September, 1989 to 2012. Water samples were collected from surface water (0.25 m to 0.5 m depth) near reservoir dams on three or four occasions per year. Analyses of water samples included chlorophyll-*a*, suspended sediments, and CDOM. Chlorophyll-*a* and sediments were measured from 1989 to 2012, while CDOM was measured from 2002 to 2012.

Suspended sediments were measured gravimetrically as non-volatile suspended solids (NVSS). NVSS was the ash-mass of solids collected by filtration with Whatman 934-AH filters and then incineration of the filter at 500°C. Samples for CDOM were filtered through 0.2 µm membrane filters. CDOM was measured by the absorption coefficient at 440 nm wavelength (A440nm). A440nm could be affected by small inorganic particles and colloids that pass through the filter, however that effect only contributes from 2% to 8% of the absorption (Sipelgas et al. 2003).

The dataset covered wide ranges of water quality: chlorophyll-*a* varied from 0.55 µg/L to 171.80 µg/L with mean = 18.39 µg/L; NVSS varied from 0.01 mg/L to 36.20 mg/L with mean = 4.20 mg/L; and A440nm varied from 1.00 m⁻¹ to 798.00 m⁻¹ with mean = 79.08 m⁻¹. The data distributions for chlorophyll-*a*, NVSS, and A440nm were skewed with mostly low values and a few samples having extremely high values (Table 3-1). Linear regression is sensitive to extreme values and uneven distributions. Therefore, chlorophyll-*a*, NVSS, and A440nm were natural log-transformed to meet the

data normality requirement of linear regression. The transformed variables were denoted as $\ln(\text{Chl})$, $\ln(\text{NVSS})$, and $\ln(\text{A}440\text{nm})$.

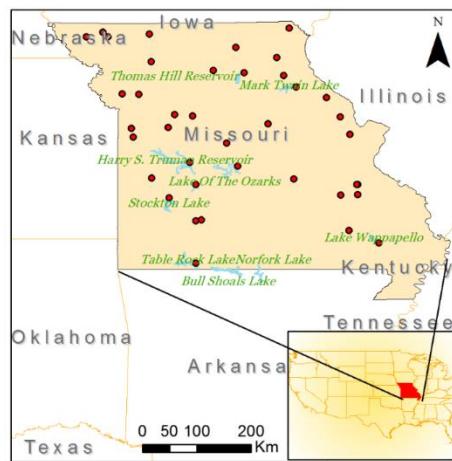


Figure 3-2 Thirty-nine sampling locations (indicated by dots) in Missouri, USA.

Table 3-1 Statistics summary of in-situ measurements

	Chlorophyll- <i>a</i> ($\mu\text{g/L}$)	NVSS (mg/L)	A440nm (m^{-1})
Min.	0.55	0.01	1.00
1st Qu.	6.80	1.80	24.00
Median	13.30	3.20	37.00
Mean	18.39	4.20	79.08
3rd Qu.	23.40	5.50	81.00
Max.	171.80	36.20	798.00

Table abbreviations: NVSS – non-volatile suspended solids; A440nm – absorbance coefficient of filtered water measured at 440 nm wavelength to estimate concentration of colored dissolved organic matter.

3.2.1.2 Remote sensing data

TM on board Landsat-5 had data from March 1984 to June 2013, which covered the entire period when water quality data were collected (*i.e.*, 1989-2012). Data of ETM+ on board Landsat-7 were available from April 1999 to present (2017), which only partly overlapped with the time period of the water quality data. ETM+ is similar to TM except for slight differences in Band 4 and Band 7: ETM+ Band 4 wavelength is 0.77-0.90 μm , compared to 0.76-0.90 μm in TM; ETM+ Band 7 wavelength is 2.09-2.35, compared to 2.08-2.35 μm in TM. TM and ETM+ images from Landsat-5 and Landsat-7 were taken on different dates. Regardless of the small differences, the images from both TM and ETM+ were used to provide as many “ground-satellite” data pairs as possible.

TM and ETM+ images were downloaded from the on-demand ESPA Data Access Interface (<http://espa.cr.usgs.gov>, accessed on July 1, 2014). The Land Surface Reflectance were products of the Climate Data Record (CDR) (<http://landsat.usgs.gov>, accessed on July 1, 2014). Atmospheric correction was processed in the Landsat Ecosystem Disturbance Adaptive Processing System (LEDAPS) reusing MODIS land surface architecture based on the 6s algorithm (Masek et al. 2006). Even though the atmospheric correction algorithm for the surface reflectance products was designed for terrestrial surfaces without considering water-specific problems like specular reflectance, we chose it for potentially less atmospheric impact than the top of atmospheric reflectance products.

To ensure a large amount of data as well as strong ground-satellite correlations, we picked both TM and ETM+ images that were less than or equal to 8 days before or after the ground sampling dates. A 3×3 set of image pixels surrounding a ground sampling site was used in TM/ETM+ imagery to calculate a mean reflectance value of each band corresponding to the ground sampling site. Each ground sampling location was checked in Google Earth (Google, CA USA) to make sure all pixels in the 3×3 window were pure water pixels. If a sampling point was too close to the shoreline, its location was adjusted. The

adjustment distance was less than 100 m. Gaps due to the scan line corrector (SLC) failures in ETM+ were excluded as well as saturated pixels. The “*Fmask*” layer in the land surface reflectance product was used to mask clouds and cloud shadows. In addition to that, any pixel with Band 2 < Band 4 (land character), or reflectance > 15% (land or cloud character), or reflectance < 0% (over-corrected in the atmospheric correction) was excluded. Ground sampling records without corresponding satellite pixels were excluded. As a result, the final dataset had 963 pairs of “ground-satellite” measurements.

3.2.2 Chlorophyll- α model development

BRT is a new machine-learning algorithm based on decision trees that has significant potential in remote sensing of water. Some of our unpublished work with other datasets has shown that BRT performs better than GAM or ANN. BRT uses a large number (commonly, thousands) of boosted decision trees to minimize the model deviance (Friedman 2001). BRT inherits all the good features of decision tree algorithms, such as low sensitivity to outliers, efficient treatment of collinear variables including variable interactions, simulation of both non-linear and linear relationships, and no data distribution requirements. Non-linear relationships between water quality and remote sensing reflectance have been shown in previous studies (Han et al. 1994; Kutser et al. 2005).

Model predictors included all band ratios (*i.e.*, Band 1/2, 1/3, 1/4, etc.) as well as all bands (*i.e.*, Band 1, 2, 3, etc.) since bands and band ratio combinations might improve chlorophyll- α estimation for turbid waters by partly removing atmospheric effects and enhancing remote sensing signals (Kloiber et al. 2002; Pattiarchi et al. 1994). Band 6, the thermal band, was not included in the model predictors, because it measured lake surface temperature instead of light reflectance. The remote sensing chlorophyll- α (RS-Chl) model was:

$$\ln(\text{Chl}) = f(\text{bands, band ratios}) \quad \text{Equation 3-1}$$

where f is MLR (multiple linear regression) or BRT. An MLR model was included in our analysis to compare a more traditional approach with a BRT model. All models were developed and analyzed using R software (<http://www.r-project.org>, accessed on July 2, 2015). The MLR models were built with the “*lm*” function in R. BRT models were built with the “*gbm*” package, version 1.5–7 (Ridgeway 2004). We adapted codes from Elith et al. (2008) to calibrate parameters (*i.e.*, tree number, learning rate, and bagging rate) for the BRT models. Model performance was measured by the Nash–Sutcliffe model efficiency coefficient (Nash and Sutcliffe 1970):

$$\text{NSE} = 1 - \frac{\sum_{i=1}^n (O_i - M_i)^2}{\sum_{i=1}^n (O_i - \bar{O})^2} \quad \text{Equation 3-2}$$

where NSE is the Nash–Sutcliffe model efficiency coefficient; O_i is the observation value with mean as \bar{O} ; and M_i is the modeled value. NSE ranges from $-\infty$ to one, where one is a perfect fit and a negative value indicates model failure. NSE indicates the proportion of the total measured variance explained by the model.

Model predictive performance was estimated by 10-fold cross-validation. Specifically, the whole dataset was divided into 10 groups. Each group was used once to validate the model that was calibrated by the other nine groups. As a result, the predictive performance of each model was estimated 10 times to get a mean NSE. MLR and BRT performance was compared with a *t*-test between the two mean NSEs from 10-fold cross-validation with variation in observed NSE calculated with the 10 NSE values calculated with 10-fold cross-validation.

3.2.3 Residual analyses

The chlorophyll- α model residual (ε_i) was calculated as:

$$\varepsilon_i = O_i - M_i \quad \text{Equation 3-3}$$

where O_i is the observation value, and M_i is the modeled value. The sediment and CDOM relationships

with model residuals were characterized by GAM (generalized additive models) using the R “*mgcv*” package, version 1.8-6 (Wood 2001). GAM was picked to account for potential non-linear trends. Only the BRT model residuals were analyzed. The residuals were calibration residuals with the full dataset as training data (not the residuals from 10-fold cross-validation). The BRT residuals were related to $\ln(\text{NVSS})$ and $\ln(\text{A440nm})$, respectively using the GAM model:

$$\varepsilon = \text{GAM}(x) \quad \text{Equation 3-4}$$

where ε is residuals of the BRT model, and x is $\ln(\text{NVSS})$ or $\ln(\text{A440nm})$. The magnitude of residual trend was indicated by (1) significance of the GAM model and (2) the percentage of the total residual explained by the GAM model (*i.e.*, R^2 of the GAM model). Significance (p value) of the GAM model was an approximate estimation using the “*summary*” function (Wood 2012) in the “*mgcv*” package.

In addition to the GAM smooth line, the residual trend was quantified by adding $\ln(\text{NVSS})$ and $\ln(\text{A440nm})$ as independent variables in the RS-Chl model:

$$\ln(\text{Chl}) = \text{BRT}[\text{bands, band ratios, } \ln(\text{NVSS}), \ln(\text{A440nm})] \quad \text{Equation 3-5}$$

The increase in the model performance indicated the contribution of sediments and CDOM in the residual of the original model, *i.e.*, the one without $\ln(\text{NVSS})$ and $\ln(\text{A440nm})$.

$\ln(\text{Chl})$ was correlated with $\ln(\text{A440nm})$ (Spearman $\rho = 0.30$, $p < 0.05$) and $\ln(\text{NVSS})$ (Spearman $\rho = 0.35$, $p < 0.05$) in the Missouri dataset (Figure 3-3). The residual trends related to $\ln(\text{NVSS})$ and $\ln(440\text{nm})$ could be correlated with $\ln(\text{Chl})$ itself. Therefore, the model improvement in Equation 3-5 may be misleading due to the correlations. To parse out the sediment and CDOM correlations with $\ln(\text{Chl})$, a residual BRT model was built:

$$\varepsilon = \text{BRT}[\ln(\text{Chl}), \ln(\text{A440nm}), \ln(\text{NVSS})] \quad \text{Equation 3-6}$$

The residual trends related to $\ln(\text{NVSS})$ and $\ln(440\text{nm})$ were fitted by the partial dependences in the BRT residual model. For example, the trend related to $\ln(\text{NVSS})$ was indicated by the fitted ε against $\ln(\text{NVSS})$ in the residual model when $\ln(\text{Chl})$ and $\ln(\text{NVSS})$ were controlled at mean values. We hypothesized that the partial dependence trends were consistent with the theoretical trends caused by sediments or CDOM if sediments or CDOM caused error in the RS-Chl model (Equation 3-1). The theoretical trends were simulated by changing band reflectance in the RS-Chl model. More specifically, to simulate the sediment effect, band reflectance was increased by a gradient of percentages (Equation 3-7), then the model residual was measured to test how it changed as the concentration of sediments changed. To simulate the CDOM effect, band reflectance was decreased by a gradient of percentages, then the model residual was measured to test how it changed as the concentration of CDOM changed. Band reflectance was adjusted using Equation 3-7:

$$R = R_0 \times (1 + c) \quad \text{Equation 3-7}$$

where R is the simulated reflectance affected by sediments or CDOM; R_0 is the original reflectance; c is the percentage of reflectance change due to sediments or CDOM, with a range from 0 to 500% for the simulation of sediment effects, and from 0 to -100% for the simulation of CDOM effects. The interval number for each range was 20. The ranges of reflectance changes were based on the ranges of sediments and CDOM in the Missouri dataset and the literature on how reflectance is affected by sediments and CDOM (Han 1997; Carder et al. 1989; Gould, Arnone, and Sydor 2001). It was necessary to use simulated residual trends since the effects (positive or negative) of sediments and CDOM in the residuals of the RS-Chl BRT model (Equation 3-1) were unknown.

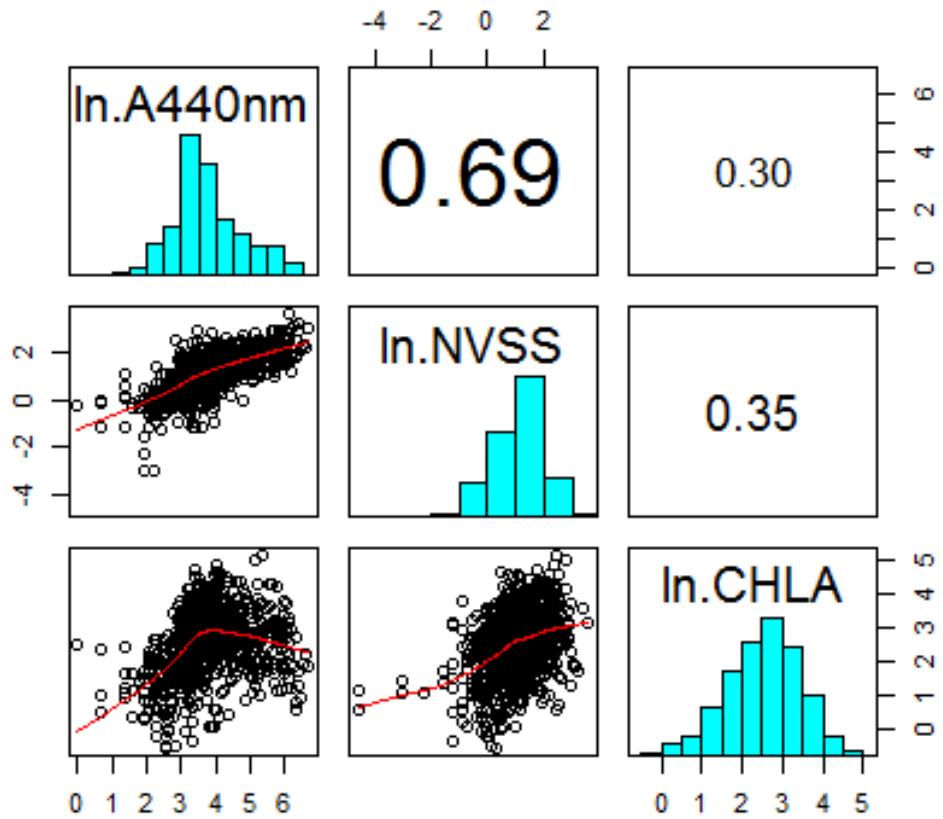


Figure 3-3 Spearman correlation matrix between ln-transformed chlorophyll-a concentration (ln.CHLA), ln-transformed absorption coefficient at 440 nm wavelength (ln.A440nm), and ln-transformed concentration of non-volatile suspended solids (ln.NVSS). The solid line in the scatter plot is the LOWESS (locally weighted scatterplot smoothing) smooth line. All correlations are significant ($p < 0.05$).

3.3 Results

NSE from 10-fold cross-validation showed the predictive performance of the BRT model for RS-Chl (NSE = 0.350, se = 0.026) was significantly (t -test $p < 0.05$) better than that of MLR (NSE = 0.214, se = 0.003) (Figure 3-4).

In the BRT model, the residual significantly ($p < 0.05$) increased with ln(Chl). However, the trend fitted by GAM only explained 4.42% of the total residual variance, indicating a weak trend in the residuals (Figure

3-5). After replacing GAM with the linear model, the trend explained 4.28% of the total residual variance, which was even lower than GAM that accounted for non-linear trends.

Systematic trends ($p < 0.05$) in the RS-Chl BRT model residuals were related to $\ln(\text{NVSS})$ (*i.e.*, sediments) and $\ln(\text{A}440\text{nm})$ (*i.e.*, CDOM), but the GAM functions indicated these trends were relatively weak (Figure 3-6). They only explained 6.73% and 4.64% of the total residual variance, respectively. The RS-Chl BRT model residual increased with $\ln(\text{NVSS})$, levelling off near zero with $\ln(\text{A}440\text{nm})$.

Adding sediments and CDOM in the RS-Chl BRT model increased model performance significantly ($p < 0.05$), from $\text{NSE} = 0.350$ ($\text{se} = 0.026$) to $\text{NSE} = 0.453$ ($\text{se} = 0.019$). The improved performance confirmed that the systematic errors were *related to*, but not necessarily caused by, sediments and CDOM. Parsing out the chlorophyll- a correlations with sediments and CDOM, the new residual (*i.e.*, partial residual) trends were different from the corresponding theoretical ones (Figure 3-7, Figure 3-8). More specifically, the partial residual slightly increased with $\ln(\text{NVSS})$ at first and then dipped down and bounced up. Theoretically, the residuals should have increased and then plateaued with higher reflectance due to higher sediment concentrations. For CDOM, the partial residual dipped down then bounced up with $\ln(\text{A}440\text{nm})$. Theoretically, the residuals should have linearly decreased then plateaued with increasing CDOM that resulted in lower reflectance. The differences in observed and theoretical relationships indicated that the residual trends in the RS-Chl BRT model was not likely caused by sediments or CDOM. Moreover, the magnitude of the partial residual change over $\ln(\text{NVSS})$ or $\ln(\text{A}440\text{nm})$ was much smaller than the original ones without parsing out the chlorophyll- a correlation. Specifically, the range of residual change over $\ln(\text{NVSS})$ decreased from 1.2 to 0.11 after parsing out the chlorophyll- a correlation. The range of residual change over $\ln(\text{A}440\text{nm})$ decreased from 0.7 to 0.30 (Table 3-2). That indicated a weaker trend related to sediments or CDOM after parsing out the chlorophyll- a correlation.

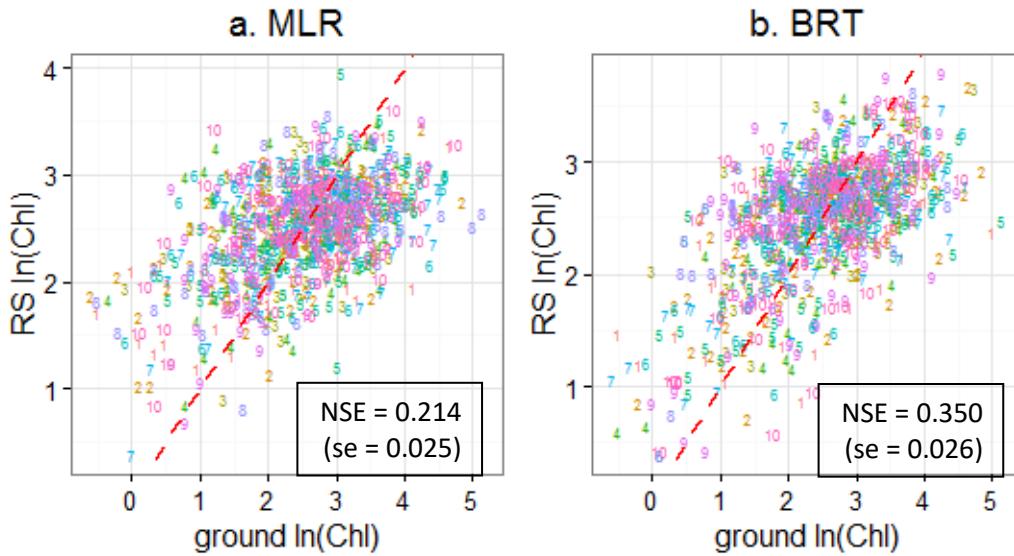


Figure 3-4 Ten-fold cross-validation for remote sensing (RS) of chlorophyll- α concentrations (Chl, $\mu\text{g/L}$) using two different algorithms: (a) multiple linear regression (MLR), and (b) boosted regression trees (BRT). The dashed line is the one-to-one ratio line. Predicted values of 10 cross-validations are coded with corresponding numbers where number i indicates the i -th validation.

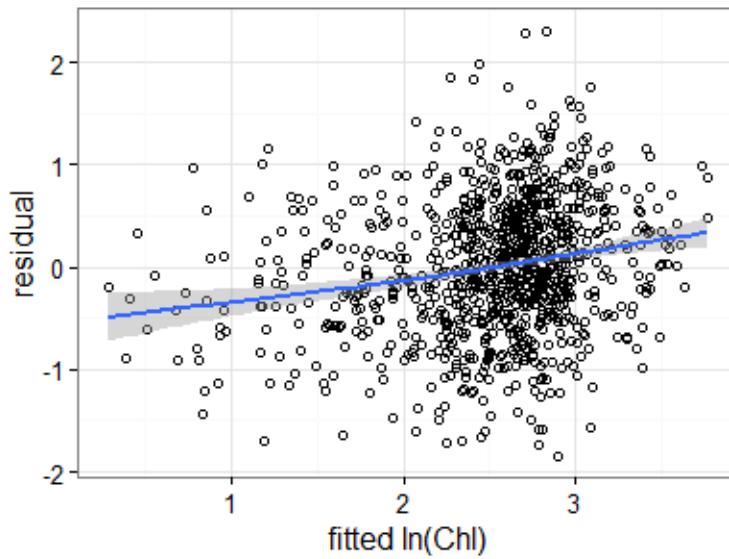


Figure 3-5 Residual plot of the remote sensing BRT model for chlorophyll- α (Chl). The solid line is the GAM (generalized additive models) smooth line with 95% confidence intervals on two sides.

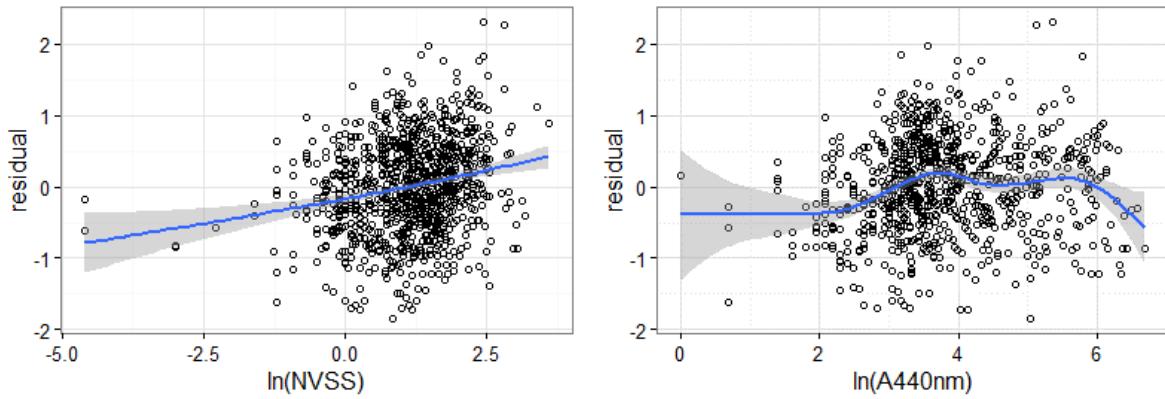


Figure 3-6 Residuals related to (a) sediments and (b) CDOM (colored dissolved organic matter). Solid lines are GAM (generalized additive models) smooth lines with 95% confidence intervals on two sides. NVSS – non-volatile suspended solids; A440nm – absorbance coefficient measured at 440 nm wavelength.

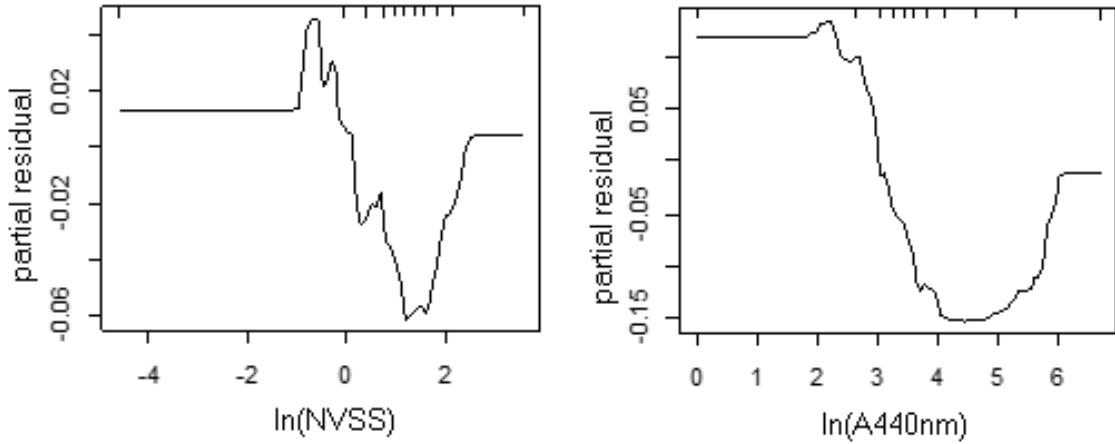


Figure 3-7 Partial dependence plots indicating residual changes over (a) $\ln(\text{NVSS})$ (suspended sediments), and (b) $\ln(\text{A}440\text{nm})$ (colored dissolved organic matter, CDOM). The bars on the top indicate data distribution in deciles.

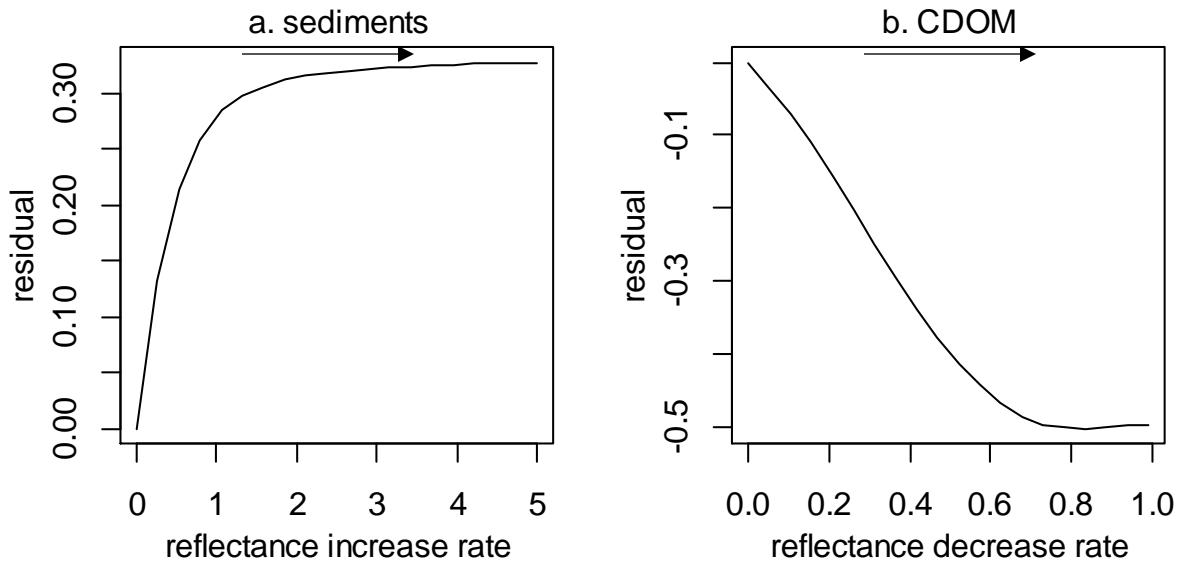


Figure 3-8 Theoretical residual changes: (a) residual increases with higher sediment concentrations then reaches a plateau, and (b) residual decreases with higher CDOM (colored dissolved organic matter) concentrations then reaches a plateau.

Table 3-2 The range of residual trend decreased after parsing out the sediment and CDOM correlations with chlorophyll-*a*.

	Min.	Max.	Max.- Min.
Partial residual changing with $\ln(\text{NVSS})$	-0.06	0.05	0.11
Partial residual changing with $\ln(\text{A}440\text{nm})$	-0.15	0.15	0.30
Original residual changing with $\ln(\text{NVSS})$	-0.8	0.4	1.2
Original residual changing with $\ln(\text{A}440\text{nm})$	-0.5	0.2	0.7

3.4 Discussion

3.4.1 Model performance

The MLR algorithm for chlorophyll-*a* explained 21.4% of *in-situ* chlorophyll-*a* variance in 39 Missouri reservoirs over 24 years. Although there are models for chlorophyll-*a* using Landsat TM/ETM+ with higher performances in the literature, those models were often calibrated for one lake or multiple lakes

covered by one scene of a satellite image where atmospheric conditions and perhaps water constituents were more homogeneous than in our study. For example, Brivio et al. (2001) found that the model “ $\text{Chl} = 9.82(\text{Band 1} - \text{Band 3})/\text{Band 2}$ ” explained 81.8% of *in-situ* chlorophyll-*a* (Chl) variance over one TM scene in March 1993 in Lake Garda, but the model explained less than 20% of variance in another TM scene in February 1992. In the latter TM scene, a different model was the best, *i.e.*, “ $\ln(\text{Chl}) = 0.52 \ln(\text{Band 1}) - 0.79 \ln(\text{Band 2})$ ”. Even though they had applied an atmospheric correction using the “integrally image-based” method in the TM images, the models still could not be transferred between two scenes (dates) covering the same lake. In our study, TM/ETM+ images were gathered over 24 years, and over a large area with 39 reservoirs that spanned 15 Landsat scenes. A relatively low MLR model performance was therefore expected considering the spatial and temporal variations of atmosphere and water optical characteristics.

BRT had better performance than MLR for estimating chlorophyll-*a* from Landsat TM/ETM+ surface reflectance. That better performance might be due to (1) insensitivity to extreme values, (2) capability to fit complicated non-linear relationships, and/or (3) machine learning to fit interactions among variables. The predictive performance of BRT was stronger than MLR. Therefore, BRT is recommended over MLR as the algorithm for chlorophyll-*a* remote sensing in the future.

3.4.2 Sediments and CDOM effects

3.4.2.1 The method for detecting effects

A relationship between sediments or CDOM with residuals from the RS-Chl model could be due to a missing variable, a missing higher-order term of a variable, or a missing interaction between variables. BRT had likely taken care of non-linear relations like having a higher-order term to explain non-linearities in other model types, and BRT also likely accounted for interactions. Therefore, the residuals are likely related to variables that were not included in the original model, such as sediments or CDOM.

However, BRT is based on thousands of decision/regression trees, which do not show direct relationship between independent and dependent variables as MLR does. So, it was hard to predict how residuals changed with sediments or CDOM based on the BRT model. Alternatively, this study simulated theoretical residual trends by changing the bands and band ratios in the RS-Chl BRT model according to the sediments and CDOM effects on band reflectance. Remote sensing reflectance may increase less at very high sediment concentrations. However, within the range of our sediment data, it was reasonable to assume reflectance decreased linearly with sediment concentrations (Han 1997). The same applied to the CDOM effect. In water with very high CDOM concentrations, the reflectance is very low due to light absorption of CDOM and a less reflectance decrease is expected at higher CDOM concentrations. Nonetheless, the general increase or decrease in the theoretical trends still held even when sediments or CDOM concentrations were very high.

3.4.2.2 Explanations for the insensitivity to suspended sediments and CDOM

After parsing out the chlorophyll- a correlation, the residual trends related to sediments and CDOM did not agree well with the theoretical trends that generally increased with sediments and decreased with CDOM. There is no doubt that sediments and CDOM can affect water-leaving radiance. However, at-sensor radiance might not be sensitive to sediments or CDOM considering a great amount of errors introduced by the atmosphere, specular reflectance, and so on. The water-leaving radiance in Landsat TM/ETM+ bands only accounts for about 3%-13% of total sensor signal in visual bands, and most radiance is from the atmosphere and from specular reflections from the water surface (Hu et al. 2001). Although atmospheric corrections had been applied in the Landsat TM/ETM+ data we used, the products were prepared for land surface applications and the correction accuracy might not meet the higher requirements for waters and their weaker signals. Moreover, specular reflectance had not been corrected in the Landsat products. When wind speed was high (> 10 m/s), the specular reflectance could

dominate sensor signals (Hu et al. 2001). Note that the RS-Chl BRT model only explained 35.0% of the total variance in the measured chlorophyll-*a*. The model accuracy might not high enough to capture the change of water-leaving radiance due to sediments or CDOM.

Alternatively, the BRT algorithm might be relatively insensitive to sediments or CDOM. Band ratios were found independent of sediments since sediments caused each band to increase by almost the same proportion (Han 1997). At higher wavelength the CDOM absorption is small and has less impact on remote sensing of chlorophyll-*a* (Kutser et al. 2001). Therefore, it was possible for decision trees in BRT using bands and band ratios and their interactions to discriminate sediments and CDOM effects on chlorophyll-*a* estimates.

3.4.3 Model correction

In the RS-Chl BRT model residuals, there was a trend indicating that the model over-predicted the low chlorophyll-*a* concentration values and under-predicted the high ones (Figure 3-5). This bias could be caused by chlorophyll-*a* concentration. When the concentration is low, bottom reflectance might be interpreted as suspended chlorophyll-*a*, resulting in over prediction. When the concentration is higher, we might see more bias if reflectance was saturated and failed to respond to the concentration change. Additionally, other factors that affect the chlorophyll-*a* model performance could contribute to the residual trend, including image signal quality that was affected by atmosphere and wind, and ground measurement quality that was affected by spatial and temporal heterogeneity of algae biomass. Also likely was the effect of the model algorithm that narrowed down the range in the modeled values compared to the measured values (Figure 3-4). Disregarding the error sources, the trend in the model residual could be corrected by using traditional deshrinking approach (Birks et al. 1990; Legendre and Legendre 1998). Specifically, in this case the modeled values were corrected by the equation:

$$M'_i = M_i(1 + 0.25) - 0.62$$

Equation 3-8

where M'_i is the corrected modeled value; and M_i is the original modeled value. This empirical equation was derived from the linear regression function of the original residual against fitted $\ln(\text{Chl})$ (Figure 3-9 a). The correction basically rotated the regression line to the relationship between residuals and fitted $\ln(\text{Chl})$ has both slope and intercept close to zero (*i.e.*, no bias in the new modeled values) (Figure 3-9 b). After correction, the model fitting performance increased from $\text{NSE} = 0.513$ to $\text{NSE} = 0.534$. The range of modeled value expanded from $[0.28, 3.77]$ to $[-0.27, 4.09]$, the latter of which was closer to the measured range, *i.e.*, $[-0.60, 5.15]$. This could be a valuable way to correct the model bias when we do not know what caused the bias.

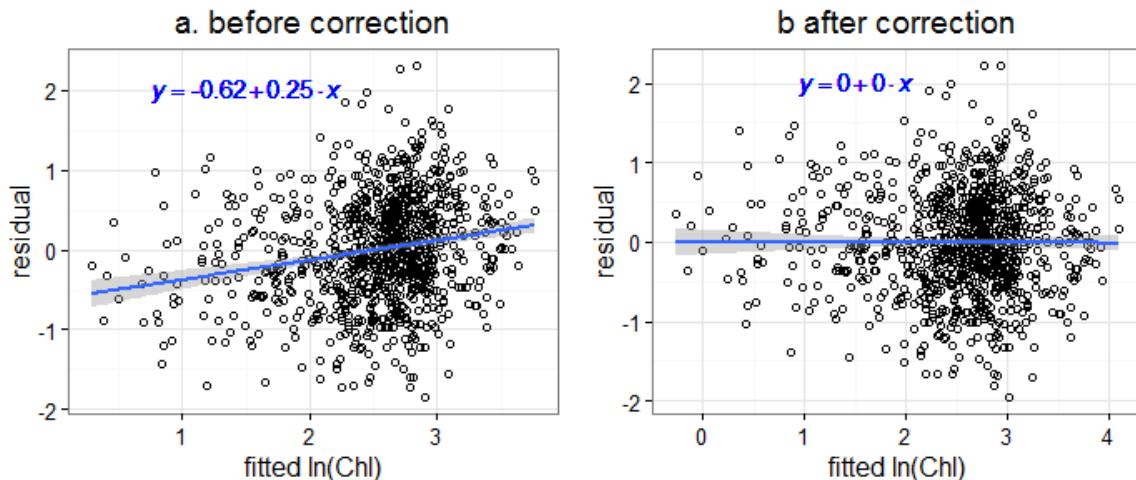


Figure 3-9 Model bias correction using deshrinking. Solid line is the linear regression line with its equation on the top and 95% confidence intervals shown in grey.

3.4.4 Application of the findings

This study showed that BRT is a sophisticated machine-learning algorithm for estimation of chlorophyll- a concentrations in lakes. It performed better than MLR, and was not sensitive to sediments and CDOM. Like other empirical models, the RS-Chl BRT model has limitations for performance in water bodies

having conditions outside the ranges tested in this study. For water bodies with chlorophyll-*a*, CDOM, and NVSS concentrations higher or lower than this study, the findings may not hold true. The data distribution of chlorophyll-*a* concentrations in the reservoir dataset analyzed here is similar to that in the 2007 National Lake Assessment (NLA) in USA (<http://water.epa.gov>, accessed on July 13, 2015). The A440nm median (37.0 m^{-1}) was higher than concentrations reported in other studies, *e.g.*, $0.68 - 11.13 \text{ m}^{-1}$ in 18 lakes over southern Finland and southern Sweden (Kutser et al. 2005) and $0.6 - 19.4 \text{ m}^{-1}$ in 15 Minnesota lakes (Brezonik, Menken, and Bauer 2005). Extremely high NVSS values (NVSS $> 200 \text{ mg/L}$) have been reported in some lakes and rivers, but for most inland lakes, NVSS is less than 20 mg/L (*e. g.*, Lenhart et al. 2009; Pollard et al. 1998; Graham et al. 2004). The NVSS concentrations ranged from 0.01 mg/L to 36.2 mg/L in this study. The RS-Chl BRT model was tested over a relatively wide range of chlorophyll-*a*, sediments, and CDOM compared to other reported ranges, so the findings here can be extended to many other lakes.

3.5 Conclusion

We used a long-term dataset covering 39 Missouri reservoirs and 24 years to compare algorithm performances of MLR and BRT for chlorophyll-*a* estimates in turbid inland waters. We have found that BRT was a better choice than MLR for empirical chlorophyll-*a* models using Landsat TM/ETM+ imagery. Moreover, the BRT-Chl model was not sensitive to sediments and CDOM. Systematic trends were found *related* to sediments and CDOM, but not *caused* by sediments and CDOM.

Acknowledgement

This work was supported by the Environmental Protection Agency (EPA), USA under Grant R835203. The views and opinions expressed in this article are those of the authors and do not necessarily reflect the official policy or position of U.S. EPA, or any other agency of the U.S. government.

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4 LANDSAT SURFACE REFLECTANCE PRODUCTS FOR REMOTE SENSING OF INLAND LAKES: THE PROBLEM OF ATMOSPHERIC INTERFERENCE

Abstract

Inland lake remote sensing has been problematic for both complexity of optical properties in water and the difficulty of atmospheric correction. Atmospheric effects account for most satellite-borne at-sensor radiance over waters. The Landsat surface reflectance products corrected for atmospheric interference are new and have recently been made available. The atmospheric correction method was designed to better account for land surface reflectance for Landsat products. However, whether the new, atmospherically corrected products have the potential to improve inland lake water quality estimates has not been tested. In this study, we examined the relationships between bands and band ratios with three optically sensitive agents in inland lake water, chlorophyll-*a*, sediments, and colored dissolved organic matter (CDOM), using Landsat imagery before and after the atmospheric correction. The results indicated that the atmospheric correction did not improve the signal of chlorophyll-*a*, sediments, and CDOM. The remote sensing accuracy of chlorophyll-*a*, sediments, and CDOM indicated by validation R^2 was 0.329, 0.508, and 0.733, respectively. The atmospheric correction also did not significantly change the predictive model performances. Our findings suggest that improvements for atmospheric correction of Landsat imagery may still be insufficient for inland lake water quality assessments. A more sophisticated method for atmospheric correction is still needed for water applications.

Keywords: Landsat, chlorophyll-*a*, sediment, CDOM, water quality, atmospheric correction

Highlights

- The existing Landsat imagery is useful to monitor water color.
- The corrected imagery did not significantly improve the water color measurements.

4.1 Introduction

Remote sensing of turbid inland lakes has been problematic because optically sensitive agents in water are complex and variable in space and time (Witte et al., 1982) and because atmospheric correction of remotely sensed reflectance is difficult (Wang & Shi, 2007). Hu et al. (2001) estimated that the radiance off water in Landsat ETM+ Band 1 (B1), Band 2 (B2), and Band 3 (B3) respectively only accounted for 13%, 10%, and 3% of the total radiance measured by the sensor for a windless day (wind speed < 2 m/s), the rest of which was mostly contributed by the atmosphere. Therefore, atmospheric correction is critical for remote sensing of inland lakes, especially for long-term and/or large scale studies, where atmospheric effects are variable.

The U.S. Geological Survey recently published a provisional version of surface reflectance (SR) products for Landsat 4-5 TM and Landsat 7 ETM+ that can be freely downloaded (<http://landsat.usgs.gov>, accessed on July 3rd, 2014). The SR products are derived from the TOA (top of atmosphere) reflectance products by removing atmospheric effects using the Landsat Ecosystem Disturbance Adaptive Processing System (LEDAPS), which has the same atmospheric correction routines as MODIS (Moderate Resolution Imaging Spectroradiometer). The latter are based on the 6S (Second Simulation of a Satellite Signal in the Solar Spectrum) radiative transfer models (Masek et al., 2006). The SR products are designed for land applications and may improve the accuracy over waters where atmospheric effects account for most of the at-sensor signal.

The goal of our work was to evaluate these two sets of Landsat data (*i.e.*, SR and TOA) for long-term and/or large-scale studies over inland lakes. More specifically, we evaluated the signal enhancement provided by the atmospheric correction and its impact on remote sensing of water optical characteristics in inland lakes. The image signal was indicated by the relationships between individual bands or band ratios (band/band ratio) and three optically sensitive agents—chlorophyll-*a* (Chl), Non-Volatile Suspended Sediment (NVSS), and Colored Dissolved Organic Matter (CDOM). Both linear and

non-linear empirical algorithms were used to demonstrate how the atmospheric correction affected remote sensing of water optical characteristics. In our evaluation, we took advantage of a set of inland water quality data that included simultaneous measurements of all water color variables over 23 years from 39 reservoirs spanning the long history of Landsat TM/ETM+ images.

4.2 Methodology

4.2.1 Study area and data

Water quality data cover 24 years (1989-2012) of sampling of 39 reservoirs in Missouri, U.S.A. (Jones et al. 2008). Water samples were taken 3-4 times per summer from the surface water column (0.25 m – 0.5 m) near dams in the reservoirs. Chl, NVSS, and CDOM concentrations were measured in composite samples using standard methods (APHA, 1985). CDOM was measured by the absorption coefficient at 440 nm wavelength ($A_{440\text{nm}}$, m^{-1}). The dataset covered wide ranges of water quality: Chl varied from 0.40 $\mu\text{g/L}$ to 184.70 $\mu\text{g/L}$ with mean = 20.03 $\mu\text{g/L}$; NVSS varied from 0.00 mg/L to 107.38 mg/L with mean = 3.39 mg/L; and $A_{440\text{nm}}$ varied from 0.40 m^{-1} to 184.70 m^{-1} with mean = 59.7 m^{-1} .

Both the Landsat TM/ETM+ TOA and SR products were downloaded from the on-demand ESPA Data Access Interface (<http://espa.cr.usgs.gov>, accessed on July 1st, 2014). Remote sensing reflectance of each water quality sample was characterized by average values of a “3 × 3” pixel window with the water quality sampling location as the center pixel. Sampling locations were adjusted (adjusted distance < 100 m) to make sure no mixed pixel with land and water was in the window. Both TM and ETM+ data within 8 days before or after the water quality sampling dates were used to provide as many data pairs with water quality sampling as possible. Pixels with clouds, shadows, saturated values, and ETM+ gaps due to SLC (Scan Line Corrector) failure were excluded using the “*Fmask*” layer in the SR products. We applied extra criteria to remove any SR pixel with reflectance less than zero, or $B2 < B4$ (to remove pixels of land or shadows), or $B2 > 0.015$ (to remove pixels of clouds or with strong “whitecap” reflectance). In total,

963 remote sensing records (SR and TOA) corresponding to *in-situ* water quality samples were produced. This long-term dataset should cover Landsat TM/ETM+ with a variety of atmospheric conditions.

4.2.2 Signal enhancement evaluation

We built a non-linear machine-learning model by using the random forest algorithm (RF) (Breiman, 2001) for each band/band ratio with the optically sensitive agents in water as independent variables:

$$Bi = RF (\text{Chl}, \text{NVSS}, \text{A440nm}) \quad \text{Model 4-1}$$

where Bi is reflectance (dimensionless) of the i^{th} Landsat TM/ETM+ band or band ratio from the SR or TOA products, *i.e.*, B1, B2, B4, B5, B7, B1v2 (ratio of B1 vs. B2), B1v3, B1v4, B2v3, B2v4, *etc.* (the thermal band, B6, was not included since it indicates object temperature regardless of the agent concentration); RF is the random forest algorithm; Chl, NVSS, and A440nm are indicators of optically sensitive agents. If the signal of the SR products has been enhanced over the original TOA products, then the Bi of the SR products should be better explained by the optically sensitive agents rather than the Bi of the TOA products. The model performance was indicated by the coefficient of determination (R^2) from the out-of-bag validation.

The contribution of each optically sensitive agent in Model 4-1 was measured to further investigate the signal combinations and their changes resulting from the atmospheric correction. The contribution is indicated by a partial R^2 , which is the model total R^2 multiplied by the relative importance of the optically sensitive agent (predictor). The relative importance of each predictor is the sum of instances that the predictor is used to split over a random forest, weighted by the model deviation decrease due to each split, and rescaled to have a sum predictor importance of one.

The R package “*gradientForest*” (version 0.1-17) (Ellis, Smith, & Pitcher, 2011) was used to calculate the total R^2 and partial R^2 in Model 4-1. The package “*gradientForest*” is a revised version of “*randomForest*” (Breiman, 2001) with extra functions and improvements including those that address correlated predictors and allowing multiple random forests to be built for multiple response variables (the bands and band ratios in our case) analyzed in one run. The significance of the improvement resulting from the atmospheric correction was evaluated by the pairwise *t*-test using the “*t.test*” function in R (version 3.2.1). More specifically, the R^2 s of Model 4-1 using TOA and SR were compared pairwise for each band/band ratio. The Shapiro-Wilk normality test (Royston, 1995), using the “*shapiro.test*” function in R, was run on ΔR^2 to make sure the data were normally distributed before the pairwise *t*-test was applied.

4.2.3 Remote sensing of water optical characteristics

The signal change in the individual bands/band ratios may or may not affect the remote sensing models for water color that use those bands/band ratios. To test whether performance of the remote sensing model was changed by the atmospheric correction in the SR products, we built separate models for each

$$\text{Optically sensitive agent} = f(\text{bands, band ratios}) \quad \text{Model 4-2}$$

optically sensitive agent measurement using either multiple linear regression (MLR) or RF algorithm and either TOA or SR dataset:

where optically sensitive agent was Chl, NVSS, or CDOM (indicated by A440nm); f was MLR or RF; bands and band ratios were from both the SR or TOA products. Model 4-2 was the same as Model 4-1, except the independent and dependent variables were reversed. Model performance was indicated by R^2 from the 10-fold cross validation. The R package “*randomForest*” was used to build random forest models and the “*lm*” function in R was used to build MLR models. The significance of the improvement resulting from the atmospheric correction was evaluated using the Welch two-sample *t*-test (the “*t.test*” function in R). More specifically, each model had 10 R^2 values from the 10-fold cross validation; the R^2 values of

the TOA model were compared with the R^2 values of the SR model using the *t*-test. The Shapiro-Wilk normality test using the “*shapiro.test*” function in R was run on each group of R^2 s ($N = 10$) from the 10-fold cross validation to make sure the data were normally distributed before the Welch two-sample *t*-test was applied.

4.3 Results

4.3.1 Signal change

Indicated by the *total* R^2 of Model 4-1, the atmospheric correction did not significantly (pairwise *t*-test $p = 0.602$) improve relationships between individual bands or band ratios and the water optically sensitive agents (*i.e.*, Chl, NVSS, and CDOM) (Figure 4-1a, b). More specifically, some bands and band ratios appeared to have relatively weaker relationships with the water optically sensitive agents after the atmospheric correction, but the others did not. The R^2 for TOA bands and band ratios ranged from 0 to 0.633 (mean = 0.271). The R^2 for SR bands and band ratios ranged from 0 to 0.577 (mean = 0.226). B1v3, B2v3, B1v2, and B3 were four bands/band ratios had total $R^2 \geq 0.5$ in the TOA models, with total R^2 of 0.634, 0.624, 0.522, and 0.521. After the atmospheric correction, the total R^2 did not increase but decreased by 8.9%, 13.2%, 45.7%, and 4.5%. Some bands/band ratios had higher total R^2 after the atmospheric correction, such as B3v4 with total R^2 increasing from 0.291 to 0.552.

The *partial* Chl R^2 for most of the bands and band ratios significantly (pairwise *t*-test $p = 0.011$) increased after the atmospheric correction, with the average (aggregated for all bands and band ratios) partial R^2 changing from 0.059 of the TOA models to 0.063 of the SR models (Figure 4-1 c). The partial R^2 of NVSS and CDOM did not change significantly (pairwise *t*-test $p = 0.844$ for NVSS, 0.848 for CDOM) with the atmospheric correction (Figure 4-1 d and e).

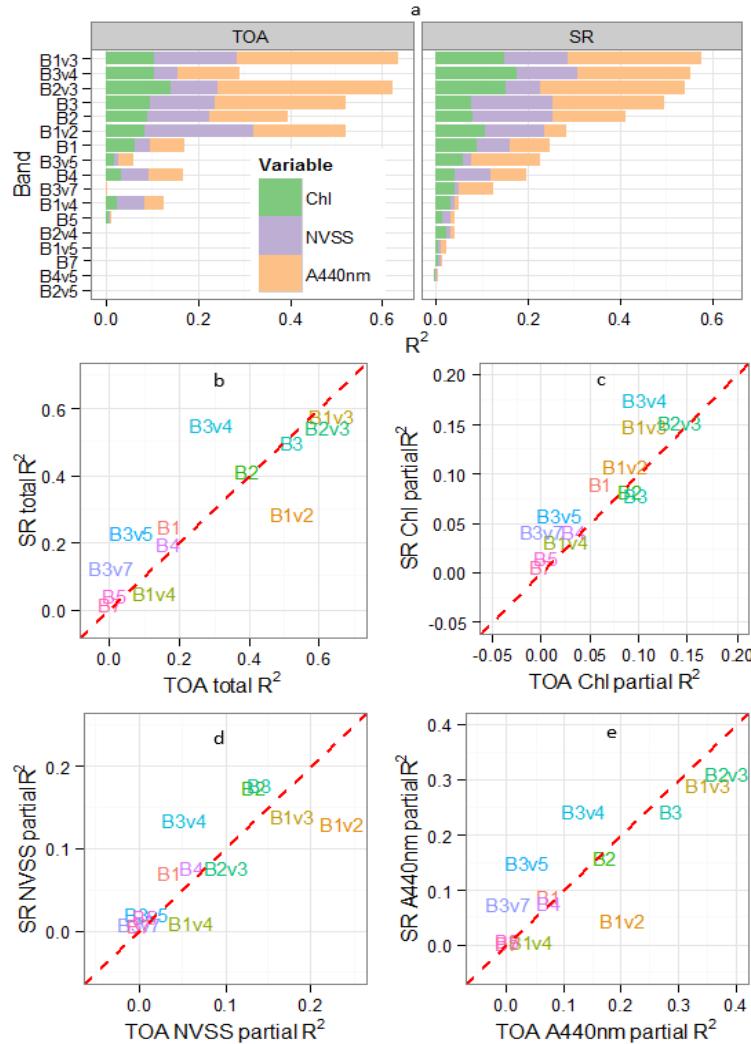


Figure 4-1 Water color signal in Landsat TM/ETM+ as changed by the atmospheric correction. The image signal is indicated by R^2 of models for bands/band ratios: $B_i = RF$ (Chl, NVSS, A440nm), where B_i is the TOA (top of atmosphere) or SR (surface reflectance) band/band ratio with i indicating the band number or combination of bands in ratios, e.g., $B_1 = \text{Band } 1$, and $B_{1v2} = \text{ratio of Band } 1 \text{ vs. Band } 2$. RF is the random forest algorithm. Chl is chlorophyll-a concentration. NVSS is concentration of non-volatile suspended solids. A440nm is absorbance coefficient at 440 nm wavelength (indicator of colored dissolved organic matter). Figure a has the same information as b-e, which are scatter plots comparing either the total or partial R^2 before and after the atmospheric correction. The dashed line is the 1:1 line in b-e.

4.3.2 Remote sensing of water optics

No significant (two-sample t -test $p > 0.05$) improvement was found in remote sensing of water optical characteristics with the new atmospheric correction of Landsat imagery, except for Chl measurements when using the MLR algorithm (Table 4-1). More specifically, the Chl measurement accuracy indicated by the R^2 from 10-fold cross validation was improved significantly (two-sample t -test $p = 0.038$) by the atmospheric correction when MLR was used as the algorithm, with R^2 increasing from 0.148 ($SD = 0.068$) to 0.219 ($SD = 0.065$). However, when the RF algorithm was used to measure Chl, which performed better than the MLR algorithm, the improvement was not significant (two-sample t -test $p = 0.585$), changing from 0.312 ($SD = 0.061$) to 0.329 ($SD = 0.068$). The NVSS and A440nm measurement accuracies were not affected by the atmospheric correction no matter which algorithm was used (MLR or RF). Remote sensing of NVSS and A440nm using RF algorithm had 10-fold cross validation R^2 of 0.508 ($SD = 0.042$) and 0.733 ($SD = 0.054$), respectively.

4.4 Discussion

4.4.1 Why did the atmospheric correction produce no obvious signal enhancement?

The atmospheric correction with SR products did not significantly improve relationships between Landsat data and optically sensitive agents (*i.e.*, Chl, NVSS, and CDOM). The amount of variation explained in bands and band ratios by the three optically sensitive agents varied with band/band ratio, but was not consistently higher for SR than TOA products. The most informative bands and band ratios, *i.e.* B1v3, B2v3, B1v2, and B3, even decreased after the atmospheric correction. Partial R^2 values were consistently but only slightly higher for Chl with SR versus TOA products, but there was no difference in partial R^2 for NVSS and CDOM.

Table 4-1 Effects of the atmospheric correction on performances of water color models when using MLR and RF algorithms for models. The *t*-test compares the R^2 for 10 cross validations of TOA and SR models with either MLR or RF algorithms.

Optically sensitive agent	Algorithm f	Image	10-fold CV R^2		<i>t</i> -test <i>p</i> value*
			Mean	SD	
Chl	MLR	TOA	0.148	0.068	0.038
		SR	0.219	0.066	
	RF	TOA	0.312	0.061	0.585
		SR	0.329	0.068	
NVSS	MLR	TOA	0.477	0.081	0.813
		SR	0.487	0.086	
	RF	TOA	0.505	0.092	0.917
		SR	0.508	0.042	
A440nm	MLR	TOA	0.614	0.095	0.192
		SR	0.671	0.080	
	RF	TOA	0.731	0.062	0.934
		SR	0.733	0.054	

Table notes: (1) **p* of two tails in the Welch two-sample *t*-test; two samples are two rows on the left. (2)

Water color model: optically sensitive agent = f (bands, band ratios). (3) Model performances are indicated by R^2 of 10-fold cross validation (CV). (4) Abbreviations: Chl, chlorophyll *a* concentration; NVSS, concentration of non-volatile suspended solids; A440nm, absorbance coefficient at 440 nm wavelength (indicator of coloured dissolved organic matter); MLR, multiple linear regression; RF, random forest; TOA, top of atmospheric reflectance; SR, surface reflectance; SD, standard deviation.



Figure 4-2 (a) Average reflectance in the 39 reservoirs as changed by the atmospheric correction; (b) band signal (indicated by R^2) as changed by the atmospheric correction. Figure 4-2 b is the same as Figure 4-1 a except that the band ratios are excluded and the bands are in a different order for comparison with Figure 4-2 a. See Figure 4-1 for abbreviations.

Several factors could explain why optically sensitive agents did not explain more variation in bands or band ratios when using TOA versus SR: (1) Atmospheric reflectance could have been relatively small compared to other errors such as specular reflectance (A.K.A. whitecap effect), so no obvious improvement was seen after a correction of minor errors; (2) Atmospheric reflectance could be relatively large, but with small spatial and temporal variation; so, no enhancement was seen when the atmospheric correction subtracted almost the same amount of reflectance from the TOA bands regardless of spatial and temporal variations expected for atmospheric effects; and/or (3) Atmospheric reflectance could be relatively large and could have large spatial and temporal variations, but low

accuracy of the atmospheric correction resulted in a lack of detectable improvement. We address each of these hypotheses in the following paragraphs.

First, was the atmospheric effect small relative to the total TOA reflectance? The atmosphere contributes more than 90% of sensor radiance signal over oceanic water (Gordon & Wang, 1994). The atmospheric proportion over inland waters might be less than the oceanic water due to stronger water-leaving radiance but still it is likely large (Hu et al., 2001). The total amount of atmospheric correction in our case was remarkable, especially in visual bands. The average reflectance in 39 reservoirs during 23 years decreased after the correction by 59.0%, 32.4%, 28.5%, 12.3%, 3.7%, and -8.4% respectively for bands B1, B2, B3, B4, B5, and B7 (Figure 4-2 a).

The whitecap effect was not corrected in the SR products. The specular reflectance caused by wind, waves, and resulting foam is independent of image band wavelength. The average reflectance of foam water was about 22% when taking into account the foam states (from forming to extinction) (Koepke, 1984). The fraction (r) of sea surface covered by foam is a function of wind speed (W): $r = 2.95 \times 10^{-6} W^{3.52}$ (Monahan & Muircheartaigh, 1980).

Therefore, the whitecap reflectance is about $22\% \times r$. An open area, such as Maryville, Missouri, had wind speed less than 8 m/s at 10 m above the land surface (Abatzoglou, 2013) (Figure 4-3 a). If the wind speed over water was less than 8 m/s and the TOA average reflectance over the 39 reservoirs was 0.105, 0.085, 0.061, 0.053, 0.019, and 0.013 for B1, B2, B3, B4, B5, and B7, respectively, then the whitecap reflectance should account for less than 0.81%, 1.02%, 1.40%, 1.63%, 4.44%, and 6.78% of for B1, B2, B3, B4, B5, and B7 reflectance (Figure 4-3 b). The wind speed over the reservoirs might be higher than over land for extra mesoscale winds associated with land-lake pressure gradient (lake and land breezes). On the other hand, the actual r in inland lakes might be much smaller for shorter wind fetch distance than

the ocean. If these unquantified sources of error in whitecap effects on reflectance are small or cancel each other, which is likely, then the whitecap effect should not be a major error source for reflectance.

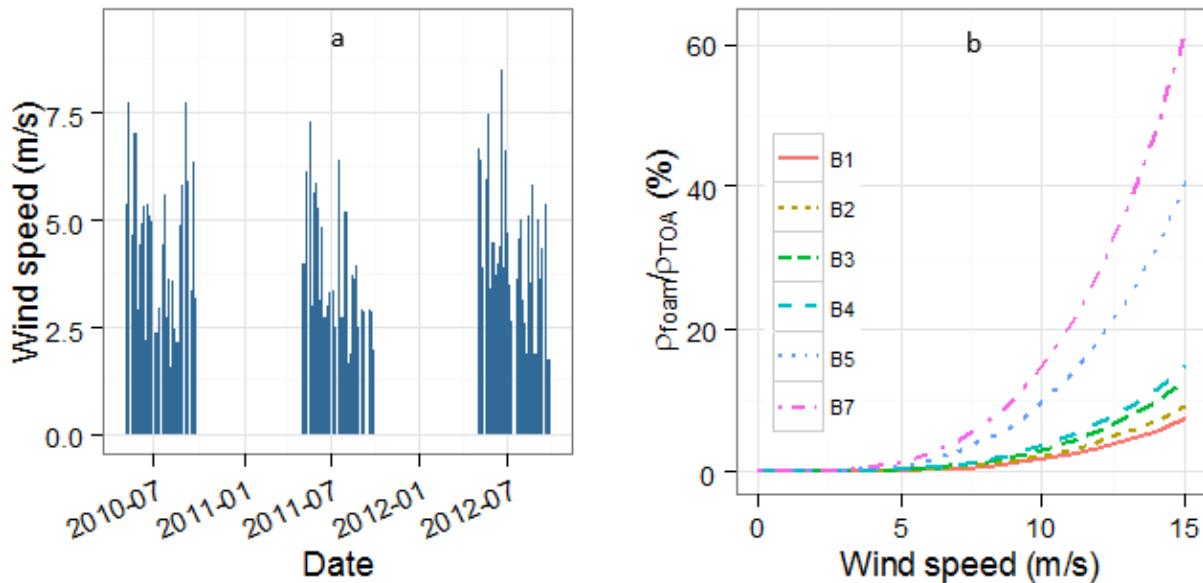


Figure 4-3 (a) Sumer wind speed at Maryville, Missouri, USA; (b) whitecap effect for each Landsat TM/ETM+ band, i.e., B1, B2, B3 etc. Wind speed data are from GRIDMET (University of Idaho Gridded Surface Meteorological Dataset) (Abatzoglou 2013). Y-axe in (b) is $(\rho_{foam}/\rho_{TOA}) * 100\%$, where ρ_{foam} is reflectance of foam caused by wind, calculated by empirical equations (Koepke 1984; Monahan and Muircheartaigh 1980); ρ_{TOA} is average TOA reflectance in the Missouri reservoirs.

Regarding the second hypothesis, the atmospheric effects likely had large variation over time and space and therefore the correction should have been effective. There are two aerosol measurement stations in Missouri: Mingo Station and S. Louis University Station in the AERONET (AErosol RObotic NETwork, <http://aeronet.gsfc.nasa.gov>, accessed on Jan 2nd, 2016). The aerosol optical depth (AOT) measured by the sun spectral photometer was highly variable over time and space (Figure 4-4), indicating a highly variable atmospheric effect that proportionally changed with the AOT. In the SR products, the correction for each reservoir varied substantially, with B1 (the band influenced by atmosphere the most)

decreasing by 30% to 80% over the TOA reflectance (Figure 4-5). Therefore, both the atmospheric effect and the correction had large variation over time and space.

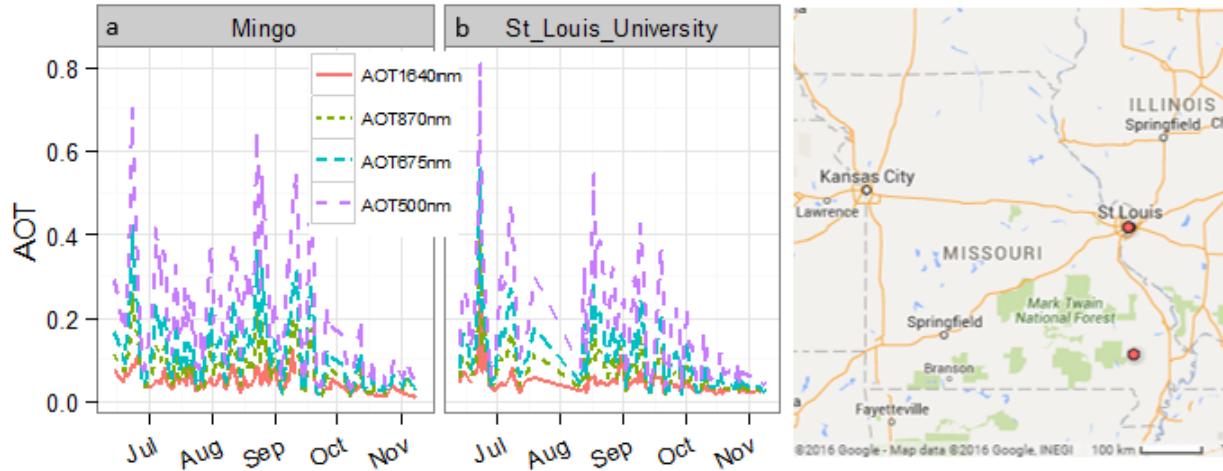


Figure 4-4 Spatial and temporal variations of aerosol optical thickness (AOT, dimensionless) in 2013 measured at the AERONET stations: (a) Mingo, Missouri; (b) St. Louis University, Missouri (data source: Pendley, <http://aeronet.gsfc.nasa.gov>, accessed on Jan 2nd, 2016). Locations of the stations are indicated on the right map: top solid dot as St. Louis University Station; bottom solid dot as Mingo Station. 550 nm, 675 nm, 870nm, and 1640nm is in the range of Landsat TM/ETM+ B1, B3, B4, and B5, respectively.

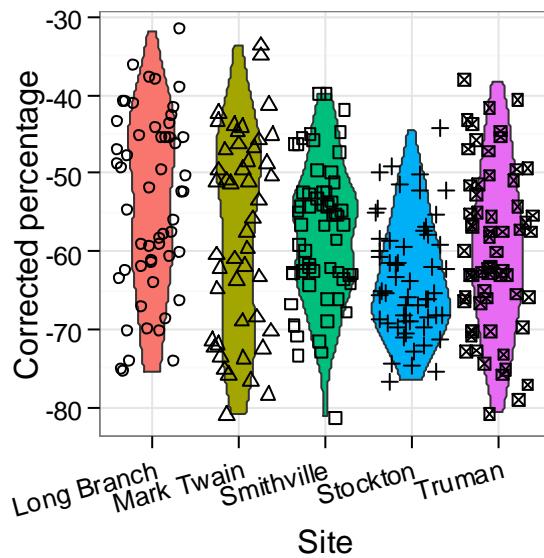


Figure 4-5 Violin plot of the atmospheric correction in band 1 (the band with the strongest atmospheric effect) in five of the Missouri reservoirs as examples. Corrected percentage = $(SR-TOA)/TOA \times 100\%$, where SR is surface reflectance and TOA is top of atmospheric reflectance. Each side of a violin is a kernel density estimation line.

After excluding the possible explanations (1) and (2) for lack of improved performance of SR versus TOA products, the final hypothesis is the atmospheric correction had not reduced signal error even though a substantial amount of “atmospheric effect” may have been removed. AOT is estimated by assuming zero water-leaving radiance at red and infrared bands over oceanic water with phytoplankton-pigment concentration less than 0.25 µg/L (Gordon & Wang, 1994). The zero assumption is not true over turbid waters and that has caused difficulty in atmospheric correction for turbid water remote sensing. The dark dense vegetation (DDV) method used in the Landsat atmospheric correction assumed that without aerosol effects the blue (B1) and red (B3) reflectance over DDV is a 0.25 and 0.5, respectively, of the reflectance at short-wave infrared (2.2 mm, B7, barely affected by atmosphere). The AOT was estimated by differentiating B7-estimated B1 and B3 (no atmospheric effect) and actual TOA B1 and B3 (with

aerosol effects). The uncertainty of the method was within 0.006 in both B1 and B3 (Kaufman et al., 1997). The 0.006 of uncertainty in the Missouri reservoirs indicates errors of 56.9% and 97.6% compared to the average reflectance of B1 and B3, respectively. The reflectance over water is very weak especially in red and infrared areas where water absorbs most of the incoming radiation. Thus, accuracy of the atmospheric correction method may be good enough for land surfaces, but probably not for water bodies. The atmospheric correction may have removed some errors associated with the atmosphere, but the same amount of magnitude of other errors might have been introduced into the data by the correction.

4.4.2 Remote sensing of water optical characteristics

Since the atmospheric correction did not significantly improve the signal related to the optically sensitive agents, it was not surprising that SR products did not produce models to measure optically sensitive agents better than TOA products. However, no improvement in the water color models did not necessarily mean no improvement in image quality, since using band ratios versus just bands are believed to be able to partly remove atmospheric errors and have been widely used (Gilerson et al., 2010; Griffin, Frey, Rogan, & Holmes, 2011; e.g., Han, Rundquist, Liu, Fraser, & Schalles, 1994; Menken, Brezonik, & Bauer, 2006). Nonetheless, if the atmospheric correction had better accuracy, more improvement should have occurred in the remote sensing of water quality variables.

Our results indicate potential uses of Landsat data in large-scale, long-term studies with or without the atmospheric correction. The RF model for A440nm was very good ($R^2 = 0.733$, SD = 0.054) in the 39 reservoirs during more than two decades (23 years), despite the water-leaving signal from water being very weak compared to land surfaces. Relatively worse performance in NVSS and Chl may be due to larger optical variation related to these properties. The size distribution and composition of suspended particles could substantially change their optical properties (Karabulut & Ceylan, 2005). Chl is only one of many pigments in algae and its optical relationship with remote sensing signal may be affected by

algal species composition and other optically sensitive agents (sediments and CDOM) (Han et al., 1994). Chl, NVSS, and A440nm are strongly correlated (Spearman $\rho > 0.4$, $p < 0.001$) in the Missouri reservoirs. It is beyond the scope of this study to investigate the discrimination capability of specific algorithms for one optically sensitive agent from the others (Lin et al., in preparation). Nevertheless, we are very optimistic about using Landsat data in large-scale, long-term ecological studies over inland lakes. Based on our knowledge, this is the first study evaluating the Landsat SR products in inland lake applications. The results will help make decisions about using the data and selecting whether to use the TOA or SR products.

4.5 Conclusion

The reflectance of visual bands in the Landsat TM/ETM+ TOA products substantially decreased after the atmospheric correction, but the predictive relationship between the SR band/band ratios and optically sensitive agents (*i.e.*, Chl, NVSS, and CDOM) was not enhanced. That indicates the accuracy of atmospheric correction was not good enough for remote sensing of water color over inland lakes. Using the SR versus TOA products may slightly but not significantly improve the water color remote sensing, especially when the machine-learning algorithm RF was used. Validation R^2 of the SR model using RF algorithm for Chl, NVSS, and CDOM was 0.329, 0.508, and 0.733 in the dataset of 23 years and 39 reservoirs in Missouri, suggesting Landsat imagery could be used in long-term and/or large-scale studies of water color.

Acknowledgement

This work was supported by the Environmental Protection Agency (EPA), U.S.A. under Grant R835203. We thank Brent Holben for establishing and maintaining the AERONET sites in Missouri.

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5 ALGAL BIOMASS RESPONSES TO CLIMATE CHANGE IN MISSOURI RESERVOIRS

Abstract

More intense precipitation projected with climate change could bring more nutrients from watersheds to lakes, which with projected warming, create conditions conducive for algal blooms. This hypothesis has rarely been tested with long-term (decadal) lake observation data mostly due to lack of whole-lake long-term algal biomass data. In this study, 28 years (1984-2011) of observations of algal biomass in four reservoirs in Missouri (USA) were derived from remote sensing imagery (Landsat TM), providing an opportunity to link the time series of climate change with the time series of algal biomass responses. The result shows that neither temperature nor precipitation was the only factor that predicted lake chlorophyll concentrations. With the increases in lake surface water temperature and precipitation intensity (mm/d), algal biomass more likely responded to temperature than precipitation. The rising temperature affected mean annual chlorophyll more than summer chlorophyll, indicating that projected warming might result in the expansion of the algal growth season rather than increasing the summer peak concentration. Summer algal biomass might increase with increasing spring precipitation in the study reservoirs.

Keywords: algal bloom, climate change, global warming, precipitation, lake surface temperature, remote sensing

Highlights

- The trend of lake chlorophyll in four reservoirs did not closely track the trend of temperature or precipitation during 28 years.
- The algal growth season may expand with global warming.
- Climate change may result in higher summer algal biomass due to higher spring precipitation.

- Daily precipitation and daily temperature together explain up to 50.6% of the variance in daily chlorophyll across 13 sites.

5.1 Introduction

5.1.1 Climate change

Climate change models have projected that surface temperature will rise during the 21st century, and it is “very likely” that extreme precipitation will be more frequent and intense in many regions (IPCC 2014). More specifically, this report indicates that over North America, mean annual temperatures are projected to rise between 2 °C and 4 °C (depending on scenario) by the end of the 21st century over most land areas. This warming is predicted to occur in all seasons, but especially in winter over high latitudes. The report also indicates that mean annual precipitation in the late century will “very likely” increase in most areas of the United States and Canada. Increasing precipitation in the United States and Canada is predicted to occur in winter, with an increasing fraction falling as rain rather than snow, due to increasing winter temperature. Extremely hot or dry summer seasons are predicted to occur over much of North America.

5.1.2 Harmful algal blooms

Harmful algae, particularly Cyanobacteria, may grow faster at higher temperatures than other algal groups (such as green algae and diatoms) (Paerl and Paul 2012). Deeper and longer stratification followed by nutrient depletion in the epilimnion favors the buoyant and nitrogen-fixing Cyanobacteria (Dokulil and Teubner 2000). On top of that, more nutrient loading due to more intense and extreme precipitation may create more favorable conditions for algal blooms (Robson and Hamilton 2003). Because of these drivers, Paerl and Huisman (2008) predicted more harmful algal blooms in the future with warmer temperature and more variable precipitation. The hypothesis was later tested by other researchers with coupled mechanistic models (HSPF, UFILS4, and AQUATOX) in Onondaga Lake (New York State, USA), and the results showed that biomass of both green algae and Cyanobacteria increased

with climate change, and Cyanobacteria did not necessarily outcompete green algae to form harmful algal blooms (Taner, Carleton, and Wellman 2011). This appears to contradict the prediction of Paerl and Huisman (2008). Additionally, observational data in the New River Estuary and Neuse River Estuary (North Carolina, USA) showed that algal biomass could not accumulate after extreme events because of flushing and light limitation (Paerl et al. 2014). Thus, algal responses to climate change may vary greatly among individual lakes depending on location, climate, basin landscape, lake morphology, internal nutrient sources, and food web interactions (Blenckner 2005).

5.1.3 Complex system

Complex processes between climate and algal production may generate different outcomes. Algal blooms occur with specific combinations of factors, not just one factor (*e.g.*, temperature) (Dokulil and Teubner 2000). For example: (1) Higher winter temperatures may cause more melting of snow and subsequent water flow, potentially producing more winter nutrient loading. On the other hand, at higher temperature, higher rates of denitrification and nutrient assimilation in soil may reduce winter nitrate concentrations in lakes (George, Jarvinen, and Arvola 2004; Marshall and Randhir 2008). (2) Extreme precipitation events in summer potentially increase peak flows and nutrient loading, but the total flow may decrease if there is also higher evapotranspiration, offsetting the additional nutrients in event flows (Taner, Carleton, and Wellman 2011; Praskievicz and Chang 2011). (3) Impacts of additional nutrient inputs to lakes may happen quickly, but it could take more than two to eight years to see long-term responses (Slavik et al. 2004; Schindler 2012). The in-lake community responses are much more complicated than lake physical or chemical responses. (4) A larger spring algal bloom may occur after a warmer winter, but the bloom may also be offset by stronger grazing pressure (Pettersson 1990; Straile 2000). (5) Warmer temperatures may change the population of keystone fish species, resulting in a cascade effect in the food web, ultimately affecting phytoplankton (McDonald, Hershey, and Miller 1996). (6) Different aquatic communities and seasonal successions may evolve depending on matches

between the timing of weather events and species-specific life-history events, such as timing of spawning (Adrian, Wilhelm, and Gerten 2006). (7) Lake morphology can also mediate the climate impacts. The effect of winter warming on phytoplankton succession persisted for less time in shallow lakes, while lasting longer (even until the next winter) in deeper lakes (Adrian et al. 1999; Gerten and Adrian 2001).

In summary, multiple processes, factors, and interactions regulate lake algal responses to climate change, some of which may cause algal biomass to increase in response to climate change while others may not. The prediction of more algal biomass or harmful algal blooms in the future is popular in the scientific climate change community, but with some assumptions that may or may not be true.

5.1.4 Objective and research questions

Long-term (*e.g.*, decadal) observations of algal biomass in lakes are rare, and future projections based on coupled models are usually incompletely validated. In this study, we generated long-term (1984–2011, 28 years), whole-lake algal biomass estimates for four reservoirs in Missouri (USA) using remote sensing (Landsat TM) observations. The new dataset allows linkage of long-term climate change with algal biomass, testing the hypothesis that higher algal biomass is associated with higher temperatures as well as more intense precipitation. First, we studied patterns of covariation among lake algal biomass, temperature, precipitation, and discharge, asking:

- 1) Does algal biomass covary with seasonal patterns of temperature, precipitation, or discharge?
- 2) Does algal biomass covary with long-term (28-year) trend with precipitation or temperature?

Then, we further quantified the relationships between algal biomass and temperature as well as precipitation, asking:

- 3) How much algal biomass variance can be explained by temperature and precipitation?

All tests were run on the upstream and downstream zones of four reservoirs, asking:

- 4) Do upstream zones have higher algal biomass and hence may be more susceptible to climate change than downstream zones?

5.2 Methodology

5.2.1 Study reservoirs

Four reservoirs, namely Smithville, Pomme de Terre, Clearwater, and Wappapello, were selected considering data availability and locations (Figure 5-1). The distances between Smithville, Pomme de Terre, and Clearwater are more than 160 km between any two reservoirs, providing potential variability in climate across the study sites. The catchments of Wappapello and Clearwater are next to each other, allowing comparison of responses to similar climate conditions. Clearwater is the smallest reservoir (6.59 km^2). Areas of the other reservoirs are 30 km^2 (Smithville), 34 km^2 (Pomme de Terre), and 28 km^2 (Wappapello). All reservoirs are fork-shaped with two up-stream branches. Three zones were assessed in each reservoir, *i.e.*, two upstream zones (east and west) and one dam zone. An extra midstream zone was also sampled in Smithville. Reservoir zones were named as Smithville Upstream West, Smithville Upstream East, Smithville Upstream Dam, etc.

In 1992, Smithville and Pomme de Terra were agricultural basins with 79% and 59%, respectively, of their catchments in cultivated lands, while Clearwater and Wappapello were relatively natural basins covered with 88% and 78%, respectively, of forest. Urban lands accounted for less than 10% of the area in all the basins. After 1992, Land use/cover changed little over the study period, < 10% (Figure A. 5-1). Small changes in land use/cover provided a good opportunity to investigate the relationship between climate change and algal biomass with minimal interference by land use/cover change over time.

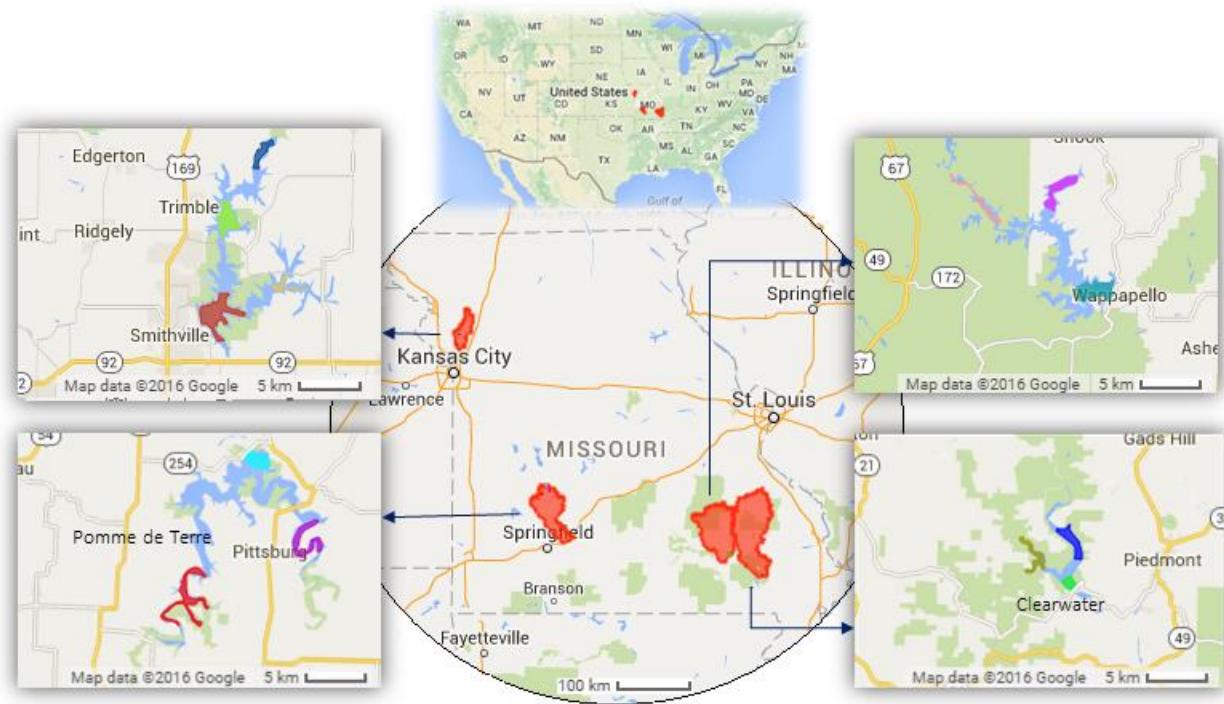


Figure 5-1 Map of study reservoirs and associated catchment basins. Locations of basins are indicated by middle maps. Polygons on reservoirs indicate study zones. Names of reservoirs are Smithville, Pomme de Terre, Wappapello, and Clearwater (from West to East).

5.2.2 Data

Lake surface temperatures (1984-2011) were estimated using the thermal band (Band 6) of Landsat 5 Thematic Mapper (TM) (Google Earth Image ID: LANDSAT/LT5_L1T_TOA). Algal biomass (1984-2011) was estimated as chlorophyll-*a* concentration (referred to as chlorophyll in the following text), which is a pigment common to all algal species that is routinely used to measure algal biomass. Chlorophyll was derived from Landsat 5 TM surface reflectance products (Google Earth Image ID: LEDAPS/LT5_L1T_SR) using a random forest model. The chlorophyll random forest model was trained by ground-measured chlorophyll (over 28 years and 39 reservoirs in Missouri). All bands and band ratios, except for the thermal band (6), were used as model predictors. In the training dataset, ground-measured chlorophyll was available for two to four dates during summers between 1989 and 2012. For each occasion, only

one sample was taken near the dam of each reservoir. Corresponding Landsat data were Landsat TM/ETM+ (Enhanced Thematic Mapper Plus) surface reflectance observed within 8 days before or after the ground-measured dates. The chlorophyll remote sensing model was trained using 963 samples. The model explained 34.7% of the total chlorophyll variance, indicated by 10-fold cross validations (Figure 5-2). The resulting lake surface temperatures and chlorophyll concentrations estimated from Landsat TM were recorded for every “7-9-7-9” day sequence, because of the Landsat 5 TM image frequency, except for cases where images were obscured by clouds. When lake surface temperatures were less than or equal to 0 °C, the chlorophyll and temperature measures were excluded from the dataset.

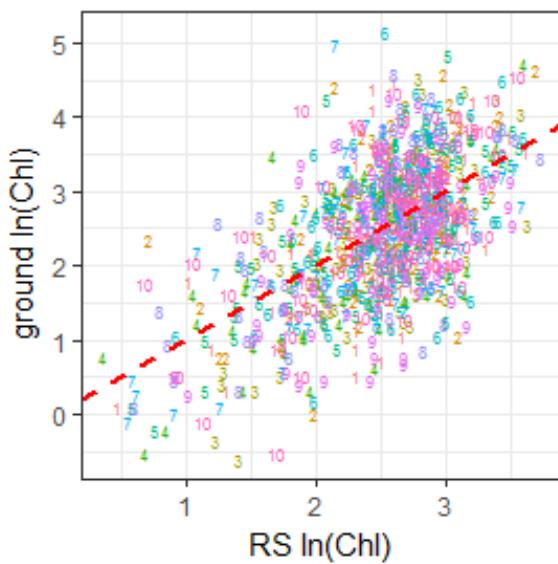


Figure 5-2 Missouri reservoir chlorophyll (Chl, natural logarithm of concentrations, $\mu\text{g/L}$) showing ground measurements compared to model remotely sensed (RS) measurements ($R^2 = 0.347$) indicated by 10-fold cross validations. Dashed line is a one-to-one ratio.

Basin daily precipitation (1983-2011) was obtained from GRIDMET (University of Idaho Gridded Surface Meteorological Dataset, Google Earth Image ID: IDAHO_EPSCOR/GRIDMET), which was a model result of regional-scale reanalysis and daily gauge-based precipitation (Abatzoglou 2013). To characterize weekly,

monthly, summer, and yearly precipitation conditions, precipitation was further characterized by number of rainy days (Pre.N, d), precipitation sum (Pre.sum, mm), and precipitation intensity (Pre.I, mm/d). For example, yearly number of rainy days was the count of days with precipitation ≥ 1 mm/d. Yearly precipitation sum was the sum of all precipitation ≥ 1 mm/d in a year. Yearly Pre.I was yearly Pre.sum divided by yearly Pre.N. Precipitation as well as temperature and algal biomass data were stored and processed in Google Earth Engine servers (Gorelick 2012).

Daily discharge (ft^3/s , $1 \text{ ft}^3 = 28.32 \text{ L}$) data were obtained from USGS hydraulic stations (<http://waterdata.usgs.gov>, accessed on March 23, 2016). Discharge data were not available until 2008. For each reservoir, the closest station in the main stream was selected. The distance between the stations and reservoirs varied from 10 to 20 km.

5.2.3 Spatial and temporal patterns

To test the biomass difference between upstream and downstream zones, mean chlorophyll concentrations in upstream zones were compared to dam zones at different times using a pairwise *t*-test. The Shapiro-Wilk test of normality was applied to the differences of pairs before conducting the pairwise *t*-test.

Seasonal patterns of precipitation, discharge, temperature, and chlorophyll were first visually examined. To have a general seasonal trend for each variable, daily precipitation, discharge, temperature, and chlorophyll over the 28 years were averaged over day of year (DOY) using LOWESS (locally weighted scatterplot smoothing).

Long-term (28 years) trends of lake surface temperature, precipitation, and chlorophyll were compared. The trends were evaluated by the non-parametric Mann-Kendall test. The Mann-Kendall test score (*S*) of time-series of data x_t ($t = 1, 2, 3...n$) is defined as:

$$S = \sum_{i=1}^{n-1} \sum_{j=i+1}^n \operatorname{sgn}(x_j - x_i)$$

where

$$\operatorname{sgn}(\theta) = \begin{cases} 1, & \text{if } \theta > 0 \\ 0, & \text{if } \theta = 0 \\ -1, & \text{if } \theta < 0 \end{cases}$$

Positive S indicates increasing trend; negative S indicates decreasing trend. The significance (p) of the trend was the probability of the S belonging to a random series with the same sample size.

The magnitude of the trend was indicated by the Sen's slope (k), which is the median slope of all slopes (k_m) in a time series:

$$k_m = \frac{x_j - x_i}{j - i}$$

where $1 \leq i < j \leq n$, $m = 1, 2, 3 \dots n \times (n-1)$, and n is the number of data. The *trend* package of R was used for Mann-Kendall test and Sen's slope calculation.

5.2.4 Univariate analyses

Summer chlorophyll (Chl.summer) and annual mean chlorophyll (Chl.annual) were compared to corresponding lake surface temperature as well as precipitation (intensity and sum) to test the hypothesis that climate change might increase peak algal biomass (indicated by Chl.summer) and the duration of high algal biomass (indicated by Chl.annual). Univariate linear regression (LM) was used to evaluate each pair of relationships in each reservoir zone. For example, Chl.summer = LM (Ts_t) and Chl.annual = LM (Pre_t) were respectively used to test the relationship between Chl.summer and Ts_t (land surface temperature with time lag t) and the relationship between Chl.annual and Pre_t (precipitation with time lag t). Only chlorophyll of the two hottest months (*i.e.*, July and August) were included in Chl.summer. Corresponding to Chl.summer, time lags for precipitation and Ts were 0, 1, 2-3,

4-7, 8-15, 16-31, and 32-63 weeks, where both delay time and statistical period increased exponentially. Time lags of 1, 2-3, and 4-7 weeks were used to test if there was any short-term (< two months) response lag. Periods for 8-15 week, 16-31 week and 32-63 week were March 18 – May 12 (roughly spring), December 27 – March 17 (roughly winter) and April 17 – December 26 (roughly spring to winter of last year), respectively. These periods were used to test if summer, winter, previous-year temperature and/or precipitation contributed to summer algal biomass of this summer (July and August). Corresponding to Chl.annual, time lags for temperature and precipitation were 0, 1, 2-3, and 4-7 years. Time lags longer than 4-7 years resulted in a sample number less than 20 so they were not included. Chlorophyll sensitivity to each variable was illustrated by the linear model slope (β) and p -value. There were 13 zones in the reservoirs (*i.e.*, four for Smithville, and three for each of the others). The slopes of linear models could be positive or negative. Based on the binomial distribution (tested by the *binom.test* function of R), if the positive slope count ≥ 10 in 13 linear models, then it was very possible (95%) that model slope was positive in general.

5.2.5 Multivariate analyses

Univariate analyses might be misleading due to correlations between temperature and precipitation. For example, both temperature and precipitation can change vegetation and soil, thereby affecting nutrient loading to lakes. To evaluate partial effects of temperature and precipitation, a non-linear machine-learning algorithm called boosted regression trees (BRT; Ridgeway 2004) was used to quantify how daily chlorophyll responded to daily lake surface temperature. BRT was used because it can fit hidden relationships, linear or non-linear, by learning from the data. Models were built separately for individual zones of study reservoirs. Model predictors included daily lake surface temperature and daily precipitation. Time lags were considered in the models. Time lags for precipitation included 0, 1, 2, 4, 8, 16, 32, 64, and 128 days. The frequency of lake surface temperature was not daily but with “7-9-7-9” period gaps, so time lags of lake surface temperature were: 0, 7 & 9, 16, 23 & 25, 32, and 39 & 41 days,

where two closely timed observations were grouped and averaged as one lag. Variables with different time lags were put in the model at the same time. Chlorophyll sensitivity to each variable was illustrated by partial dependence variation, which was the response of chlorophyll over one independent variable when the other variables were controlled at their means. The contribution of each variable to chlorophyll variation was indicated by partial R^2 , which was: (total model R^2) \times (relative importance). The relative importance of a variable in boosted regression trees was the percentage that the sum of deviation reductions related to the tree splits using the variable was relative to total deviation reduction by all the variables. Model performance (R^2) was defined by the commonly used Nash-Sutcliffe coefficient (Nash and Sutcliffe 1970):

$$R^2 = 1 - \frac{\sum_{i=1}^n (O_i - P_i)^2}{\sum_{i=1}^n (O_i - \bar{O})^2}$$

where O_i is observation value; P_i is model predicted value and \bar{O} is the mean of O_i . R^2 ranges from $-\infty$ to one, where one is a perfect fit and $R^2 < 0$ indicates residual variance is larger than the observation variance. Total model R^2 was calculated from 10-fold cross-validations.

Only daily chlorophyll, rather than summer or annual chlorophyll, was evaluated in the multivariate analyses because 28 years of measurements were not enough for the BRT modeling with yearly chlorophyll, especially when time lags were considered.

5.3 Results

5.3.1 Spatial and temporal patterns

In each reservoir, the chlorophyll of the upstream zones was significantly ($p < 0.05$, same α level for the following significance without specification) higher than chlorophyll of the midstream or dam zone, indicating algal blooms, were more likely to occur in upstream zones than in dam zones (Figure 5-3). For example, in Pomme de Terre, the chlorophyll of the Upstream West was significantly higher than the

Dam by 2.8 µg/L, and the chlorophyll of the Upstream East was significantly higher than the Dam by 2.5 µg/L. Chlorophyll of upstream zones had higher variations than dam zones measured by Landsat TM. For instance, in Pomme de Terre the standard deviation of the chlorophyll estimates in Upstream West was the same as Upstream East ($\delta = 5.7$ µg/L), while they were higher than the Dam zone ($\delta = 4.0$ µg/L).

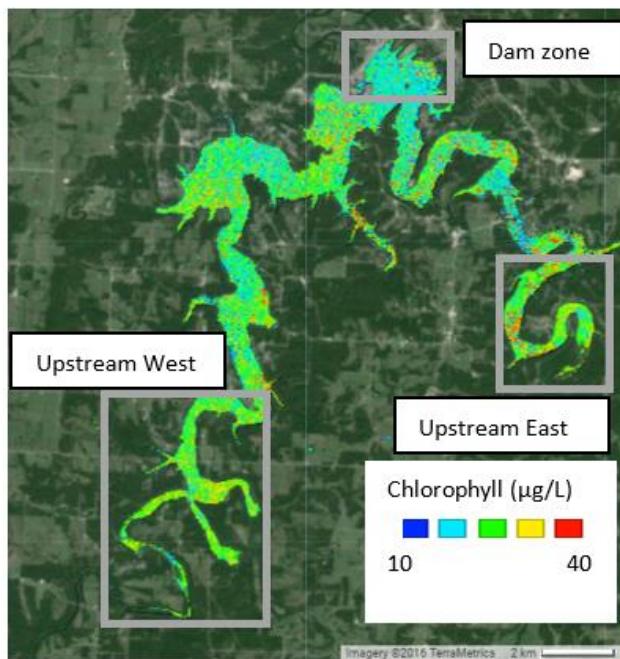


Figure 5-3 Average chlorophyll concentration of Pomme de Terra Lake (Missouri) during July-August 2011. Higher chlorophyll was found in the upstream branches than the dam zone (on the top figure).

Similar spatial patterns were found in the other study reservoirs.

Seasonal cycles were obvious in the time series data for both algal biomass and lake surface temperatures (Figure 5-4). Discharge peaks were found after precipitation events. We did not observe obvious chlorophyll peaks corresponding to precipitation events.

When the 28 years of data were aggregated over day of year (DOY), seasonal patterns of lake surface temperatures in all the study zones were similar, with peak values around DOY = 200 (in July) and low values at the beginnings and ends of the years (Figure 5-5). However, the peak of chlorophyll was not

always on the same day as the corresponding temperature peak. Specifically, the peak day could be later (e.g., DOY = 220 in Smithville Upstream West, Figure 5-5 a), the same (e.g., Pomme de Terre Upstream West, Figure 5-5 b), earlier (e.g., DOY = 180, Wappapello Upstream West, Figure 5-5 d), or in a different shape (e.g., two peaks at DOY = 200 and 280 in Clearwater Upstream East, Figure 5-5 c). This indicated that temperature was not the only factor controlling chlorophyll. Seasonal patterns of precipitation and discharge were relatively weak, compared to chlorophyll and lake surface temperature. On days with very intense precipitation (> 50 mm/d), chlorophyll did not show corresponding extremes. For example, during April and October there were some very high-intensity precipitation events in Pomme de Terre, Wappapello, and Clearwater. However, very high chlorophyll was not measured by Landsat for the same periods (Figure 5-5 b-d). This indicated weak or no chlorophyll response to precipitation events.

When annual trends were viewed over 28 years, increasing trends of yearly lake surface temperatures were found in all reservoir zones ($N = 13$), with Sen's slope ranging from 0.0556 (Clearwater Upstream West) to 0.163 (Smithville Upstream West), but only four of the slopes were significantly different than zero (Figure 5-6, Table A. 5-1). Yearly total precipitation did not increase significantly from 1984 to 2011 in all basins ($N = 4$), but yearly counts of rainy days decreased significantly. Thus, precipitation intensity increased significantly in all basins, with Sen's slope ranging from 0.0832 (Pomme de Terre) to 0.141 (Smithville). Although there were similar environmental pressures of increasing temperature and increasing precipitation intensity, lake chlorophyll responded individually. Significant increases of the annual mean chlorophyll were only found in Pomme de Terre Upstream West and all zones in Wappapello. No significant trend was found in the other zones ($N = 9$). Mean chlorophyll in July-August significantly increased only in Wappapello Upstream East. Lakes with significant positive trends of precipitation intensity or lake surface temperature did not necessarily have significant positive trends in algal biomass (either mean of the whole year or mean of July-August), suggesting algal biomass might also be controlled by factors other than lake surface temperature or precipitation.

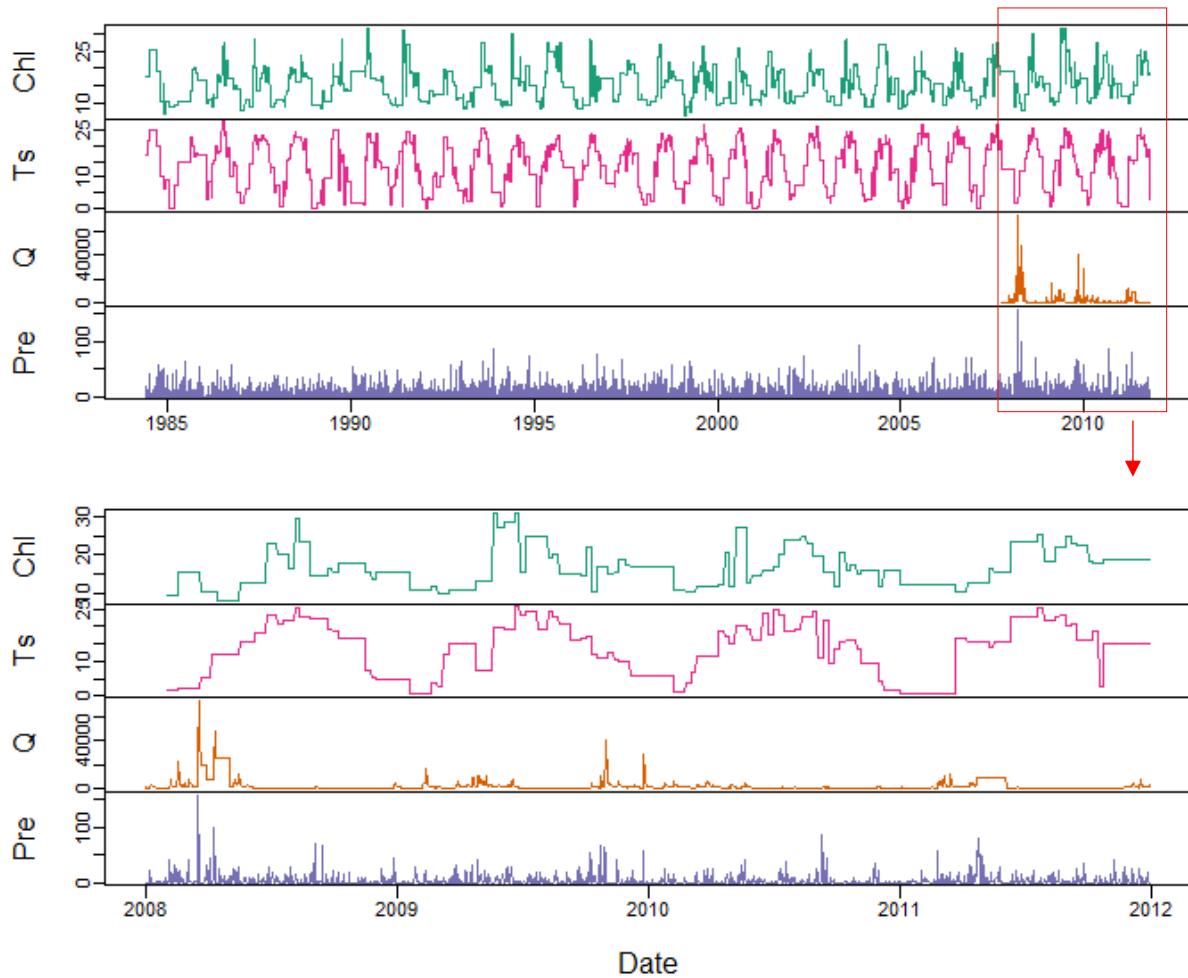
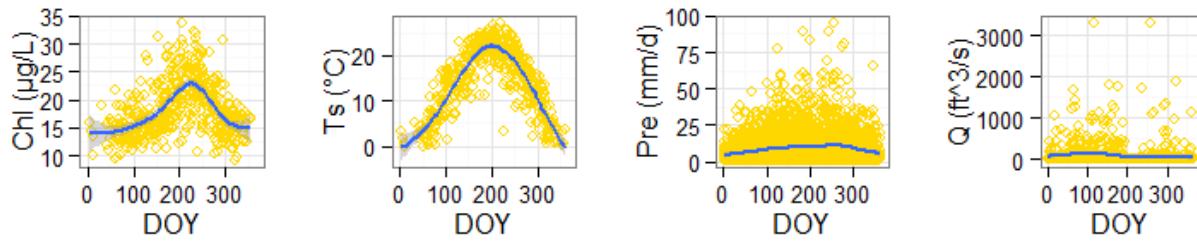
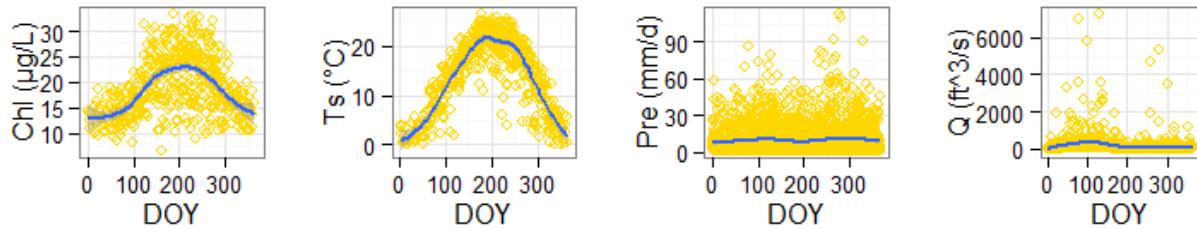


Figure 5-4 Daily time series of chlorophyll concentration (Chl, $\mu\text{g/L}$), lake surface temperature (Ts, $^{\circ}\text{C}$), discharge (Q, ft^3/s , 1 ft = 30.48 cm), and precipitation (Pre, mm/d) from 1984 to 2011 at Wappapello Upstream West. Data gaps were interpolated with the method of “last one carried forward.” There was no discharge data available before 2008.

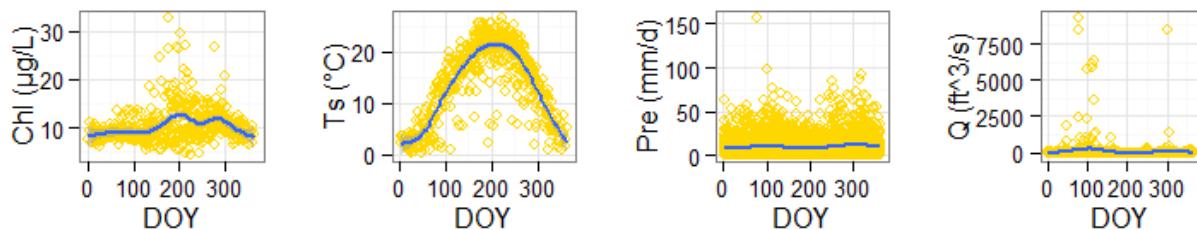
a. Smithville Upstream West



b. Pomme de Terre Upstream West



c. Clearwater Upstream East



d. Wappapello Upstream West

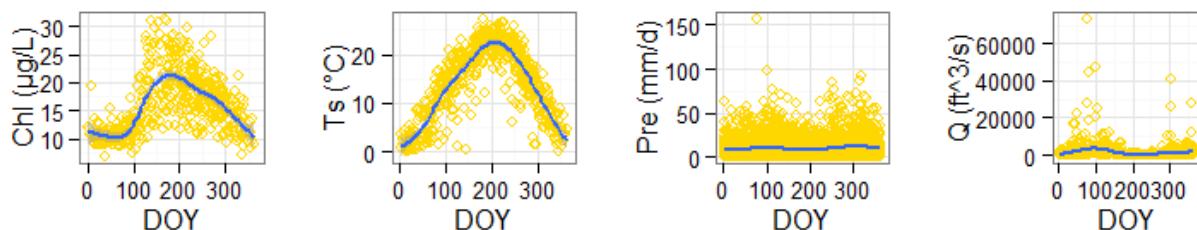


Figure 5-5 Chlorophyll (Chl), lake surface temperature (Ts), precipitation (Pre) and discharge (Q) changed over day of year (DOY) in four upstream zones that are associated corresponding main sub-basins of study reservoirs. Values were measured from 1984-2011, except for discharge data that were only available in 2008-2011. Solid lines are smooth lines with 95% confidence intervals. See Figure A. 5-2 for all zones of the reservoirs.

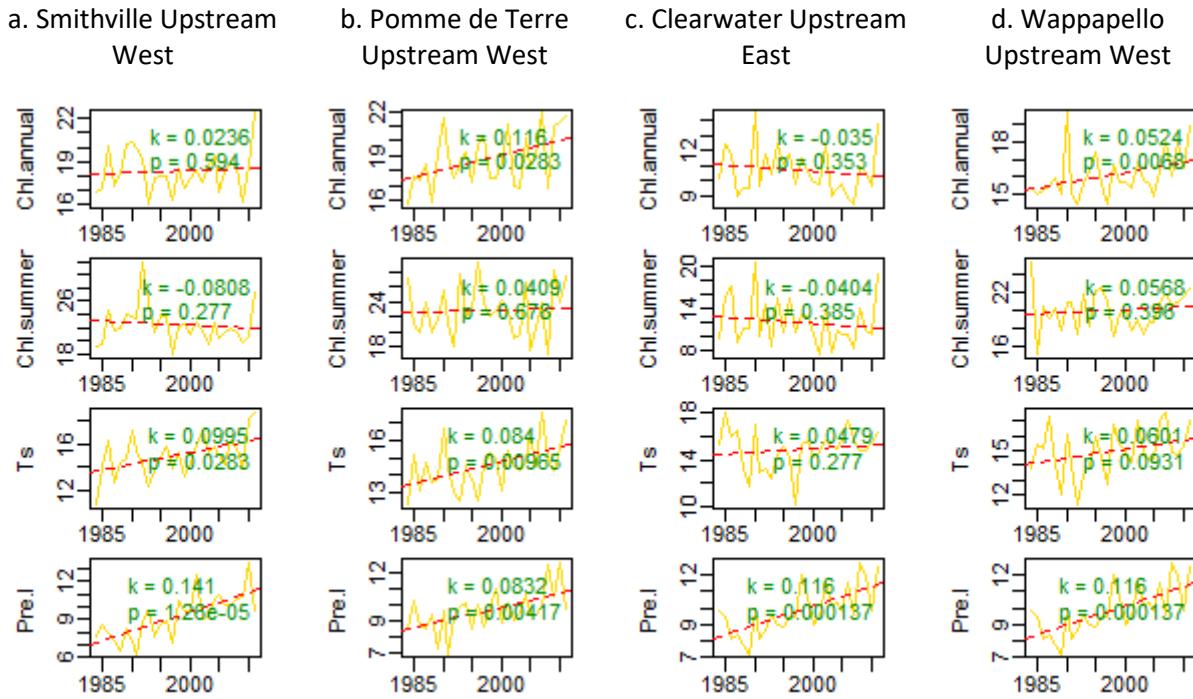


Figure 5-6 Annual average time series of mean annual chlorophyll (Chl.annual $\mu\text{g/L}$), chlorophyll in July-August (Chl.summer $\mu\text{g/L}$), lake surface temperature (Ts, $^{\circ}\text{C}$), and precipitation intensity (Pre.I, mm/d, excluding days with precipitation < 1 mm/d) from 1984 to 2011 at four upstream zones that are associated to the main sub-basins of study reservoirs. Magnitude (Sen's slope, k) and significance (p) of the trends are shown. Dashed lines are linear regression lines. See Table A. 5-1 for the full summary of all zones.

5.3.2 Single-factor analyses

5.3.2.1 Lake surface temperature effects on chlorophyll

Linear regression models (model $N = 13$ for 13 zones) indicated only the model for *summer* chlorophyll in Wappapello Upstream was significantly related (positively) to lake surface temperature (lag = 0 week). Specifically, six model slopes were positive, and seven model slopes were negative, in all of which only

one slope (Wappapello Upstream) was significant, indicating July-August chlorophyll was unlikely related to changes in lake surface temperature over the 28-year period. Taking time lags (ranging from 1 to 63 weeks) into consideration, no new significant positive slope was found in the models, indicating no time lag between July-August chlorophyll and lake surface temperature. Five out of 78 summer chlorophyll models with time lags had significant negative slopes (Table 5-1).

All models ($N = 13$) of *annual* chlorophyll and lake surface temperature (lag = 0 week) had positive slopes, six of which were significant. Compared to 6 positive slopes (one significant) in summer chlorophyll models, annual chlorophyll more likely increased with lake surface temperature than summer chlorophyll did in the study zones. Taking time lags (ranging from 1 to 7 years) into consideration, no new significant positive slopes were observed in the models with time lags, indicating no time lag between annual chlorophyll and lake surface temperature. Two significant negative slopes occurred in the models with time lag = 1 year (Table 5-1).

5.3.2.2 Total precipitation effects on chlorophyll

Total precipitation in the mid-summer months (July-August) showed one significant negative effect (*i.e.*, negative slope in the model, same meaning hereafter) and three positive effects (*i.e.*, positive slopes in the models, same meaning hereafter) in chlorophyll over the same period (lag = 0 week). In total, only 7 out of 13 linear-model slopes were positive, suggesting a mixed effect of total precipitation on summer (July-August) chlorophyll.

Total precipitation in the 8-15 weeks prior to sampling (March 18 – May 12, spring) and 32-63 weeks prior (April 17 – December 26, previous water year) more likely had positive than negative impacts on summer chlorophyll because of 13 (5 significantly positive) and 12 (3 significantly positive) positive linear-model slopes, respectively. Thus, summer chlorophyll might increase with total precipitation of

spring and the previous water year. However, the number of significant slopes was less than 10, so the positive effects of time lags are uncertain.

Table 5-1 Number of models with slope > 0 and number of models with p -value < 0.05 (in brackets) in linear regression models for individual zones ($N = 13$) of study reservoirs ($N = 4$).

Lag	$x = Ts$	$x = Pre.l$	$x = Pre.sum$
$y = \text{mean chlorophyll of July - August}$			
0 week	6 (1+)	8	7 (3+1-)
1 week	9	6	7
2-3 week	9 (1+)	3	4
4-7 week	3 (2-)	7	9 (1+)
8-15 week	7 (1-)	8 (4+)	13 (5+)
16-31 week	8	3	6
32-63 week	3(2-)	9	12(3+)
$y = \text{annual mean chlorophyll}$			
0 year	13 (6+)	10 (4+)	12 (4+)
1 year	5 (2-)	8	5
2-3 year	10 (2+)	7 (2+)	8
4-7 year	13 (1+)	11 (4+)	5 (1-)

Table notes: Ts, Pre.l, and Pre.sum is lake surface temperature ($^{\circ}\text{C}$), precipitation intensity (mm/d), and total precipitation (mm), respectively. Lag period of “8-15 week”, “16-31 week” and “32-63 week” is March 18 – May 12, December 27 – March 17 and April 17 – December 26, respectively. Number in brackets is the count of positive (+) and negative (-) slopes with $p < 0.05$. Bold font indicates positive slope number ≥ 10 (*i.e.*, significantly more than negative slopes). See Table A. 5-2 for more details of individual models.

In the models with *annual* total precipitation and mean chlorophyll over the same period (lag = 0), 12 out of 13 reservoir zones had positive slopes, four of which were significant, suggesting that annual mean chlorophyll had significantly more positive effects than negative effects due to annual total precipitation over the same year. There was one significant negative slope in the model with time lag of

4-7 years. The number of significant slopes was less than 10, so the positive effects and the time lags were uncertain.

5.3.2.3 Precipitation intensity effects on chlorophyll

Precipitation intensity strongly correlated with total precipitation of the same period when statistical periods were less than one year, with Pearson r ranging from 0.48 to 0.91. However, when the statistical period was longer than one year, *i.e.*, 2 years and 4 years, the correlation was weak with Pearson r ranging from 0.025 to 0.36. Annual total precipitation did not significantly increase over the 28 years, but precipitation intensity did. Thus, annual precipitation intensity might characterize precipitation impacts due to climate change in study reservoirs better than total precipitation.

Precipitation intensity with lag = 8-15 weeks (March 18 – May 12, spring) had 8 positive (4 insignificant positive) slopes in the summer (July-August) chlorophyll models, and no significant slope was found in the other summer chlorophyll models, including those with lag = 0 week (8 positive, but not significant). In the models with precipitation intensity lag = 32-63 weeks (April 17 – December 26, previous water year), nine slopes were positive, none of which was significant. This indicated that summer chlorophyll might increase with precipitation intensity of spring in some study zones, but the uncertainty was large based on the number (4 out of 13) of significant slopes.

Precipitation intensity with lag = 0 year had 12 positive slopes, 4 of which were significant, in 13 annual chlorophyll models. That indicated that annual chlorophyll might increase with precipitation intensity of the same year. When the time lag increased to 1 year or 2-3 year, no new significant slope occurred. When the time lag increased to 4-7 years one new significant slope appeared in another zone, indicating a possible time lag for that zone. Based on the number of significant slopes, the effects and time lags for the effects of precipitation intensity on annual chlorophyll were very uncertain.

5.3.3 Multiple-factor analyses

Using models built with boosted regression trees to simulate relationships between daily chlorophyll and daily weather (*i.e.*, lake surface temperature and precipitation) with different time lags, model performance indicated by 10-fold cross-validation R^2 varied from -0.004 (Pomme de Terre Dam) to 0.506 (Wappapello Upstream East) (Figure 5-7, Table 5-2). That suggested that the daily variations of chlorophyll in some zones such as Pomme de Terre could not be explained by temperature and precipitation, but some others such as Wappapello Upstream East were correlated with temperature and precipitation.

In models with 10-fold cross-validation $R^2 > 0.005$, the model performance was mostly (> 50%) affected by lake surface temperature (lag = 0 day). When the temperature (lag = 0 day) varied from 0 °C to 25 °C, chlorophyll increased by 6-10 µg/L, varying with zones. Temperatures with time lags (*i.e.*, 7 & 9, 16, 23 & 25, 32, and 39 & 41 days) had minor (< 10%) contributions in the models, indicating no time lag for chlorophyll responding to lake surface temperature. Precipitations with different lags (*i.e.*, 0, 1, 2, 4, 8, 16, 32, 64, and 128 days) had very small contributions in the models. All precipitation variables had less than 10% of relative importance in total variance reduction of models, indicating chlorophyll was weakly explained by precipitation, regardless of the time lags. Precipitation with time lags of 32 days or 64 days had the highest relative importance, compared to the other precipitation variables, indicating possible one- or two-month time lags for chlorophyll to respond to precipitation events. However, the evidence was weak due to very small contribution (< 5%) of the precipitation variables in the models.

The model performances for the upstream zones were better than the mid-stream or dam zones. Specifically, average R^2 for eight upstream zones was 0.334, with maximum $R^2 = 0.506$ (Wappapello Upstream East), while average R^2 for four dam zones was lower (0.138), with maximum $R^2 = 0.347$ (Wappapello Dam) (Table 5-2).

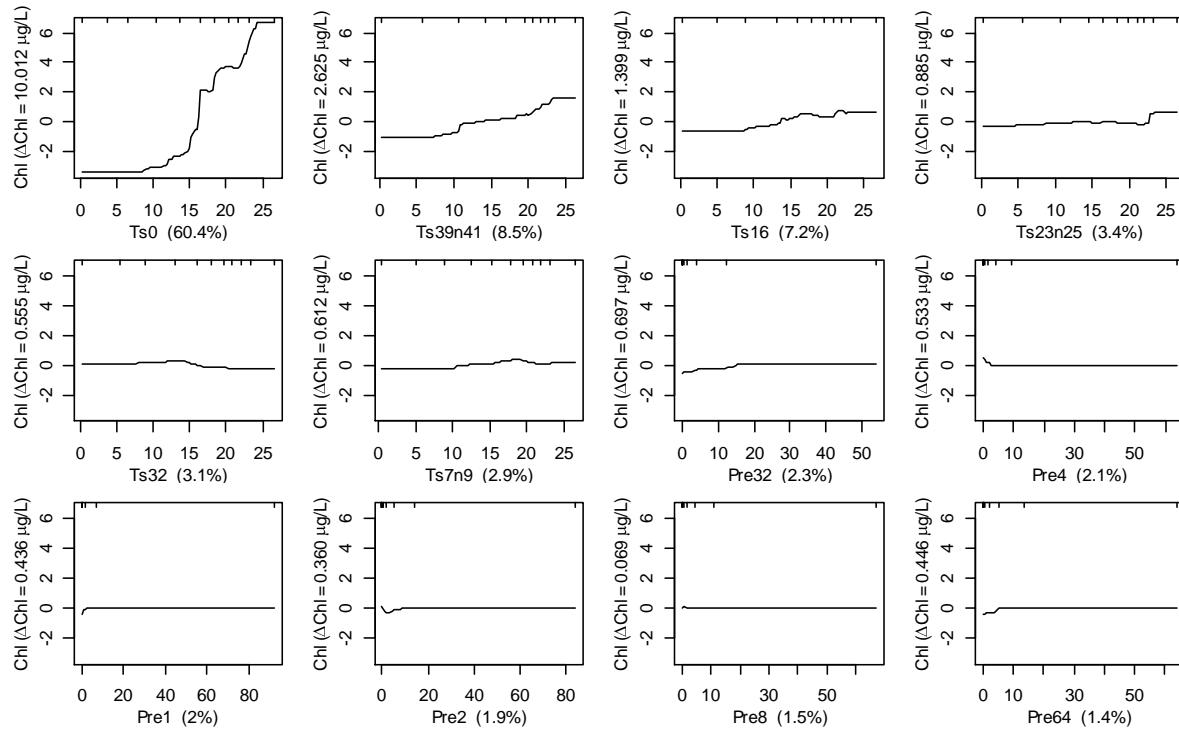


Figure 5-7 Partial dependent plots of the Wappapello Upstream East chlorophyll (Chl, $\mu\text{g/L}$) model (10-fold cross validation $R^2 = 0.505$). ΔChl (= max - min) indicates the magnitude of chlorophyll change over the variable of x-axis. Numbers in brackets are the relative importance of predictors. For comparison purposes, y-axis variable is centered to have a zero mean. Bars at the top of plots show distribution of x-axis variables in deciles. The model predictors include Ts0, Ts7n9, Ts16, Ts23n25, Ts32, Ts39n41, Pre0, Pre1, Pre2, Pre4, Pre8, Pre16, Pre32, Pre64, and Pre128, where the number at the end of each variable is the number of lag days, and “n” links two lags that are grouped together. Ts, lake surface temperature ($^{\circ}\text{C}$); Pre, precipitation (mm/d)

Table 5-2 Variations of daily chlorophyll contributed mostly by lake surface temperature (Ts) other than precipitation (Pre), indicated by 10-fold cross validation R^2 of the daily chlorophyll models.

Reservoir zone	Total R^2	Subtotal partial R^2 of Ts	Subtotal partial R^2 of Pre
Smithville Upstream West	0.390	0.315	0.076
Smithville Upstream East	0.327	0.260	0.067
Smithville Midstream West	0.180	0.136	0.044
Smithville Dam	0.180	0.131	0.048
Pomme de Terre Upstream West	0.384	0.285	0.099
Pomme de Terre Upstream East	0.364	0.285	0.079
Pomme de Terre Dam	-0.004	-0.002	-0.002
Clearwater Upstream West	0.195	0.135	0.059
Clearwater Upstream East	0.025	0.017	0.008
Clearwater Dam	0.024	0.015	0.009
Wappapello Upstream West	0.481	0.412	0.069
Wappapello Upstream East	0.506	0.430	0.076
Wappapello Dam	0.347	0.262	0.085
minimum	-0.004	-0.002	-0.002
maximum	0.506	0.430	0.099
mean	0.262	0.206	0.055

5.4 Discussion

5.4.1 Temperature effects

Lake surface temperature in the four Missouri reservoirs was related to algal biomass in some reservoirs and zones, but not in the others. The increase of algal biomass with lake temperature might be caused by a faster growth rate of algae at higher temperature due to higher efficiency of enzyme activity and light-harvesting (Raven and Geider 1988; Coles and Jones 2000). The environmental carrying capacity of algae might also increase with temperature (Tilman, Kilham, and Kilham 1982; Stomp et al. 2011).

However, temperature is not the only determinant of algal biomass. In oligotrophic lakes, seasonal patterns of algal biomass may not coincide with temperature patterns, but algal biomass is regulated by nutrients and lake turnover (Hasson 1990). For example, algal biomass in Lake Woodrail (Missouri) showed that high chlorophyll peaks ($> 12 \mu\text{g/L}$) happened not just in warm seasons, but also in winters

(Jones and Knowlton 2005). In Lake Erie, algal biomass has not correlated significantly with inter-annual temperature differences in summer, but rather with nutrient loadings (Stumpf et al. 2012). In this study, two chlorophyll peaks, instead of one, appeared in the chlorophyll-DOY relationship of Lake Wappapello, where the average chlorophyll concentration was lower than the other reservoirs (Figure 5-5 c). These suggested that temperature impacts on algal biomass were also strongly mediated by nutrients.

Algal biomass of the dam zones was significantly lower than associated upstream zones. Compared to upstream zones, the variation in algal biomass in dam zones was explained less by lake surface temperature in both one-factor models (Table A. 5-1) and multiple-factor models (Table 5-2). Dam areas with lower nutrient levels might be subjected to stronger nutrient mediation than the upstream zones. Both temperature and nutrients regulate algal biomass, and it would be interesting for future research to investigate how the sensitivity of algal biomass to temperature changes with nutrient levels and N/P ratios.

The results show that the temperature effect, indicated by the number of significant slopes in the univariate linear models, was more likely found in annual chlorophyll than summer (July – August) chlorophyll. The reason for that could be mathematical or ecological. Annual chlorophyll had lower variance than summer chlorophyll, so annual models were more likely to be statistically significant than summer models. On the other hand, algal biomass might be less sensitive and even saturated at high temperature, so summer chlorophyll responded less to temperature than annual chlorophyll, which included chlorophyll in cold months when algal biomass response to temperature was not saturated. Lake surface temperatures in the study reservoirs varied from 16 °C to 30 °C. Growth rates of algae might be stimulated at temperature > 25 °C (Lürling and De Senerpont Domis 2013).

5.4.2 Precipitation effects

5.4.2.1 Nutrient and light availability

Weak and mixed (positive and negative) correlations were found between precipitation (total precipitation and precipitation intensity) and chlorophyll (annual and summer) in the studied Missouri reservoirs. This might be due to complex hydrologic processes between precipitation events, nutrient loading to lakes, and lake conditions. For instance, nutrients and light conditions might vary with individual events and lakes. In Western Lake Superior after an extreme precipitation event on June 19–20, 2012, both nutrients and turbidity (due to sediments and colored dissolved organic matter) increased, then both returned to pre-event levels in two months; thus the temporal mismatch between availability of nutrients and light resulted in no change in algal biomass over two months after the event (Minor, Forsman, and Guildford 2014). However, if precipitation events bring more nutrients with less turbidity, algal biomass might increase after the event. In our results, all four zones of Smithville Lake had positive slopes in the July-August chlorophyll models (time lag = 0 week), three of which were significant. That might be because Smithville Lake had a relatively high percentage of disturbed lands (*i.e.*, cultivated and urban lands) that might generate event flows from with higher nutrient concentrations and potentially higher nutrient loading compared to other lands (Table 5-3). On the other hand, one significantly negative slope was found in the Wappapello univariate models of July-August chlorophyll. Wappapello watershed had a relatively low percentage of disturbed lands and thereby potentially relatively low nutrient loads in the event flows. The negative correlation might be due to the dilution effect of the low concentration flows. A predictable relationship between light and the ratio of algal biomass to total phosphorus was shown in Lake Woodrail (Missouri) after precipitation events, supporting the hypothesis of a mixed precipitation effect depending on nutrients and light combination (Jones and Knowlton 2005).

Table 5-3 Reservoir characteristics that may affect algal biomass responses to precipitation. Z scores of reservoir characteristics are compared to the first National Lake Assessment (NLA) lakes. Algal biomass responses are indicated by number of slope $\theta > 0$ in linear regression models: July-August chlorophyll = LM (total precipitation with time lag).

Reservoir	Z score						Count of $\theta > 0$	
	Lake area (km ²)	Basin/lake ratio	Soil K factor	Conductivity (cm/h)	Slope (°)	Disturbed lands (%)	Lag = 0 week	Lag = 8-15 week
Smithville (4 zones)	0.23	-0.13	1.4	-0.95	-0.58	2.15	4 (3+)	4(1)
Pomme de Terre (3 zones)	0.27	-0.12	0.29	-0.6	-0.43	0.97	2	3
Clearwater (3 zones)	-0.07	-0.01	0.26	-0.58	0.57	-0.4	1	3 (3+)
Wappapello (3 zones)	0.21	-0.09	0.31	-0.5	0.16	-0.22	0 (1-)	3 (1+)

Table notes: Lake character data including soil K factor (*i.e.*, the soil erosion factor of the Universal Soil Loss Equation) and disturbance lands (*i.e.*, cultivated and developed lands in 2005) were from Charles P. Hawkins at Utah State University; See Table A. 5-2 for details of the linear regression models.

5.4.2.2 Residence time of water in the reservoirs

More intense precipitation events result in shorter reservoir water residence times (Knowlton and Jones 1995), and potentially less algal biomass accumulation if residence times fall below a few weeks. That would potentially cause an inverse relationship between precipitation and chlorophyll. Lake Wappapello was in an area with relatively steep slopes and relatively undisturbed lands. And the ratio of basin to lake was higher than the other reservoirs (Table 5-3). Thereby, it potentially had higher peak flows with lower nutrients and shorter flow travel time compared to the other reservoirs. Residence time might contribute to the significant negative slope in the univariate model of Wappapello Upstream West, *i.e.*, July-August chlorophyll = LM (total precipitation) (lag = 0 week). Similar to this finding, the study in

estuaries of North Carolina showed that algal biomass decreased after floods because of flushing and shorter residence time (Paerl et al. 2014).

5.4.2.3 Time lags in algal biomass responses

The possibility of one- or two-month time lags was found in both univariate and multivariate models for precipitation effects on chlorophyll. The lag might be the time for event flows to disperse and be mixed in lakes, or/and the time for light to recover to a suitable level for algal biomass to catch up. For a distance of 45 km between river outlet and dam in Mark Twain Lake (Missouri), it took about one month for the turbid headwater to reach the dam in the 1990 flood event (Knowlton and Jones 1995). In Western Lake Superior, it took about two months for turbidity to return to pre-event level (Minor, Forsman, and Guildford 2014). The time periods of these observations were on a similar scale as the time lags in this study (*i.e.*, 1 and 2 months). Variation in time lags might be related to lake morphology and events themselves. Time lags for algal biomass to respond to precipitation events have been reported in the literature. For example, in Lake Erie where blooms consistently occurred in July-August, average discharge during the March-June period was found exponentially related to annual algal biomass ($r^2 = 0.97$) during 2002 to 2011 (Stumpf et al. 2012). Extreme algal blooms in 2011 happened after extreme springtime precipitation events in Lake Erie (Michalak et al. 2013).

5.4.2.4 Internal nutrient legacy sources

Internal nutrient sources may have more important effects on algal biomass than nutrient loading of the same period caused by precipitation events. Nutrients deposited in lake bottoms could still influence algal biomass far beyond the precipitation event periods, such as the next spring turnover time or even years later. That might contribute to the weak correlations between precipitation and chlorophyll in both univariate and multivariate models, and then there were additional complex effects of inflow nutrients and light conditions.

5.4.2.5 Phytoplankton adaptation

Some algae may be able to adapt to low light conditions after precipitation events. In the Swedish Lake Mälaren, the biomass of flagellate group Cryptophyceae , which can adjust their position to a surface with abundant light, was 19 times higher than the past 20-year median level after an unusual precipitation event in May 2001 (Weyhenmeyer, Willén, and Sonesten 2004). The adaptation of algal community could result in an increase of algal biomass after precipitation events. However, algal community adaptation might differ over lakes. That contributed to different individual responses of algal biomass to precipitation.

In summary, compared to temperature, precipitation indirectly affected lake algae by mediating conditions, including nutrient and light availability, water residence time, lag time, internal nutrient sources, and phytoplankton adaptation; and all of these together generated more uncertainties in how algal biomass responded to precipitation events. Moreover, these conditions were further controlled by more factors, such as land use/cover, soil nutrients, basin hydraulic conditions, lake morphology, and the ‘food web’ in lakes (Blenckner 2005). All these factors constituted a complex system with different resilience and outcomes to climate change.

5.5 Conclusion

Characterizing climate change impacts on algal biomass has been hindered by the limited availability of long-term observational lake data. This study differed from others in using long period (1984-2011, 28 years) of algal biomass data generated by remote sensing observations. In our study area, lake surface temperature and precipitation intensity (mm/d) generally increased over 28 years. However, the trend of lake chlorophyll did not necessarily follow the trend of temperature or precipitation over the 28 years, indicating that temperature and precipitation were not the only factors controlling reservoir chlorophyll. Annual chlorophyll was more likely to increase with temperature than summer chlorophyll,

suggesting that with global warming the algal growth period might expand while the peak biomass during summer might saturate. More precipitation in spring as predicted by the climate models might result in higher summer algal biomass. Annual chlorophyll might increase with higher total precipitation or precipitation intensity without time lags. The uncertainty of the climate change impacts was high since only a few of the univariate models were statistically significant. The multivariate models further revealed that daily temperature and daily precipitation together explained as less zero and as high as 50.6% of the variance in daily chlorophyll. These findings are based on four Missouri reservoirs and may not be applied to other lakes with different conditions of nutrients, turbidity (light), lake morphology, soil hydraulic properties, soil nutrients, and land use/cover.

Acknowledgement

This work was supported by the U.S. Environmental Protection Agency (EPA) under EPA STAR Grant #835203. The views and opinions expressed in this article are those of the authors and do not necessarily reflect the official policy or position of U.S. EPA, or any other agency of the U.S. government.

APPENDIX

APPENDIX

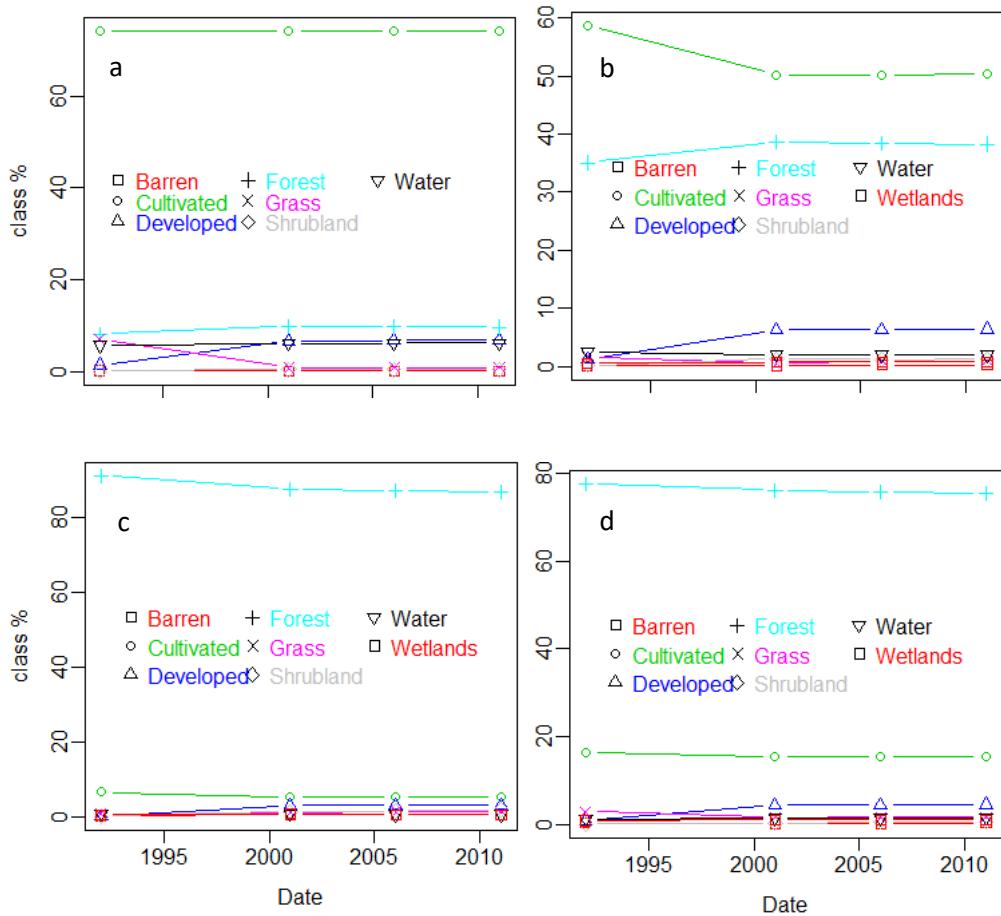


Figure A. 5-1 Basin Land use/cover changes of (a) Smithville, (b) Pomme de Terra, (c) Clearwater, and (d) Wappapello. Data source: USGS National Land Cover Database (Google Earth Image ID: USGS/NLCD).

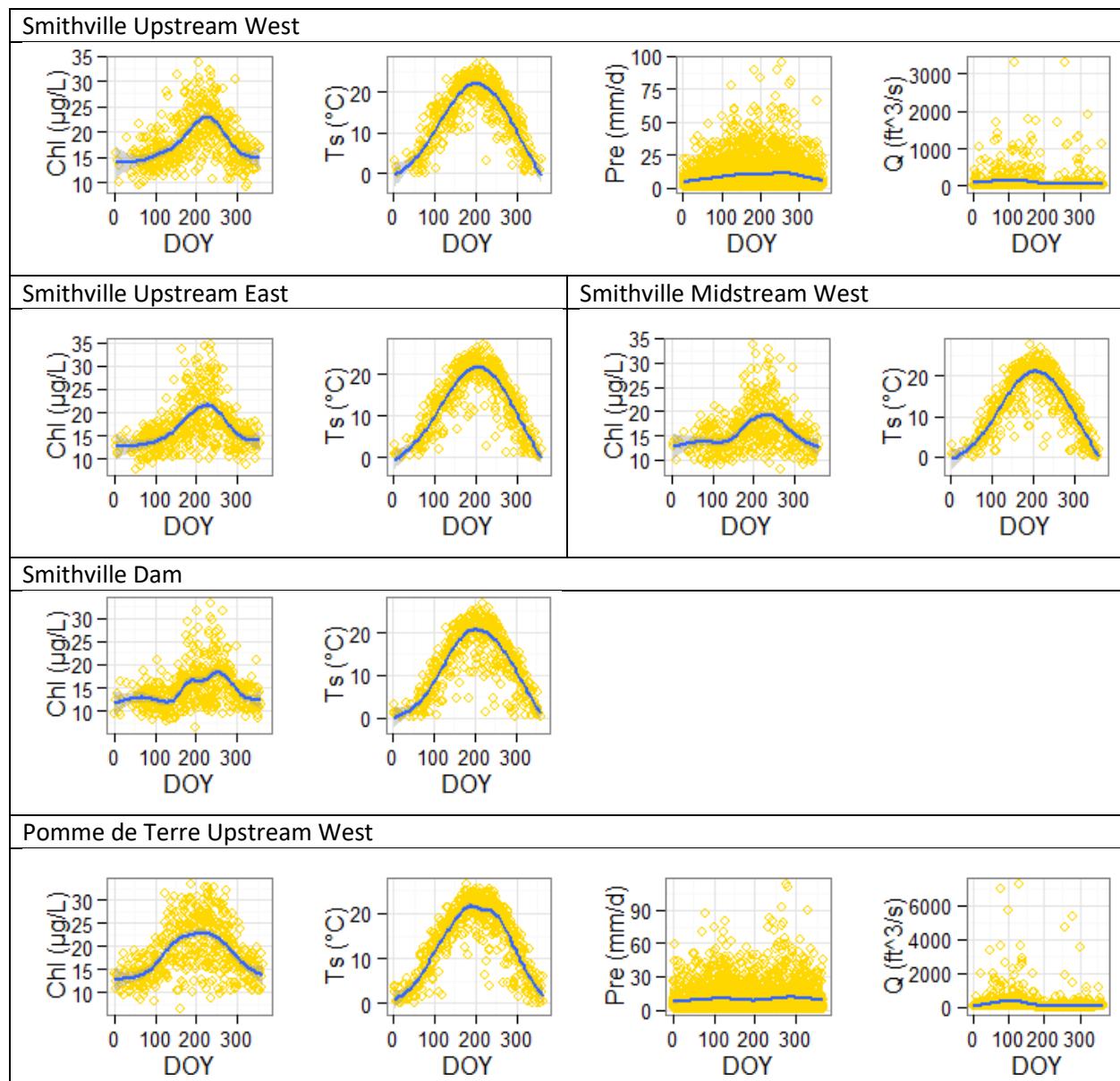


Figure A. 5-2 Chlorophyll (Chl), lake surface temperature (Ts), precipitation (Pre) and discharge (Q) changed over day of year (DOY). Values were measured from 1984-2011, except for discharge data that were only available in 2008-2011. Solid line is smooth line with 95% confidence interval.

Figure A. 5-2 (cont'd)

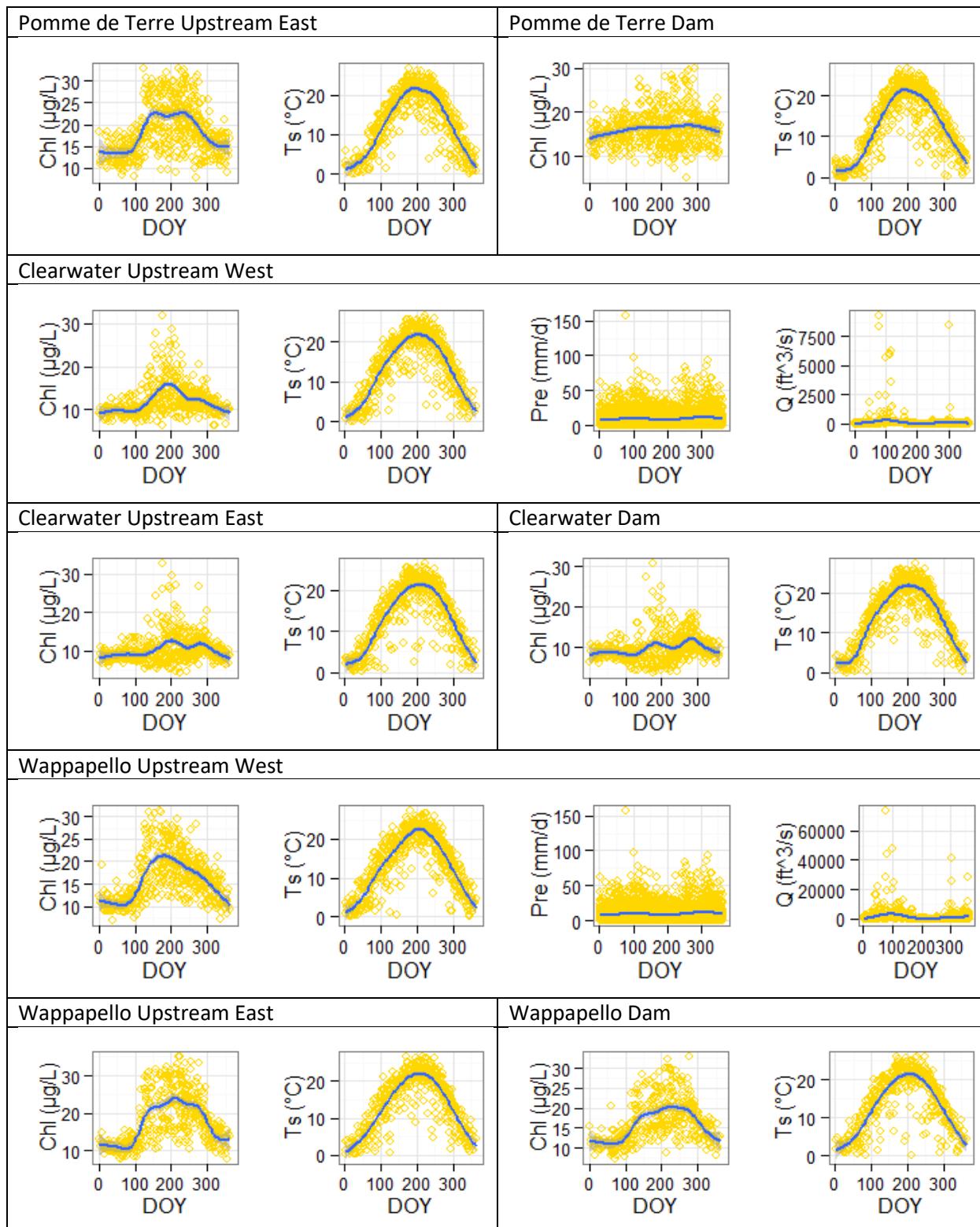


Table A. 5-1 Magnitude (Sen's slope, k) and significance (p) of yearly mean algal biomass and climate during 1984-2011 at upstream, midstream, and dam zones of Smithville, Pomme de Terre, Clearwater, and Wappapello in Missouri, United States. Table indicates significant increase trends in precipitation intense (Pre.I), while different responses of chlorophyll at different reservoir zones.

Reservoir zone	Chl.annual	Chl.summer	Ts	Pre.sum	Pre.N	Pre.I
Smithville Upstream West	0.0236	-0.808	0.163**	1.82	-1.55**	0.141***
Smithville Upstream East	-0.0187	0.0749	0.110*	1.82	-1.55***	0.141***
Smithville Midstream West	-0.0237	0.00710	0.0852	1.82	-1.55**	0.141***
Smithville Dam	-0.0194	0.000772	0.100.	1.82	-1.55**	0.141***
Pomme de Terre Upstream West	0.116*	0.0409	0.0943.	-1.63	-1.30**	0.0832**
Pomme de Terre Upstream East	0.0832	-0.0432	0.0927*	-1.63	-1.30**	0.0832**
Pomme de Terre Dam	0.0255	0.0385	0.0721.	-1.63	-1.30**	0.0832**
Clearwater Upstream West	0.0223	0.0153	0.0556	1.57	-1.40**	0.116***
Clearwater Upstream East	-0.035	-0.0404	0.0602	1.57	-1.40**	0.116***
Clearwater Dam	-0.0443	-0.0371	0.0544	1.57	-1.40**	0.116***
Wappapello Upstream West	0.0524*	0.0568	0.0784.	1.57	-1.40**	0.116**
Wappapello Upstream East	0.208***	0.190*	0.128*	1.57	-1.40**	0.116**
Wappapello Dam	0.107**	0.0856	0.102	1.57	-1.40**	0.116**

Table notes: Symbol of significance: “***”, $p < 0.0001$, “**”, $p < 0.01$, “*”, $p < 0.05$, and “.”, $p < 0.1$.

Column variables: Chl.annual ($\mu\text{g/L}$), yearly mean chlorophyll; Chl.summer ($\mu\text{g/L}$), mean chlorophyll of July-August; Ts ($^{\circ}\text{C}$), yearly lake surface temperature; Pre.sum (mm), sum of precipitation higher or equal to 1 mm/d in a year; Pre.N (d), count of rainy days with precipitation higher or equal to 1 mm/d in a year; Pre.I (mm/d), average intensity of precipitation in a year, *i.e.*, Pre.sum/Pre.N.

Table A. 5-2 Slope (β) and p-value of linear regression models (LMs). $P < 0.05$ is marked as red.

Model 1.1: chlorophyll of July-August = LM (lake surface temperature)														
Reservoir zone	lag = 0 week		lag = 1 week		lag = 2-3 week		lag = 4-7 week		lag = 8-15 week		lag = 16-31 week		lag = 32-63 week	
	β	p	β	p	β	p	β	p	β	p	β	p	β	p
Smithville Upstream West	0.087	0.787	0.085	0.705	-0.067	0.737	-0.201	0.267	-0.114	0.522	0.088	0.628	-0.352	0.431
Smithville Upstream East	-0.321	0.397	-0.104	0.724	0.224	0.352	0.031	0.892	0.079	0.790	0.213	0.327	-0.240	0.630
Smithville Midstream West	0.013	0.966	0.041	0.858	0.152	0.479	0.116	0.495	0.149	0.609	-0.016	0.940	0.172	0.737
Smithville Dam	-0.097	0.720	0.078	0.715	0.070	0.693	-0.058	0.689	0.189	0.513	0.030	0.872	-0.210	0.590
Pomme de Terre Upstream West	0.001	0.997	-0.104	0.673	0.111	0.598	-0.003	0.988	0.252	0.388	-0.388	0.254	0.514	0.303
Pomme de Terre Upstream East	-0.189	0.704	-0.073	0.839	-0.125	0.595	-0.118	0.574	0.199	0.517	-0.062	0.856	-0.425	0.449
Pomme de Terre Dam	0.020	0.960	0.304	0.156	-0.203	0.293	-0.323	0.068	-0.009	0.971	0.184	0.565	-0.068	0.875
Clearwater Upstream West	0.028	0.920	0.036	0.816	0.079	0.531	-0.223	0.138	-0.226	0.288	-0.072	0.759	-0.645	0.073
Clearwater Upstream East	-0.666	0.051	0.076	0.745	0.228	0.329	-0.405	0.031	-0.539	0.056	0.329	0.316	-1.413	0.009
Clearwater Dam	-0.456	0.146	0.036	0.853	0.102	0.600	-0.696	0.003	-0.688	0.021	0.029	0.918	-0.988	0.031
Wappapello Upstream West	0.532	0.029	0.169	0.184	0.277	0.012	0.125	0.304	0.133	0.270	0.313	0.217	0.514	0.091
Wappapello Upstream East	-0.114	0.705	0.021	0.914	0.144	0.499	-0.243	0.168	-0.050	0.810	0.274	0.361	-0.115	0.787
Wappapello Dam	-0.157	0.272	-0.119	0.270	-0.028	0.814	-0.144	0.206	0.029	0.861	-0.023	0.923	-0.202	0.396

Table A. 5-2 (cont'd)

Model 1.2: chlorophyll of July-August = LM (precipitation intensity)

Reservoir zone	lag = 0 week		lag = 1 week		lag = 2-3 week		lag = 4-7 week		lag = 8-15 week		lag = 16-31 week		lag = 32-63 week	
	β	p	β	p	β	p	β	p	β	p	β	p	β	p
Smithville Upstream West	0.192	0.284	0.046	0.533	-0.137	0.206	-0.173	0.205	-0.249	0.338	-0.031	0.915	-0.146	0.532
Smithville Upstream East	0.313	0.165	0.077	0.419	0.052	0.711	0.131	0.465	0.068	0.842	-0.083	0.820	0.236	0.411
Smithville Midstream West	0.114	0.595	-0.009	0.917	-0.037	0.780	-0.115	0.490	0.076	0.810	-0.076	0.824	-0.060	0.838
Smithville Dam	0.176	0.315	-0.013	0.863	-0.047	0.663	0.080	0.566	-0.019	0.943	-0.023	0.934	0.003	0.991
Pomme de Terre Upstream West	0.323	0.373	-0.092	0.176	-0.069	0.574	0.022	0.927	-0.126	0.554	-0.097	0.738	0.419	0.345
Pomme de Terre Upstream East	0.089	0.830	-0.139	0.062	-0.203	0.135	-0.118	0.666	-0.217	0.364	-0.170	0.603	0.124	0.807
Pomme de Terre Dam	0.093	0.789	-0.012	0.853	-0.079	0.495	0.082	0.721	-0.010	0.960	-0.353	0.190	0.720	0.071
Clearwater Upstream West	-0.181	0.576	0.136	0.479	-0.075	0.600	0.090	0.606	0.297	0.036	-0.008	0.975	-0.190	0.654
Clearwater Upstream East	0.196	0.623	-0.024	0.920	-0.085	0.632	0.397	0.055	0.411	0.016	-0.159	0.601	-0.049	0.926
Clearwater Dam	-0.140	0.702	0.035	0.874	-0.105	0.517	0.227	0.243	0.430	0.005	-0.105	0.708	0.057	0.909
Wappapello Upstream West	-0.250	0.311	0.058	0.646	-0.171	0.117	-0.243	0.063	0.092	0.353	0.145	0.452	0.000	0.999
Wappapello Upstream East	-0.320	0.398	-0.055	0.802	0.010	0.953	-0.164	0.419	0.323	0.054	0.362	0.208	0.349	0.507
Wappapello Dam	-0.269	0.345	0.100	0.570	0.040	0.767	-0.268	0.087	0.338	0.005	0.159	0.488	0.086	0.831

Table A. 5-2 (cont'd)

Model 1.3: chlorophyll of July-August = LM (total precipitation)

Reservoir zone	lag = 0 week		lag = 1 week		lag = 2-3 week		lag = 4-7 week		lag = 8-15 week		lag = 16-31 week		lag = 32-63 week	
	β	p	β	p	β	p	β	p	β	p	β	p	β	p
Smithville Upstream West	0.015	0.013	0.010	0.734	-0.015	0.382	0.001	0.913	0.001	0.921	-0.004	0.713	0.004	0.171
Smithville Upstream East	0.019	0.014	0.027	0.488	0.016	0.457	0.014	0.282	0.022	0.076	-0.010	0.468	0.010	0.005
Smithville Midstream West	0.014	0.057	0.002	0.957	-0.001	0.947	-0.002	0.858	0.024	0.036	-0.004	0.752	0.005	0.156
Smithville Dam	0.012	0.042	-0.004	0.908	0.005	0.780	0.013	0.214	0.013	0.194	-0.002	0.876	0.006	0.051
Pomme de Terre Upstream West	0.008	0.567	-0.001	0.986	0.011	0.624	0.002	0.876	0.003	0.719	-0.003	0.704	0.008	0.047
Pomme de Terre Upstream East	0.001	0.929	-0.022	0.558	-0.013	0.604	0.008	0.568	0.001	0.940	-0.007	0.428	0.009	0.056
Pomme de Terre Dam	-0.002	0.906	-0.023	0.473	0.007	0.730	0.016	0.162	0.008	0.290	-0.010	0.147	0.012	0.001
Clearwater Upstream West	-0.006	0.598	0.011	0.804	-0.025	0.180	0.017	0.146	0.013	0.010	0.003	0.551	0.002	0.584
Clearwater Upstream East	0.004	0.797	-0.046	0.375	-0.016	0.476	0.034	0.014	0.017	0.004	0.002	0.735	0.005	0.290
Clearwater Dam	-0.011	0.432	-0.034	0.492	-0.021	0.329	0.019	0.155	0.018	0.000	0.003	0.603	0.005	0.249
Wappapello Upstream West	-0.020	0.025	0.028	0.320	-0.021	0.132	-0.014	0.129	0.005	0.179	0.002	0.688	0.001	0.789
Wappapello Upstream East	-0.015	0.280	0.001	0.979	-0.027	0.221	-0.006	0.684	0.011	0.064	0.007	0.283	0.000	0.945
Wappapello Dam	-0.012	0.281	0.016	0.687	-0.018	0.319	-0.017	0.143	0.010	0.018	0.000	0.962	-0.001	0.780

Table A. 5-2 (cont'd)

Model 2.1: annual mean chlorophyll = LM (lake surface temperature)									
Reservoir zone	lag = 0 year		lag = 1 year		lag = 2-3 year		lag = 4-7 year		
	β	p	β	p	β	p	β	p	
Smithville Upstream West	0.590	0.000	0.267	0.145	0.053	0.860	0.725	0.272	
Smithville Upstream East	0.276	0.234	0.053	0.839	0.375	0.350	1.246	0.109	
Smithville Midstream West	0.124	0.407	0.050	0.754	0.031	0.902	0.883	0.107	
Smithville Dam	0.188	0.253	0.055	0.761	0.229	0.412	0.906	0.075	
Pomme de Terre Upstream West	0.735	0.002	-0.290	0.280	0.558	0.163	1.059	0.364	
Pomme de Terre Upstream East	0.451	0.034	-0.299	0.186	0.416	0.228	1.055	0.163	
Pomme de Terre Dam	0.134	0.610	-0.085	0.761	-0.113	0.778	0.817	0.287	
Clearwater Upstream West	0.188	0.143	-0.229	0.085	-0.070	0.680	0.490	0.090	
Clearwater Upstream East	0.252	0.147	-0.374	0.033	-0.004	0.986	0.721	0.128	
Clearwater Dam	0.048	0.803	-0.470	0.016	0.070	0.805	0.471	0.401	
Wappapello Upstream West	0.516	0.000	-0.124	0.470	0.435	0.062	0.731	0.085	
Wappapello Upstream East	0.733	0.000	-0.122	0.534	0.544	0.033	0.961	0.005	
Wappapello Dam	0.340	0.001	0.048	0.677	0.397	0.011	0.344	0.267	

Model 2.2: annual mean chlorophyll = LM (precipitation intensity)									
Reservoir zone	lag = 0 year		lag = 1 year		lag = 2-3 year		lag = 4-7 year		
	β	p	β	p	β	p	β	p	
Smithville Upstream West	-0.041	0.807	0.007	0.968	0.004	0.987	0.474	0.155	
Smithville Upstream East	0.013	0.946	0.083	0.664	-0.054	0.847	0.703	0.082	
Smithville Midstream West	-0.098	0.513	-0.078	0.607	-0.094	0.666	0.381	0.195	
Smithville Dam	-0.055	0.736	-0.067	0.691	-0.172	0.488	0.827	0.008	
Pomme de Terre Upstream West	0.283	0.305	0.337	0.201	0.496	0.333	1.050	0.255	
Pomme de Terre Upstream East	0.195	0.446	0.404	0.092	0.343	0.472	0.773	0.367	
Pomme de Terre Dam	0.297	0.293	0.338	0.232	-0.328	0.541	0.652	0.517	
Clearwater Upstream West	0.301	0.040	-0.173	0.292	0.011	0.962	0.259	0.364	
Clearwater Upstream East	0.293	0.160	-0.377	0.095	-0.202	0.530	-0.260	0.565	
Clearwater Dam	0.234	0.290	-0.435	0.066	-0.353	0.308	-0.480	0.295	
Wappapello Upstream West	0.438	0.010	0.100	0.609	0.353	0.202	0.786	0.030	
Wappapello Upstream East	1.049	0.000	0.476	0.184	1.141	0.011	1.567	0.000	
Wappapello Dam	0.652	0.000	0.389	0.057	0.671	0.013	0.825	0.019	

Table A. 5-2 (cont'd)

Model 2.3: annual mean chlorophyll = LM (total precipitation)									
Reservoir zone	lag = 0 year		lag = 1 year		lag = 2-3 year		lag = 4-7 year		
	β	p	β	p	β	p	β	p	
Smithville Upstream West	-0.001	0.437	-0.002	0.148	0.000	0.960	0.000	0.973	
Smithville Upstream East	0.002	0.137	0.001	0.557	-0.001	0.810	0.000	0.932	
Smithville Midstream West	0.000	0.838	-0.001	0.631	-0.001	0.477	0.000	0.935	
Smithville Dam	0.002	0.275	0.001	0.677	-0.002	0.451	0.001	0.804	
Pomme de Terre Upstream West	0.001	0.595	-0.001	0.627	0.001	0.672	-0.012	0.088	
Pomme de Terre Upstream East	0.001	0.542	0.001	0.580	0.001	0.630	-0.011	0.105	
Pomme de Terre Dam	0.003	0.131	0.002	0.224	0.001	0.687	-0.015	0.038	
Clearwater Upstream West	0.003	0.006	-0.001	0.341	0.000	0.847	-0.005	0.242	
Clearwater Upstream East	0.005	0.001	-0.001	0.666	0.000	0.983	-0.005	0.421	
Clearwater Dam	0.004	0.006	-0.001	0.461	0.000	0.966	-0.005	0.436	
Wappapello Upstream West	0.003	0.025	-0.001	0.533	0.000	0.853	-0.002	0.648	
Wappapello Upstream East	0.004	0.081	-0.003	0.198	-0.003	0.515	-0.004	0.616	
Wappapello Dam	0.002	0.089	0.000	0.884	-0.001	0.829	0.000	0.951	

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6 ALGAL BIOMASS RESPONSES TO CLIMATE CHANGE IN LAKES ACROSS THE CONTINENTAL UNITED STATES

Abstract

Climate change is expected to create conditions conducive to harmful algal blooms. However, in complex watersheds and aquatic systems, it is not clear how algae in lakes respond to changes in climate factors and nutrient loadings. It is even more challenging to predict climate change impacts on lake algae that involve complex effects of climate change on interactions between watersheds and aquatic systems. This study investigated relationships between algal biomass and climate change utilizing a space-for-time substitution method with data from more than 1000 lakes across a large gradient of climate in continental United States. Lake algal biomass was characterized using remote sensing observations as well as in-lake measurements. Statistical models using boosted regression trees indicated that (1) algal biomass increased with temperature; and (2) algal biomass increased with higher precipitation intensity, but decreased with higher annual total precipitation. The climate scenario analyses predicted that algal biomass would increase in the future climate. Specifically, algal biomass would increase in all CO₂ emission scenarios, and higher CO₂ emission would result in higher algal biomass increase.

Keywords: climate change, lakes, water quality, phytoplankton

Highlights

- Algal biomass increased with temperature.
- Algal biomass sensitivity to temperature increased with higher nutrient concentrations in lakes.
- Algal biomass decreased with total precipitation, but increased with precipitation intensity.
- Algal biomass sensitivity to precipitation intensity increased with soil erodibility.
- Algal biomass will increase more in the “high” CO₂ emission scenario than the “low” one.

6.1 Introduction

An algal bloom is a rapid increase or accumulation of algae in water. Harmful algal blooms are significant global and local threats to public health and aquatic ecosystems (Anderson 1989; Lopez et al. 2008). Freshwater algal blooms are often dominated by cyanobacteria, some of which can release toxins and cause sickness or death in the wildlife and humans who use the water for drinking or recreation (Falconer, Beresford, and Runnegar 1983). The economic damages incurred from freshwater eutrophication were conservatively estimated at 2.2 billion dollars per year in the United States, considering recreational water usage, waterfront real estate, and recovery of biodiversity and drinking water (Dodds et al. 2009). Predicted changes in climate may cause more algal blooms, especially harmful cyanobacteria blooms, based on the following hypotheses (Paerl and Huisman 2008):

- Increased atmospheric CO₂ enhances carbon availability for all phytoplankton species, especially surface-dwelling cyanobacteria;
- Higher water temperatures, resulting in lower water viscosity and stronger thermal stratification, facilitates buoyant cyanobacteria to out-compete other phytoplankton species;
- Higher temperatures accelerate growth of all phytoplankton species, especially cyanobacteria that have a warmer temperature optimum than other algal groups;
- Higher hydrologic variability introduces more nutrients, especially particulate phosphorus (P), which stimulates phytoplankton growth in inland lakes that are mostly P-limited.

Recently, some of these hypotheses have been questioned as being too simplistic to apply to the complex conditions in lakes and their watersheds. Lürling et al. (2013) found that cyanobacteria did not have significantly higher optimum temperatures than the other species, after taking more algal species into consideration than Paerl and Paul (2012). Moreover, at optimum temperatures, cyanobacteria did not grow significantly faster than the other species. Based on an extensive literature review, Reichwaldt

and Ghadouani (2012) found that harmful algae and total biomass of all species responded to rainfall events variably on a case by case basis, not necessarily increasing with the changes of rainfall pattern.

Numerous laboratory experiments have supported some of the hypotheses, but natural ecosystems are much more complicated than the incubation and mesocosm conditions of most experiments. Even large-scale observations that include natural ecosystem complexities may not be long enough to account for the hysteresis effect that nutrient legacies in lake sediments can have on algal production (Schindler 2012).

Climate change impacts on algal biomass involve the complexity of algal responses to nutrient loading, as well as the complexity of watershed-based nutrient loading that responds to climate change. Scholars continue to debate how algal biomass responds to phosphorus and nitrogen control (Lewis and Wurtsbaugh 2008; Conley et al. 2009; Schindler and Hecky 2009; Lewis, Wurtsbaugh, and Paerl 2011; Schindler 2012). Above-ground vegetation and soil nutrients may shift to new regimes due to climate change resulting in new combinations of CO₂, temperature, and precipitation. Subsequently, inflow nutrient quality and quantity may change. Additional processes in watersheds inevitably bring more possible outcomes and uncertainties than solely considering in-lake processes and the phosphorus/nitrogen control debate. Ultimately, despite a good deal of research, a consensus has not yet been reached regarding sensitivity of algal blooms to climate change. This lack of consensus leaves policy makers in a dilemma when planning for climate change, as they lack strong and consistent scientific evidence for the impacts of climate change on eutrophication and harmful algal blooms (Whitehead et al. 2009; Hudnell 2010).

The general goal of this study was to develop statistical relationships between climate variables and algal biomass in lakes across a diversity of watersheds and climatic settings. Specifically, the present study was designed to quantify the sensitivity of algal biomass to temperature and precipitation in lakes across the United States. Chlorophyll-*a* (Chl) concentration was used as a proxy for algal biomass. Algal

biomass sensitivities to climate were assessed using a “space-for-time substitution” method (Pickett 1989; Blois et al. 2013) in which lake condition was assessed during one summer/year across the continental United States, which includes a wide range of algal biomass and climatic conditions. We assumed that the trajectories of algal biomass changes along temperature and precipitation gradients over space would inform how the algal biomass would change in response to changes in the future climate. The sensitivities to climate were evaluated by statistical models, *i.e.*, boosted regression trees (BRT), which are derived by non-linear machine-learning algorithms (Friedman 2001). The following hypotheses were tested:

- A. Chl (indicated by concentration) increases asymptotically with temperature until a maximum positive effect of temperature is reached.
- B. Temperature impacts on Chl are regulated by nutrient (*e.g.*, phosphorus and nitrogen) availability.
- C. Chl increases with precipitation intensity due to soil erosion, but may decrease with total precipitation (precipitation frequency) due to the dilution of inflow nutrients and algal concentration.
- D. Precipitation impacts on Chl are mediated by natural hydraulic conditions (*e.g.*, watershed slope, soil erodibility, and soil hydraulic conductivity). Specifically, Chl sensitivity to precipitation increases with slope and soil erodibility for higher sediment loading to lakes, but decreases with higher soil hydraulic conductivity because a greater proportion of precipitation infiltrates to groundwater, resulting in less overland flow and consequent soil erosion.

6.2 Methodology

6.2.1 Study lakes

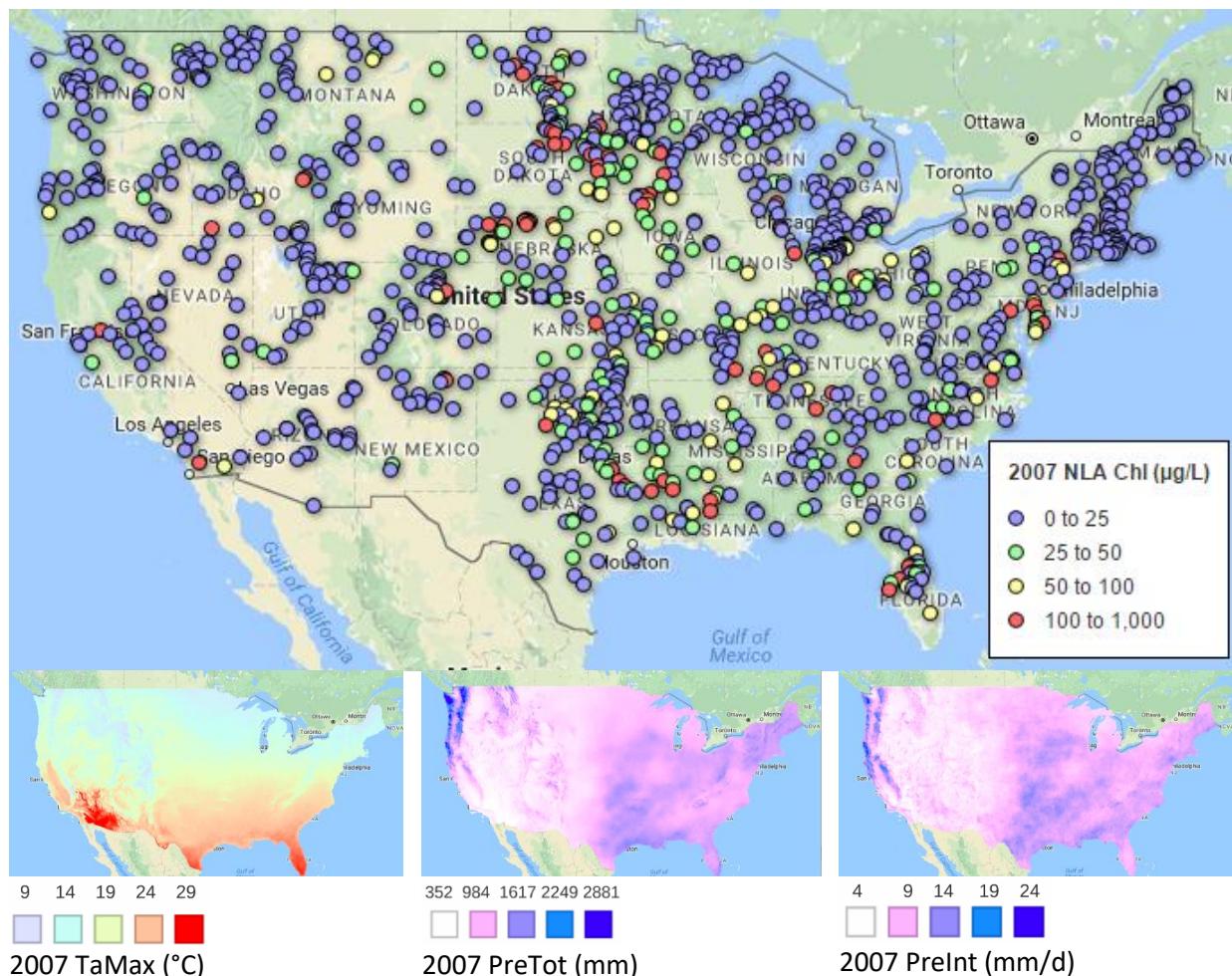


Figure 6-1 Lake chlorophyll-a (Chl) from the 2007 National Lake Assessment (NLA), 2007 daily maximum temperature (TaMax), 2007 annual total precipitation (PreTot), and 2007 precipitation intensity (PreInt).

Each Chl point represents one lake sample. Background maps are Google Map data.

A total of 1157 lakes were used in this study based on data from the 2007 National Lakes Assessment (NLA) by the United States Environmental Protection Agency (<https://www.epa.gov>, accessed on December 30, 2016). These lakes represented natural and man-made freshwater lakes and ponds greater than 10 acres (0.04 km^2) and deeper than 1 m. This sample across the continental United States

provided a wide range of algal biomass, temperature, precipitation, nutrient, and hydraulic conditions (Figure 6-1).

6.2.2 Sensitivity and partial dependence analyses

Sensitivity of algal biomass (hereafter referred to as “Chl sensitivity”) was defined as the change in Chl (dependent variable) along the gradient of an independent variable such as temperature and precipitation. Boosted regression trees (BRT) were used to quantify algal biomass sensitivity to temperature and precipitation. BRT models were calibrated with R codes adapted from Elith et al (2008). The BRT algorithm core functions were from the *gbm* R package (Ridgeway 2004). Chl sensitivity was evaluated by one-variable partial dependence analysis. Partial dependence of a predictor in a BRT model was the response of Chl to the predictor when the other predictors were held at their means. One-variable partial dependence analysis provided the trend and magnitude of Chl change along the gradient of one independent variable. One-variable partial dependence analysis used the *plot.gbm* function from the *gbm* R package. The contribution of each predictor in a BRT model was indicated by relative importance. Relative importance of a predictor in a BRT model is the sum of deviation reduced by each split using the predictor in the BRT trees, divided by the total deviation reduced by all predictors. Relative importance was calculated with the *summary.gbm* function from the *gbm* R package. The change of Chl sensitivity over the range of an independent variable, such as Chl sensitivity to temperature changes over total phosphorus, was evaluated by two-variable partial dependence analysis, *i.e.*, how Chl sensitivity to one predictor changed with the other predictor when the remaining predictors were held at their means. This was basically a two-way interaction analysis. In addition to the range of Chl change, the magnitude of the two-way interaction was also indicated by the Friedman’s *H*-statistic index (Friedman and Popescu 2008). The Friedman index ranges from zero to one (100%) with higher values indicating stronger interactions. For instance, *H* = 10% indicates the interaction explained

10% of the total variance that could be explained by two variables together. The index was calculated with the function *interact.gbm* in the *gbm* R package.

Model performance was validated by 10-fold cross validation. In a 10-fold cross validation, a dataset was randomly split into 10 subsets. Each subset was used as a holdout validation dataset once to validate a version of the model that was calibrated with a combined dataset of the remaining nine subsets. Thus, the model was validated 10 times with 10 different subsets of data. Model performance was evaluated by Nash–Sutcliffe model efficiency coefficient (NSE):

$$\text{NSE} = 1 - \frac{\sum_1^i (y_i - \hat{y}_i)^2}{\sum_1^i (y_i - \bar{y})^2}$$

- y_i is measured value
- \hat{y}_i is modeled value
- \bar{y} is mean of y_i

NSE means the portion of the total variance explained by the model. NSE is the same as the general definition of R^2 (model determination coefficient). NSE ranges from $-\infty$ to one, where one indicates a perfect fit, while $\text{NSE} \leq 0$ indicates a model failure.

Six analytical BRT models were developed to evaluate Chl sensitivity to temperature and precipitation (Table 6-1). More details about these models will be described in the following sections.

Table 6-1 Diagnostic models. See Table 6-2 for variable descriptions. Grey background indicates a new variable compared to the previous model.

Model #	Dependent Variable	In-lake independence variable				Watershed independence variable							
		In.TP	In.TN	Ts	TaMax2007Point	PreTot2007	PreInt2007	k-factor	conductivity	disturbance2005	shoreDevelopment	slope	In.basin2Lake
1	NLA.Chl (survey point)	x	x	x									
1.1	RS.Chl.1.time (3x3 pixels)	x	x	x									
1.2	RS.Chl.summer (whole lake)	x	x	x									
1.3	RS.Chl.annual (whole lake)	x	x	x									
1.4	RS.Chl.annual (whole lake)	x	x		x								
2	RS.Chl.annual (whole lake)				x	x	x	x	x	x	x	x	x

Table 6-2 Model variables and data sources.

Variable	Description and data source
NLA.Chl ($\mu\text{g/L}$)	Ground-measured chlorophyll-a (Chl). One sample for each lake ($N = 1156$). Source: 2007 National Lake Assessment (USEPA, http://www.epa.gov).
RS.Chl.1.time ($\mu\text{g/L}$)	Remote-sensing Chl measured by Landsat 5 (Google Earth Engine ImageCollection ID = "LEDAPS/LT5_L1T_SR") using the random forest algorithm. 30-m resolution. Each lake was measured by one image with the closest date ($\Delta\text{day} \leq 8$ days) to the survey date of the 2007 National Lake Assessment. Average of a 3-by-3-pixel window. $N = 482$. Source: this study.
RS.Chl.summer ($\mu\text{g/L}$)	2007 summer (May-August) average Chl measured by Landsat 5 (Google Earth Engine ImageCollection ID = "LEDAPS/LT5_L1T_SR") using the random forest algorithm. 30-m resolution. Average of whole-lake. $N = 591$. Source: this study.
RS.Chl.annual ($\mu\text{g/L}$)	2007 annual average Chl measured by Landsat 5. 30-m resolution. Average of whole-lake. $N = 658$. Source: this study.
In.TP ($\mu\text{g/L}$)	Log-transformed total phosphorus. One sample for each lake. Source: 2007 National Lake Assessment (USEPA, http://www.epa.gov).
In.TN ($\mu\text{g/L}$)	Log-transformed total nitrogen. One sample for each lake. Source: 2007 National Lake Assessment (USEPA, http://www.epa.gov).
Ts ($^{\circ}\text{C}$)	Lake surface temperature. One sample for each lake. Source: 2007 National Lake Assessment (USEPA, http://www.epa.gov).

Table 6-2 (cont'd)

TaMax2007Point (°C)	2007 average daily air maximum temperature over lake (not watershed). 4-km resolution. Source: University of Idaho Gridded Surface Meteorological Dataset (Abatzoglou 2013), Google Earth Engine Sever, ImageCollection ID = "IDAHO_EPSCOR/MACAv2_METDATA".
TaMax2099Point (°C)	2099 average daily air maximum temperature over lake. Two scenarios: RCP4.5 and RCP8.5 from CCSM4 model and r6i1p1 ensemble. Same resolution and source as TaMax2007Point.
PreTot2007 (mm)	2007 annual total precipitation of watershed. Same resolution and source as TaMax2007Point.
PreTot2099 (mm)	2099 annual total precipitation of watershed. Two scenarios: RCP4.5 and RCP8.5 from CCSM4 model and r6i1p1 ensemble. Same resolution and source as TaMax2007Point.
PreInt2007 (mm/d)	2007 precipitation intensity of watershed. Equals to average daily precipitation that has value ≥ 1 mm/d. Same resolution and source as TaMax2007Point.
PreInt2099 (mm/d)	2099 precipitation intensity of watershed. Two scenarios: RCP4.5 and RCP8.5 from CCSM4 model and r6i1p1 ensemble. Source: Same resolution and source as TaMax2007Point.
kFactor (dimensionless)	Watershed soil erodibility factor (the K factor in the Universal Soil Loss Equation). Source: State Soil Geographic (STATSGO) Database.
conductivity (in/h)	Watershed soil hydraulic conductivity. Source: State Soil Geographic (STATSGO) Database. 1 in = 2.54 cm.
disturbance2005 (%)	2005 percentage of developed lands and cultivated lands in watershed. 30-m resolution. Source: National Land Cover Dataset, Google Earth Engine Sever, ImageCollection ID = "USGS/NLCD".
shoreDevelopment (1 to 10)	Development grade of lake shore estimated by eye visual survey. 1 indicates natural shore; 10 indicates fully developed. Source: 2007 National Lake Assessment (USEPA, http://www.epa.gov)
slope (°)	Watershed average slope. 30-m resolution. Source: SRTM Digital Elevation Data, Google Earth Engine Sever, Image ID = "USGS/SRTMGL1_003".
In.basin2lake	Log-transformed ratio of basin area to lake area. Source: this study.

6.2.2.1 Chl sensitivity to temperature

Chl sensitivity to temperature was evaluated by Model 1 (Lake Model, Table 6-1), *i.e.*, NLA.Chl = BRT (In.TP, In.TN, Ts), where chlorophyll- α (NLA.Chl), total phosphorus (In.TP), total nitrogen (In.TN), and lake surface temperature (Ts) were measured in lakes during the 2007 National Lake Assessment (NLA) in the United States. All variables in Model 1 were measured in lakes, so it was called the Lake Model.

Hypothesis A, *i.e.*, Chl increases asymptotically with temperature until saturated, was tested using one-

variable partial dependence analysis between NLA.Chl and Ts. Hypothesis B, *i.e.*, Chl sensitivity to temperature was regulated by nutrient availability, was tested using two-variable partial dependence analyses between NLA.Chl, Ts, and each nutrient variable (ln.TP or ln.TN).

6.2.2.2 Chl sensitivity to precipitation

Chl sensitivity to precipitation was evaluated by Model 2 (Watershed Model, Table 6-1), *i.e.*, RS.Chl.annual = BRT (TaMax2007Point, PreTot2007, PreInt2007, kFactor, conductivity, disturbance2005, shoreDevelopment, slope, ln.basin2lake). The variables of this model will be explained in the following paragraphs. Model 2 was an upscaled version of Model 1: the statistical period of the variables increased from a summer (sampling duration) to a year; and lake nutrients were indirectly estimated by precipitation and watershed characteristics. Thus, Model 2 was called the Watershed Model.

The measurement period was scaled up to a year in the Model 2 because precipitation effects on lake Chl may have time lags that vary lake by lake and watershed by watershed (Chapter 5). Without knowing the time lags for each specific lake in the study, it was impossible to select precipitation variables to relate to lake Chl of a specific time. To address this problem, Model 2 used lake Chl and precipitation conditions during a full year, assuming that annual average Chl was related by BRT to precipitation conditions within the same year regardless of the time lags. The year of 2007 was picked for Model 2 so it could be compared best to Model 1, which used 2007 NLA data.

NLA Chl was mostly measured only one time at one location in a lake during summer 2007 and therefore could not be expected to represent the Chl of a whole year and over the whole lake. So, remote sensing (RS) was used to estimate Chl. 2007 annual RS Chl (RS.Chl.annual) was derived using Landsat TM 5 (Google Earth Engine Image Collection ID = “LANDSAT/LT5_SR”) and a machine-learning algorithm, random forest. Landsat images were Land Surface Reflectance with atmospheric correction (Masek et al. 2006). The random forest Chl model was trained with the ground-measured Chl from the 2007 NLA. The

RS Chl algorithm had a predictive accuracy of 46.2% indicated by 10-fold cross validation (Figure 6-2).

The algorithm was then applied in Google Earth Engine (Gorelick 2012) to calculate whole-lake RS Chl for 2007. Landsat TM 5 revisit time was 16 days. RS.Chl.annual was an average over all images in 2007 and all pixels in the lake for images with low cloud interference.

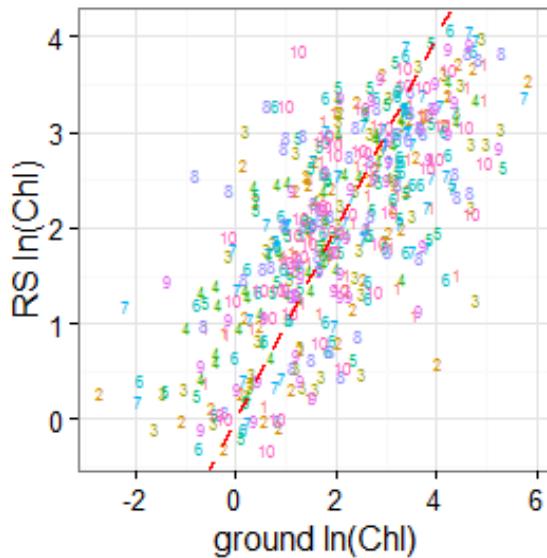


Figure 6-2 Predictive accuracy of remotely sensed chlorophyll-a (RS Chl) indicated by 10-fold cross validations. NSE = 0.462 ($\delta = 0.086$), sample $N = 483$. The dashed line is a 1:1 ratio line. Each point represents one lake sample. Ten validations were coded by corresponding numbers from 1 to 10.

Lake annual temperature (TaMax2007Point), watershed annual total precipitation (PreTot2007), and watershed annual precipitation intensity (PreInt2007) were determined with the University of Idaho Gridded Surface Meteorological Dataset (Abatzoglou 2013) (Table 6-2

Table 6-2). Even though a period of 30 minutes is the best time interval to calculate precipitation intensity regarding soil erosion (Wischmeier and Mannering 1969), due to unavailability of hourly or 30-min precipitation data, precipitation intensity was the average of daily precipitation that for days with greater than 1 mm/d (Nicholls and Kariko 1993; Groisman et al. 2005).

Nutrient conditions in Model 2 were estimated with precipitation and a set of watershed landscape variables (Table 6-1). Those landscape variables were soil erodibility factor (kFactor), soil hydraulic conductivity, percentage of developed and cultivated lands (disturbance2005), lake shore development (shoreDevelopment), watershed slope (slope), and ratio of basin area to lake area (ln.basin2lake). These variables were selected from a large variable pool ($N = 68$) of climate, soil, ecoregion, geology, hydrology, watershed morphology, lake morphology, and land use/cover, which were similar to the candidate variables in Olson and Hawkins (2013). Variables were selected by both forward and backward selection. Redundant variables were eliminated from the nutrient condition model, and were defined as variables resulting in changes in predictive deviation less than half of one standard error of the predictive deviation of the full model.

Hypothesis C, *i.e.*, Chl increases with precipitation intensity but decreases with total precipitation, was tested using one-variable partial dependence analyses between RS.Chl.annual and each precipitation variable (PreInt2007 or PreTot2007). Hypothesis D, *i.e.*, Chl sensitivity to precipitation intensity was mediated by natural hydraulic conditions, was tested using two-variable partial dependence analyses between RS.Chl.annual, PreInt2007, and each natural hydraulic variable (kFactor, conductivity, or slope).

When upscaling the Lake Model to the Watershed Model for the analyses of Chl sensitivity to precipitation, the model accuracy might be affected by (1) replacing NLA ground-measured Chl with RS Chl, (2) replacing NLA ground-measured temperature (Ts) with annual air temperature (TaMax2007), or (3) replacing NLA ground-measured nutrients with precipitation and landscape variables. To evaluate the variable replacements, four intermediate models (Model 1.1, 1.2, 1.3 and 1.4 in Table 6-1) were built to compare models in the stepwise transition from Model 1 and Model 2. Specifically:

1. Comparing NSE of Models 1 and 1.1 with ground-measured Chl (NLA.Chl) and RS Chl measured one time (RS.Chl.1.time) being related to ground-measured water temperature, TP, and TN provided a direct comparison of ground-measured Chl and RS Chl.
2. Comparing NSE of Models 1.1 and 1.2 with RS chl measure one time and RS Chl measured over the summer (RS.Chl.summer) tested whether multiple measures of RS Chl during a season provided better model performance than one measure.
3. Comparing NSE of Models 1.2 and 1.3 with RS summer Chl and RS annual Chl (RS.Chl.annual, Table 6-2) tested whether annual Chl was similarly sensitive to temperature as summer Chl.
4. Comparing NSE of Models 1.3 and 1.4 with NLA ground-measured temperatures (Ts) and annual air temperatures (TaMax2007) tested whether annual average temperature was better than the one-time temperature measure.
5. Comparing NSE of Models 1.4 and 2 with in-lake nutrient measurements and watershed nutrient proxies tested whether in-lake nutrients could be inferred by watershed proxies.

RS.Chl.1.time and RS.Chl.summer were estimated from Landsat 5 using the same algorithm as RS.Chl.annual (Table 6-2). RS.Chl.1.time was RS Chl of 3x3 pixels with the same locations as NLA.Chl. The dates of RS.Chl.1.time were the same or close (Δ day \leq 8 days) to NLA.Chl sampling dates. RS.Chl.summer was the average of summer (May-August, 2007) RS Chl. Some lakes did not have Chl values due to cloud cover or no pure water pixels in the Landsat imagery. Most of those lakes were small. 658, 591, and 482 lakes had RS.Chl.annual, RS.Chl.summer, and RS.Chl.1.time. The number and identity of lakes was the same when calculating and comparing model performance using NSE.

6.2.3 Future scenario analyses

Future algal biomass was predicted using Model 2 and replacing the 2007 measures of temperature and precipitation with predictions for 2099. The future temperature and precipitation were based upon two CO₂ emission scenarios, Representative Concentration Pathway (RCP) 4.5 (the “low” emission), and RCP

8.5 (the “high” emission). Both scenarios were produced under the fifth Coupled Model Intercomparison Project (CMIP5) (Taylor, Stouffer, and Meehl 2012). The algal biomass difference between 2007 and 2099 was evaluated by pairwise *t*-test, where the paired measurements were 2007 and 2099 Chl for each lake.

6.3 Results

6.3.1 Chl sensitivity to temperature

The Lake Model (Model 1) explained 40.6% ($\text{NSE} = 0.406$, $\sigma = 0.325$) of the total variance of ground measured Chl, indicated by the 10-fold cross validation. Relative importance analyses of variables showed that most of the model error was reduced by nutrients, *i.e.* total nitrogen (ln.TN , 64.1% of error reduction) and total phosphorus (ln.TP , 26.4% of error reduction), while the remaining 9.5% of error reduction was by lake surface temperature (Ts). One-variable partial independence analysis showed that sample site Chl increased with Ts . Specifically, when Ts increased from 10 °C (minimum) to 34 °C (maximum) and the nutrients were controlled at mean levels, Chl increased by 36.3 µg/L. In other words, Chl sensitivity to Ts was 1.5 µg/(L °C) (Figure 6-3).

Chl sensitivity to Ts increased with total phosphorus and total nitrogen, according to two-variable partial dependence analyses. Specifically, Chl sensitivity to Ts increased from 0.8 µg/(L °C) to 2.5 µg/(L °C) when total phosphorus increased from 1 µg/L (minimum) to 479 µg/L (maximum). Chl sensitivity to Ts increased from 0.8 µg/(L °C) to 4.2 µg/(L °C) when total nitrogen increased from 5 µg/L (minimum) to 26400 µg/L (maximum). Chl sensitivity to Ts did not continually increase with ln.TP or ln.TN at high concentrations as it did at low concentrations. At high ln.TN , the sensitivity was slightly decreased (Figure 6-4). Friedman's *H*-statistic in Model 1 showed that the interaction between Ts and ln.TP accounted for 27.3% of the total variance explained by Ts and ln.TP , and the interaction between Ts and

In.TN accounted for 28.3% of the total variance explained by Ts and In.TN. Both interactions were almost as strong as the interaction between In.TP and In.TN ($H = 33.4\%$).

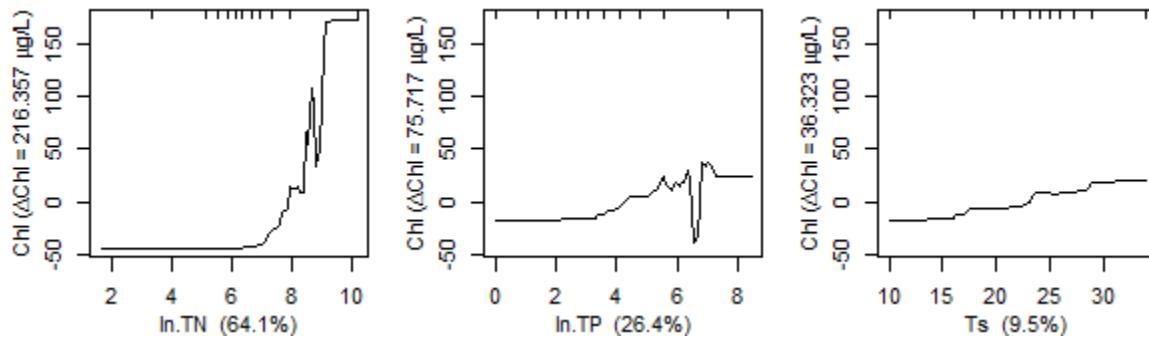


Figure 6-3 Partial dependence plots of Model 1. For comparison purposes, all plots have the same range of y-axis, and modeled Chl is centered to have a zero mean. Percentages in brackets are relative importance of the independent variables. Tick marks at the top are decile marks showing data distribution across the x-axis variable (data $N = 1156$). ΔChl is the range of modeled Chl. See Table 6-2 for variable explanations.

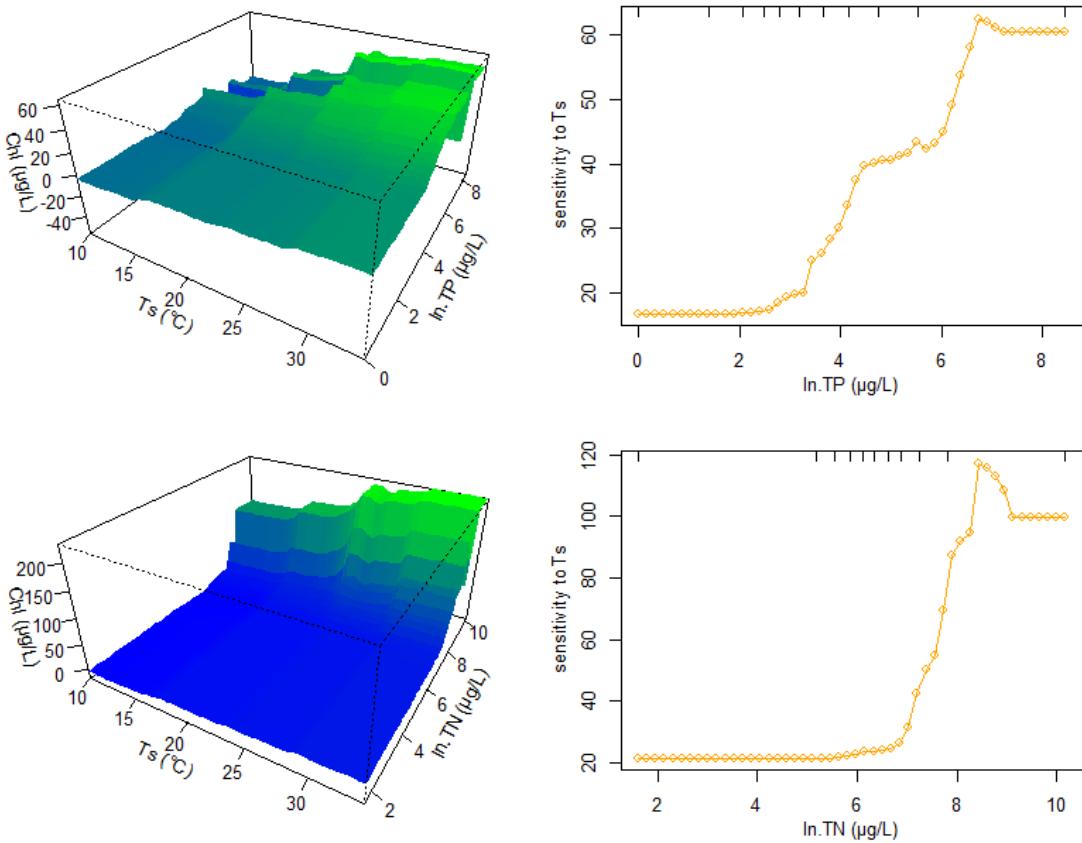


Figure 6-4 Chlorophyll- α (Chl) sensitivity to lake surface temperature (T_s) changed with nutrient concentration, *i.e.*, log-transformed total nitrogen ($\ln.TN$) and log-transformed total phosphorus ($\ln.TP$). Chl are modeled values from Model 1. Sensitivity to T_s here is the range of Chl change with T_s at the designated level of $\ln.TP$ and $\ln.TN$. Tick marks at the top are decile positions showing the data distribution across the x-axis variable (data $N = 1156$). Each point on figures on the right is one of 50 interpolation points.

6.3.2 Chl sensitivity to precipitation

Replacing ground-measured Chl (NLA.Chl) with remotely-sensed Chl (RS.Chl.1.time) in Model 1 had no effect on model performance (t -test $p = 0.899$) because NSE only changed from 0.288 ($\delta = 0.152$) to 0.292 ($\delta = 0.137$). Thus, remotely sensed Chl was accurate enough to relate algal biomass changes with

nutrients and temperature. When one-time measures of Chl (RS.Chl.1.time) were replaced by the Chl average for the summer (May – August) and for the whole lake (RS.Chl.summer), Model 1 performance increased significantly (t -test $p < 0.05$), with NSE increasing from 0.224 ($\delta = 0.179$) to 0.521 ($\delta = 0.117$). Thus, averages of multiple Chl measures during the summer and over the whole lake were better related to lake nutrients and temperatures than the one-time measurements of Chl. When the period of Chl averaging was expanded from the summer to the whole year 2007 (RS.Chl.annual), the model performance did not change significantly (t -test $p = 0.221$) (Figure 6-5).

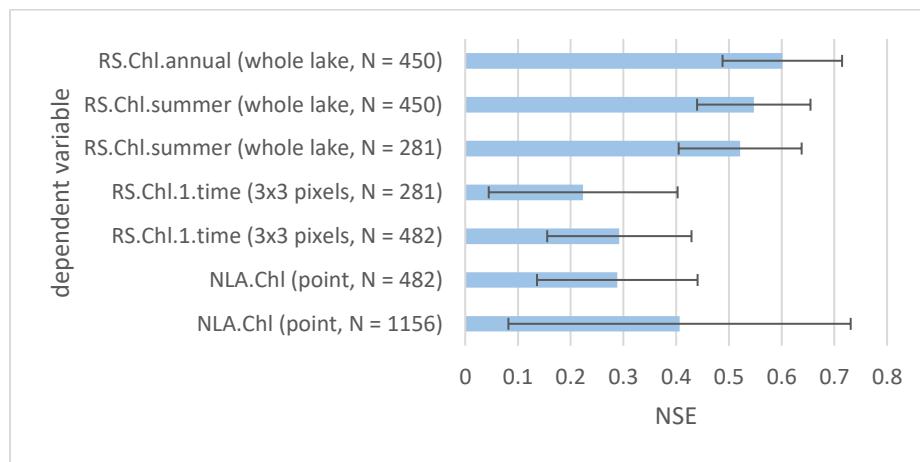


Figure 6-5 Model performance (indicated by Nash–Sutcliffe model efficiency coefficient, NSE) changes with dependent variable (y) in the model $y = \text{BRT}(\ln.\text{TP}, \ln.\text{TN}, \text{Ts})$. See Table 6-2 for variable explanations. Error bars represent one standard deviation. N is sample number of each model. For comparison purposes, lake samples were changed to have the same number and identity of lakes for each step of model comparison.

After the dependent variable in Model 1 was replaced by RS.Chl.annual, ground-measured lake surface temperature (Ts) was replaced by 2007 air maximum temperature over lake (TaMax2007Point). That replacement did not significantly (t -test $p = 0.627$) change model performance, with NSE = 0.580 ($\delta = 0.080$) changing to NSE = 0.571 ($\delta = 0.096$), indicating temporal up-scaling of temperature did not affect

the model predictive performance. When the ground-measured lake nutrients (*i.e.*, ln.TP and ln.TN) were further replaced with watershed variables (*i.e.*, PreTot2007, PreInt2007, watershed slope, kFactor, soil conductivity, ln.basin2lake, disturbance, and shoreDevelopment) to have Model 2 for assessing Chl sensitivity to precipitation, the model performance significantly (*t*-test $p < 0.05$) decreased from NSE = 0.571 ($\delta = 0.096$) to NSE = 0.428 ($\delta = 0.105$), indicating watershed predictors had a lower correlation with lake algal biomass than even one-time measures of in-lake nutrients.

Model 2 explained 42.8% of the total variance in annual Chl (RS.Chl.annual), where 2007 annual total precipitation (PreTot2007) and 2007 precipitation intensity (PreInt2007) contributed 6.7% and 2.7% of the total model explanation, respectively. The contribution of precipitation variables was relatively low compared to watershed slope (32.4%), soil K factor (17.2%), soil conductivity (12.8%), and human disturbance (7.1%). One-variable partial dependences of Model 2 showed that RS.Chl.annual decreased with PreTot2007, while it increased with PreInt2007. The partial RS.Chl.annual decreased by 2.0 $\mu\text{g/L}$ when PreTot2007 increased from 32.5 mm (minimum) to 2960.7 mm (maximum). A sharp decrease in partial RS.Chl.annual was found from PreTot2007 = 500 to 700 mm, and there was little Chl change outside this range. Partial RS.Chl.annual increased by 0.8 $\mu\text{g/L}$ when PreInt2007 increased from 2.8 mm/d (minimum) to 16.3 mm/d (maximum). The partial RS.Chl.annual trend over PreInt2007 was almost linear (Figure 6-6).

The partial RS.Chl.annual increased by 2.9 $\mu\text{g/L}$ when lake temperature (TaMax2007Point) increased from 5 °C (minimum) to 29 °C (maximum). Partial RS.Chl.annual was saturated at TaMax2007Point > 17 °C (Figure 6-6).

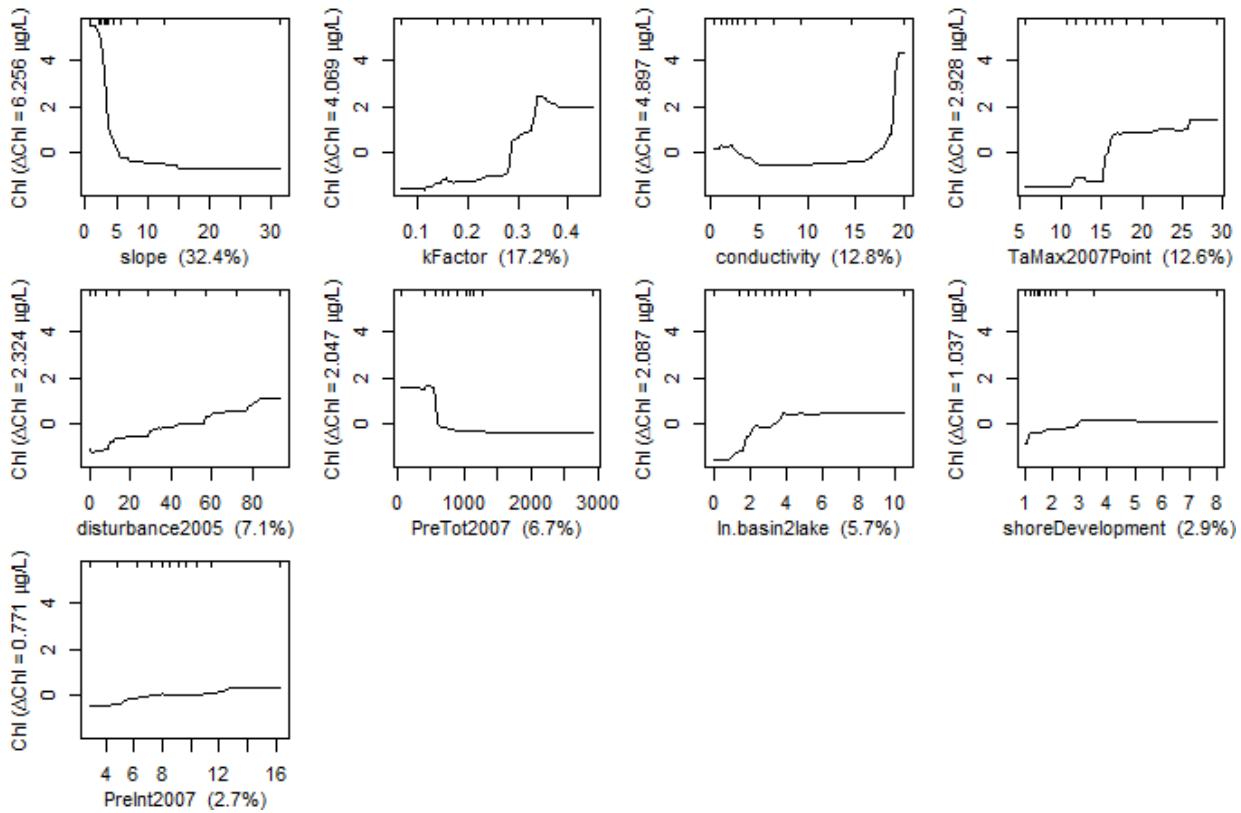


Figure 6-6 Partial dependence plots of Model 2. For comparison purposes, all plots have the same range of y-axis, and modeled Chl is centered to have zero mean. Percentages in brackets are relative importance of the variables. Tick marks at the top are decile locations showing the data distribution across the x-axis variable (data $N = 658$). ΔChl is the range of modeled Chl. See Table 6-2 for variable explanations.

Lakes in watersheds with more erosive and less hydraulically conductive soils were most sensitive to increases in precipitation intensity. Chl sensitivity to precipitation intensity (PreInt2007) increased with soil erodibility (K factor) and decreased very slightly with soil conductivity (Figure 6-7, two-variable partial dependence analyses). Specifically, Chl sensitivity to PreInt2007 increased from 0.9 $\mu\text{g/L}$ per K unit to 1.5 $\mu\text{g/L}$ per K unit when K factor increased from 0.06 (minimum) to 0.49 (maximum). Chl sensitivity to PreInt2007 decreased from 0.025 $\mu\text{g}/(\text{L in/h})$ to 0.016 $\mu\text{g}/(\text{L in/h})$ when soil conductivity

increased from 0.2 in/h (minimum) to 20.0 in/h (maximum, 1 in = 2.54 cm). Note that there was a very small increase in sensitivity at low conductivity that was not consistent with the overall negative trend in sensitivity along the soil conductivity gradient (Figure 6-7). Chl sensitivity to PreInt2007 did not increase with watershed slope. Chl sensitivity to PreInt2007 decreased with total annual precipitation in watersheds during 2007 (PreTot2007), indicating that dry areas were more sensitive to precipitation intensity (Figure 6-8).

Friedman's *H*-statistic in Model 2 showed that the interaction between PreInt2007 and PreTot2007 accounted for 22.0% of the total variance explained by PreInt2007 and PreTot2007. The remaining independent variables in Model 2 interacted relatively weakly with PreInt2007 (*H* < 5%) (Table 6-3).

Table 6-3 Variable interactions in Model 2 indicated by Friedman's *H*-statistic. Grid colors: green = low; red = high. See Table 6-2 for variable explanations.

	TaMax2007Point	PreTot2007	PreInt2007	kFactor	conductivity	disturbance2005	shoreDevelopment	slope
PreTot2007	3.1%							
PreInt2007	0.3%	22.0%						
kFactor	8.3%	5.4%	1.5%					
conductivity	5.9%	3.2%	0.7%	8.5%				
disturbance2005	1.9%	3.2%	1.4%	6.7%	9.6%			
shoreDevelopment	0.8%	3.3%	2.7%	1.6%	2.7%	7.5%		
slope	15.2%	10.6%	2.4%	6.6%	3.8%	1.3%	1.1%	
In.basin2lake	3.0%	3.3%	1.2%	6.8%	1.7%	3.6%	5.4%	3.8%

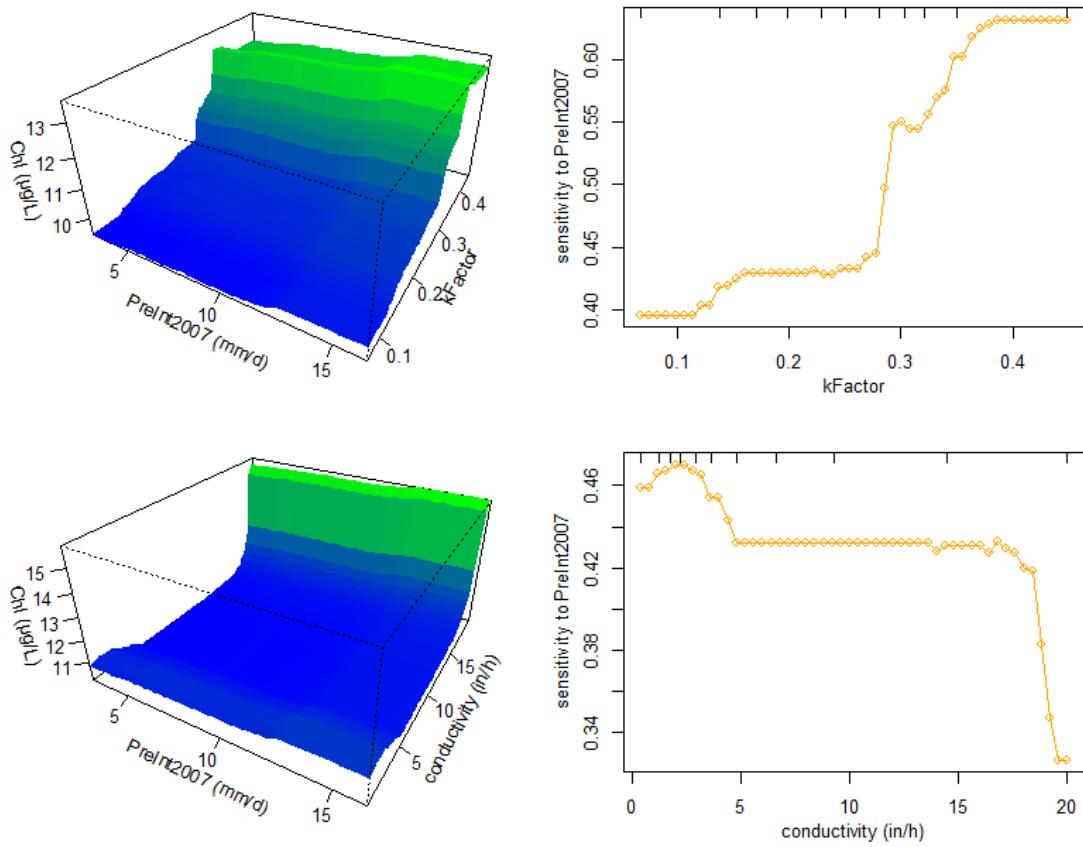


Figure 6-7 Chlorophyll-*a* (Chl) sensitivity to precipitation intensity (PreInt2007) changed with soil erodibility (kFactor) and soil conductivity. Chl values are modeled values from the two-variable partial dependence analyses with Model 2. Sensitivity to PreInt2007 is the range of Chl change with PreInt2007 at the designated level of PreInt2007. Tick marks at the top of figures on the right are decile locations showing the data distribution across the x-axis variable (data $N = 658$). Each point on figures on the right is one of 50 interpolation points.

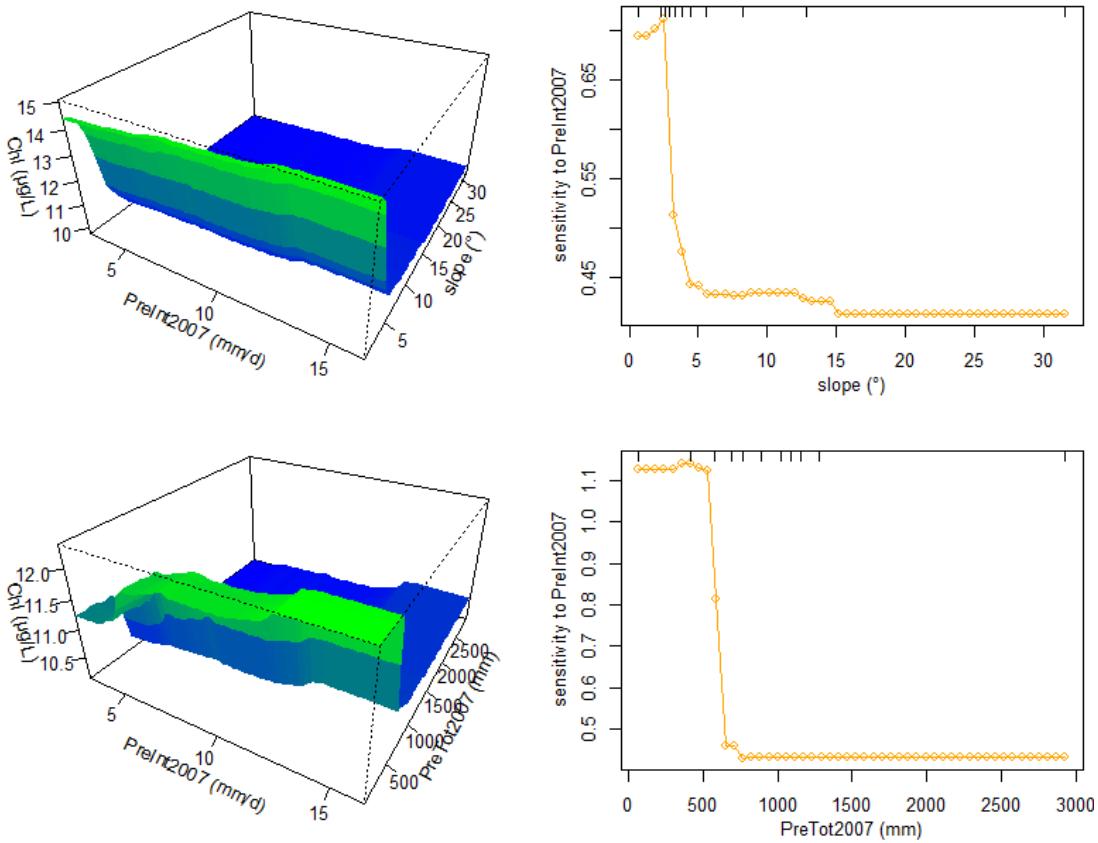


Figure 6-8 Chlorophyll- α (Chl) sensitivity to precipitation intensity (PreInt2007) changed with slope and 2007 total annual precipitation (PreTot2007). Chl values are modeled values from the two-variable partial dependence analyses with Model 2. Sensitivity to PreInt2007 is the range of Chl change with PreInt2007 at the designated level of PreInt2007. Tick marks at the top of figures on the right are decile locations showing the data distribution across the x-axis variable (data $N = 658$). Each point on figures on the right is one of 50 interpolation points.

6.3.3 Future scenario analyses

According to the climate model, the 30-year average daily air maximum temperature (TaMax) in the 2069-2099 period will increase by 4 °C over the 1977-2006 period in the “low” CO₂ emission scenario (*i.e.*, RCP 4.5). In the “high” CO₂ emission scenario (*i.e.*, RCP 8.5), temperature will increase by an extra 3

°C on top of the “low” emission scenario. Annual total precipitation (PreTot) at the end of this century (2069-2099) will increase by 20% over the 1977-2006 level in the “low” CO₂ emission scenario. All watersheds will get wetter, but the increase in wet areas is higher. In the “high” CO₂ emission scenario, the total precipitation will increase by an additional 18 mm on the top of the “low” emission scenario. Precipitation intensity (PreInt) in 2069-2099 will increase by 10% over the 1977-2006 period in the “low” CO₂ emission scenario. In the “high” CO₂ emission scenario, the precipitation intensity will increase by an additional 10% on top of the “low” emission scenario, indicating more extreme precipitation conditions in the future climate (Figure 6-9).

Using one year (2099) of future temperature and precipitation variables might not represent the future climate indicated by 30-year averages due to interannual variability. TaMax in 2099 (RCP 4.5) was higher than TaMax in 2007 by 3.5 °C; whereas, the 30-year (2069-2099) average TaMax was higher than TaMax in 2007 by 4 °C. Total precipitation in 2099 (RCP 4.5) was higher than total precipitation in 2007 by 30%; whereas total precipitation in 2069-2099 was higher than total precipitation in 2007 by 20%. No significant change (pairwise *t*-test *p* = 0.258) was found between precipitation intensity of 2007 and 2099; whereas the change in the 30-year averages was 10%. The magnitudes of the yearly changes in TaMax and total precipitation were similar to the 30-year average changes. However, the change of yearly precipitation intensity had a different trend than the 30-year average trend (Figure 6-9).

However, the scenario analyses were based on 2099 annual predictions instead of 2069-2099 average, because Model 2 was trained using annual variables. Replacing 2007 measured variables with the 2099 annual predictions (*i.e.*, TaMax2099Point, PreTot2099, and PreInt2099) as the inputs of Model 2, 2099 lake Chl was significantly (pairwise *t*-test *p* < 0.05) greater than 2007 fitted Chl in both scenarios. Specifically, in the “low” emission scenario, average lake Chl increased 0.8 µg/L, while in the “high” emission scenario average lake Chl increased 1.2 µg/L. Chl in the “high” emission scenario was significantly (pairwise *t*-test *p* < 0.05) higher than in the “low” emission scenario. The predicted Chl

change from 2007 to 2099 ranged from -2 µg/L to 5 µg/L in the “low” emission scenario and from -3 µg/L to 5 µg/L in the “high” emission scenario. Chl in most lakes (>75% of total 658 lakes) was predicted to increase in both scenarios. High increases (> 3 µg/L) were mostly at high latitudes (Figure 6-10). The predicted changes were higher in low-Chl lakes than high-Chl lakes, indicating that oligotrophic lakes were more sensitive to climate change than eutrophic lakes. Consistent with the analyses of Model 2 (Figure 6-6), lakes with temperature around 10-18 °C, or annual total precipitation around 500-600 mm had higher predicted increase in Chl than the other lakes. Lakes with different precipitation intensity had almost the same predicted Chl change (Figure 6-11).

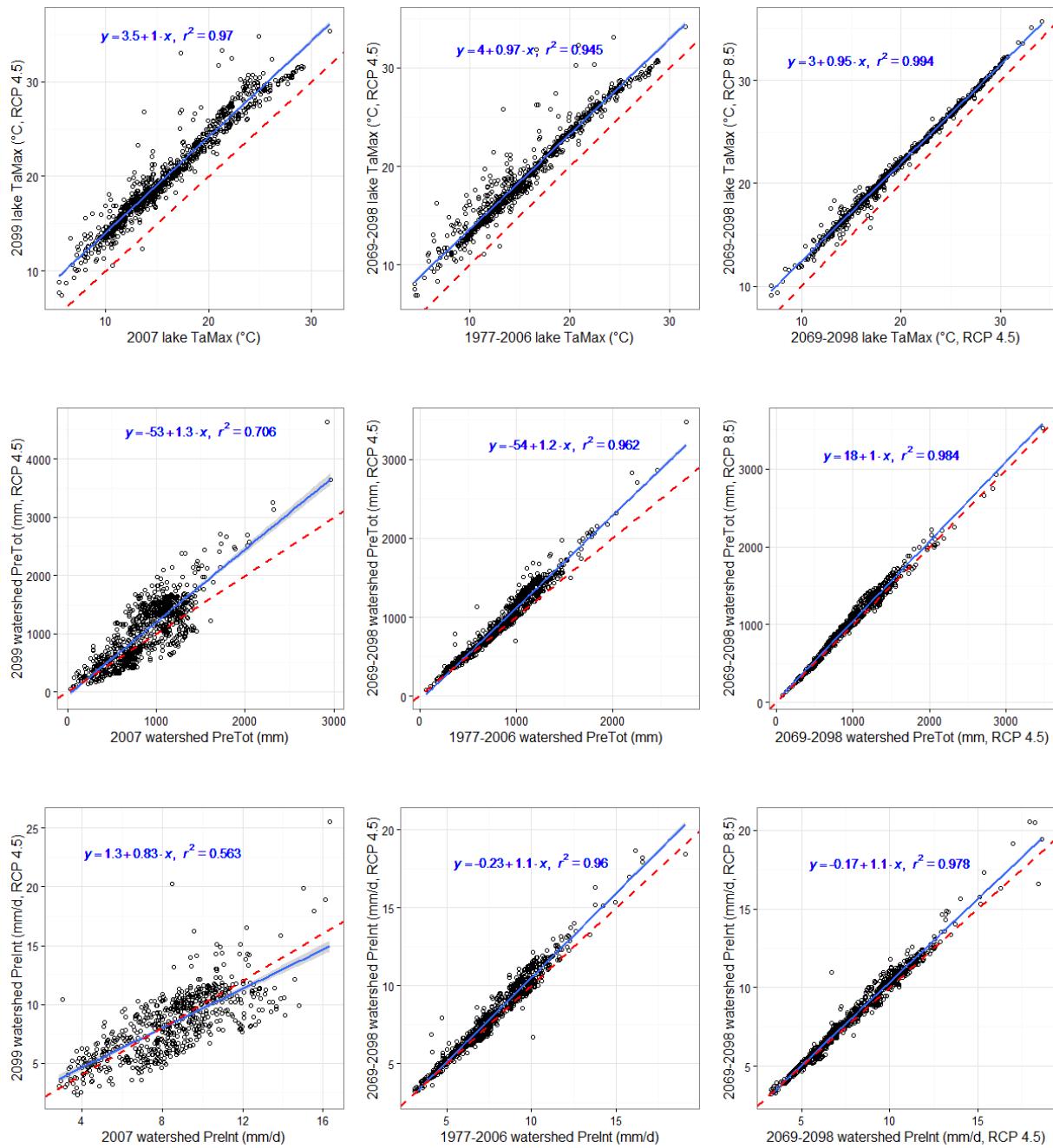


Figure 6-9 Projected changes in daily air maximum temperature (TaMax), annual total precipitation (PreTot), and precipitation intensity (PreInt) in two CO₂ emission scenarios, *i.e.*, RCP 4.5 (low) and RCP 8.5 (high). The dashed lines are 1:1 ratio lines. The solid lines are linear regression fits with functions shown on top. RCP: representative concentration pathway.

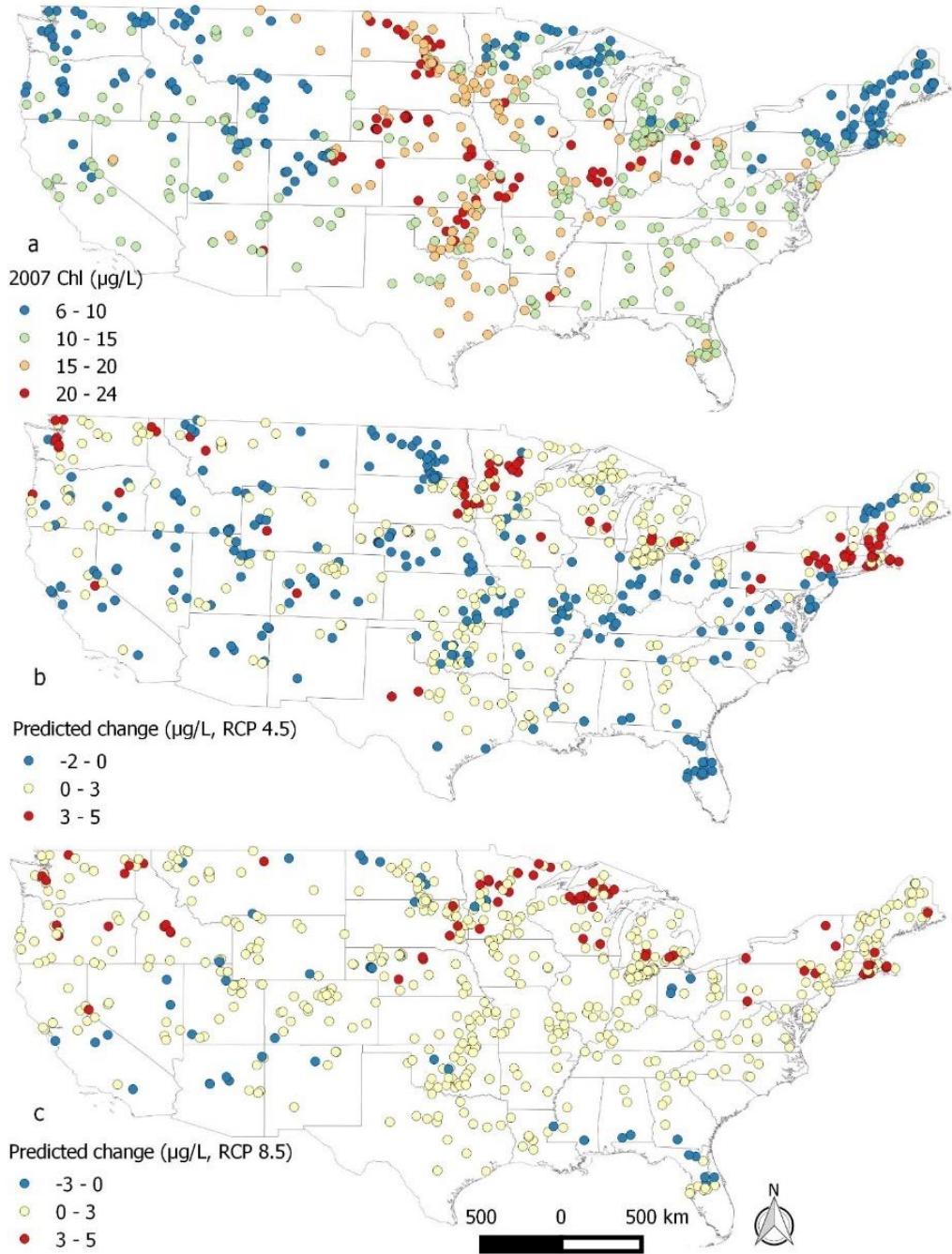


Figure 6-10 Comparison of chlorophyll-a (Chl) in 2007 (a, modeled values) and 2099 regarding two scenarios, i.e., the “low” emission scenario (b, RCP 4.5) and the “high” emission scenario (c, RCP 8.5).

Predicted change = 2099 predicted – 2007 fitted. Prediction model NSE = 0.428.

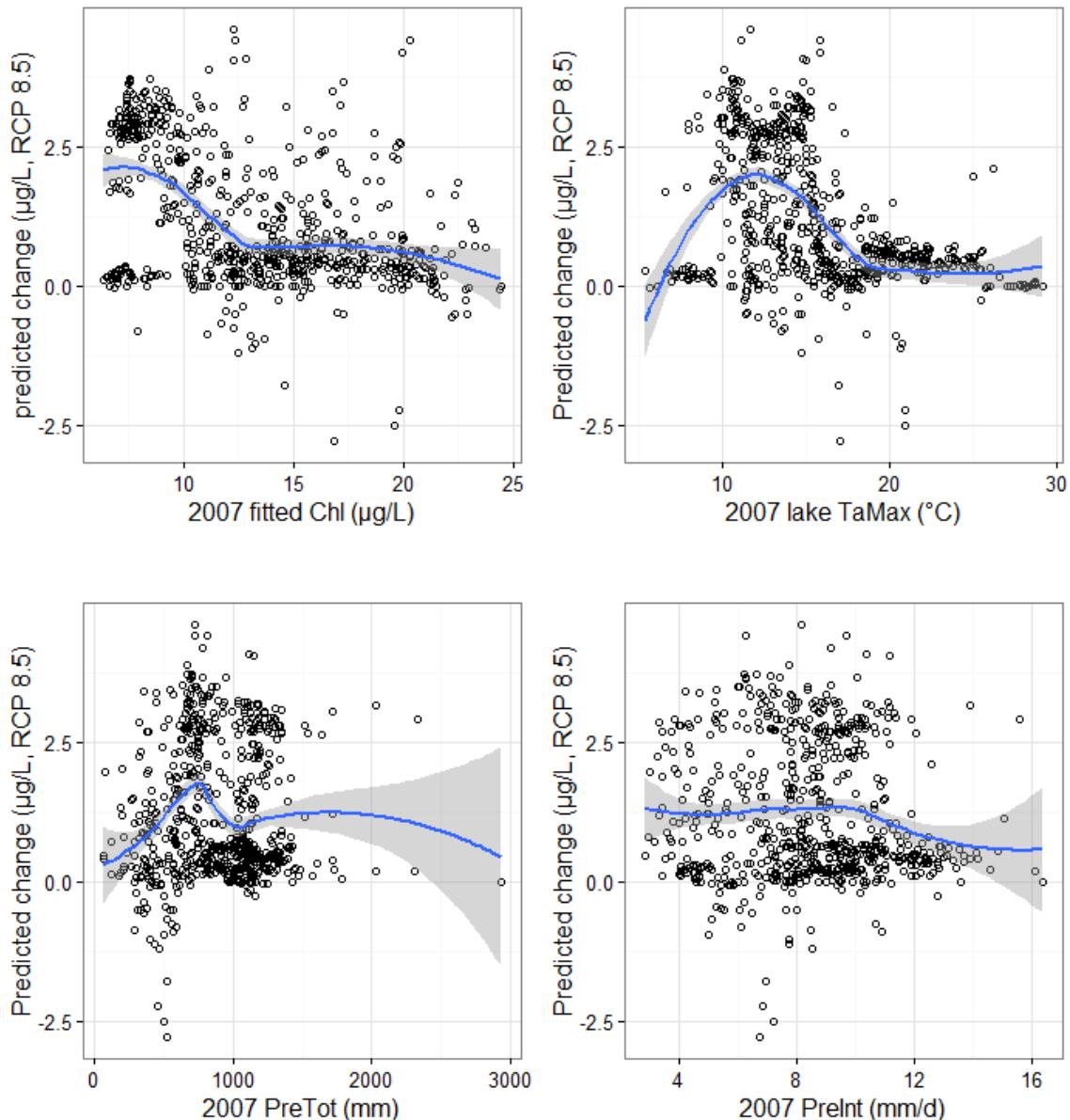


Figure 6-11 Predicted changes in chlorophyll- α (Chl) along 2007 Chl, daily maximum air temperature (TaMax,), annual total precipitation (PreTot), and precipitation intensity (PreInt). Predicted change = 2099 predicted – 2007 fitted, where 2099 weather was predicted in the “high” CO₂ emission scenario (i.e. RCP 8.5). Solid lines are LOWESS (locally weighted smoothing) smooth lines with 95% confidence interval on sides. Each point represents one lake.

6.4 Discussion

6.4.1 Chl increased with temperature but regulated by nutrients (Hypotheses A & B)

Algal growth follows Arrhenius and Michaelis–Menten enzymatic kinetics, where growth rate increases with temperature and nutrients exponentially, but the rate of increase decreases with temperature and nutrients (Gotham and Rhee 1981; Raven and Geider 1988). However, it gets more complicated when applying the kinetics to algal biomass that treats all algal species as a whole. First, “enzyme” concentration and spectrum are not constant any more, but change with algal species abundance and composition. Second, temperature can change enzymatic properties (“temperature acclimation”), which in turn change algal biomass sensitivities to temperature and nutrients (Davison 1991). Third, “substrate” concentration is not constant. Nutrients are depleted when algal biomass increases and are replenished by algal decomposition, which is also regulated by temperature and other substrate concentrations (White et al. 1991). Although lab experiments have provided evidence supporting these theories, they remain unclear in a wide range of complex aquatic systems with an almost infinite number of possible combinations within/between algal species and involving nutrients, thermal stratification, grazing, and decomposers. The findings of this paper have partly filled this knowledge gap.

The partial dependence analyses in Model 1 (Lake Model) and Model 2 (Watershed Model) illustrated that Chl increased with temperature, and was saturated at high temperature, consistent with the enzymatic kinetics responding to temperature, and Hypothesis A. More than half of Chl variation was not explained in both Model 1 and Model 2 ($NSE < 0.5$). That might be due to the complex realities mentioned above, *e.g.*, temperature acclimation, and concentration variations in enzymes and substrates. For nutrient regulation, the results confirmed Hypothesis B. Note that nutrient concentrations themselves might not be the only regulation factors. Other factors include (1) nutrient limitation, (2) grazing, and (3) light. Specifically: (1) When phosphorus availability is limited, Chl sensitivity to temperature increases with total phosphorus (TP). When phosphorus is replete, Chl

sensitivity to temperature is not controlled by TP, but other factors, such as grazing and light. The same rule applies to total nitrogen (TN). This might explain the results that Chl sensitivity to temperature did not increase with increasing TN or TP concentration. (2) In addition to that, at higher nutrient levels, algal production could be higher possibly resulting in a higher grazing rate, which offsets the increase in Chl sensitivity with temperature (Carpenter, Kitchell, and Hodgson 1985). Moreover, higher TP may favor accumulation of nitrogen-fixing cyanobacteria, which are more resistant to grazers than the other species, while higher nitrogen does not give nitrogen-fixing cyanobacteria an advantage. Species regulation of nutrient limitation might cause different nutrient regulation effects than were shown in Model 1, where Chl sensitivity to temperature slightly decreased at high TN. (3) Light might be another factor that co-varies with TN and TP and regulates Chl sensitivity to temperature. It is common that algal growth is limited by light after precipitation events, which generate higher turbidity as well as nutrient concentrations in inflows (Jones and Knowlton 2005). Higher turbidity could also reduce Chl sensitivity to temperature at higher nutrient levels as was shown in Model 1.

In summary, Chl increased with temperature, but high variability is expected due to the complex interactions among multiple abiotic and biotic factors. Chl sensitivity to temperature increased with nutrients only when the nutrients were limiting. Chl sensitivity to temperature may not increase at high nutrient levels due to grazing and light limitation, as well as nutrient saturation.

6.4.2 Chl sensitivity to precipitation (Hypothesis C) and its variations with natural hydraulic conditions (Hypothesis D)

Rainfall-induced high stream flows usually have higher total nitrogen and phosphorus concentrations than baseflow, and a few heavy rainfall events may carry most of nutrient loading to a lake over a year (McDiffett et al. 1989; Coser 1989). However, as reviewed by Reichwaldt and Ghadouani (2012), algal biomass could respond to precipitation in different ways. Algal biomass may increase after precipitation events for higher nutrients and de-stratification (*i.e.*, vertical mixing) (Kebede and Belay 1994; Nöges et

al. 2011). Opposite results may be seen for higher turbidity (including higher turbidity of inflows, and turbidity caused by inflow turbulence in shallow lakes), or dilution (especially flushing effects in reservoirs and estuaries) (Harris and Baxter 1996; Bouvy et al. 2003; Paerl et al. 2014). No change may occur for a mismatch between nutrient availability and light availability (Minor, Forsman, and Guildford 2014). This study separated precipitation into total precipitation and precipitation intensity to study precipitation impacts on algal biomass. The results from Model 2 were consistent with Hypothesis C, *i.e.*, Chl increased with precipitation intensity but decreased with total precipitation. It was interesting that Chl decreased with total precipitation when precipitation intensity was controlled as the mean. That might be due to the dilution effect (nutrient concentration decrease) mentioned above, or a rinsing effect (total nutrient loading decrease) related to a high frequency of precipitation events, *i.e.*, the nutrient generation in soils was slower than the nutrient loss due to frequent precipitation events. The rinsing effect has also been hypothesized in a stream study using spatial statistical models similar to this study (Olson and Hawkins 2013). It would be interesting to test whether nutrient loading to lakes decreases with higher precipitation frequency in a time series in future studies.

Soil erosion increases with soil erodibility and decreases with soil hydraulic conductivity. Regarding soil erodibility and conductivity, the results in the two-variable partial dependence analyses of Model 2 were generally consistent with Hypothesis D, *i.e.*, Chl sensitivity to precipitation intensity is regulated by natural hydraulic conditions, except that Chl sensitivity to precipitation intensity did not always decrease with higher soil hydraulic conductivity. There was a very small positive effect at low conductivity. The small positive effect might be due to other factors that co-varied with soil hydraulic conductivity, such as soil vegetation, which was not included in the model (Numata et al. 2003). An extra analysis showed that watershed vegetation, indicated by normalized difference vegetation index (NDVI), decreased with soil conductivity with a similar jump at low soil hydraulic conductivity (Figure 6-12). Adding NDVI in Model 2, the magnitude of the positive effect at low conductivity decreased by half, further suggesting

that the small positive effect was partly related to the correlation between soil hydraulic conductivity and vegetation cover.

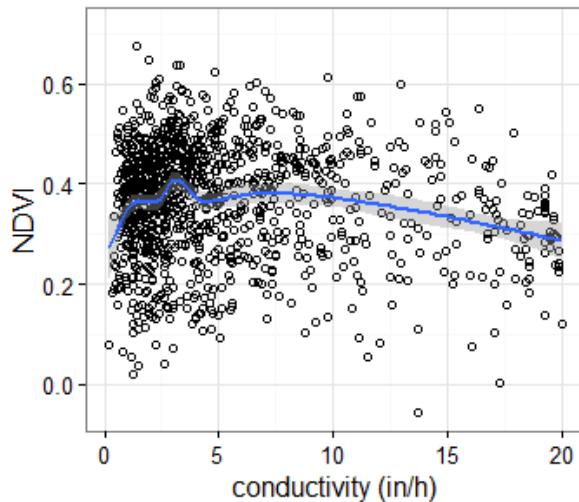


Figure 6-12 Normalized Difference Vegetation Index (NDVI) and soil hydraulic conductivity. Solid line is the LOWESS smoothed line with 95% confidence interval. Each point represents one watershed. NDVI is summer (May-August) average calculated from Landsat 8-Day NDVI Composite (Google Earth Engine ImageCollection ID = “LANDSAT/LT5_L1T_8DAY_NDVI”). 1 in = 2.54 cm.

Nutrients in soil are as important as the natural hydraulic conditions (*i.e.*, watershed slope, *K* factor, and soil hydraulic conductivity) regarding algal biomass responses to precipitation. The former determines nutrient concentration in sediments, and the latter determines the amount of sediments carried by surface water. Chl sensitivity to precipitation intensity did not increase with watershed slope as Hypothesis D expected in Model 2. Soil nutrients related to slope might play a more important role than soil erosion that was mediated by slope. Soils in low slopes usually have higher soil depths and higher nutrient stocks because of less erosion over time (Tesfa et al. 2009). An additional analysis of this study revealed that watersheds with more cultivated and developed lands (disturbance %) had lower slopes,

indicating possibly more fertile agriculture soils and fertilization in watersheds with lower slopes (Figure 6-13).

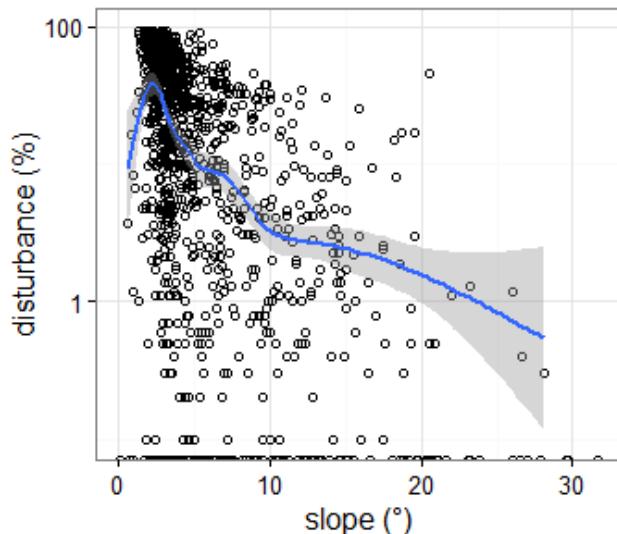


Figure 6-13 Percentage of cultivated and developed lands (disturbance %) changed with watershed slope. Solid line is LOWESS smooth line with 95% confidence interval. Each point represents one watershed.

Another interesting finding was that Chl sensitivity to annual precipitation *intensity* surprisingly did not increase with annual *total* precipitation in Model 2. More intensive rainfalls should carry more nutrients to lakes. However, soil nutrient concentration might decrease with higher total precipitation due to the rinsing effect as was previously discussed. All unexpected results, *i.e.*, the isolated positive effect in low conductivity, the opposite trend with slope, and the opposite trend with total precipitation, implied the importance of soil nutrient concentration in mediating precipitation intensity effects.

6.4.3 Future scenario analyses

This study was the first to project lake algal biomass to the end of this century across the continental United States. Chl in lakes was predicted to increase in both scenarios. The significant difference between the “low” and the “high” scenarios indicated that greenhouse gas emissions will affect lake

algal biomass. Although the predicted Chl changes in lakes were less than 5 µg/L, these changes were for annual average whole-lake Chl. The actual Chl of a specific site within a lake at a specific time might vary greatly compared to the annual average Chl of the whole lake, due to the high spatial and temporal variability of algae (Figure 6-14). Furthermore, Model 2 explained less than 50% of the spatial variation in Chl. Therefore, there would be a substantial uncertainty regarding Chl of individual lakes at specific times in the predicted future. The magnitude of uncertainty may be larger than the magnitude of predicted changes.

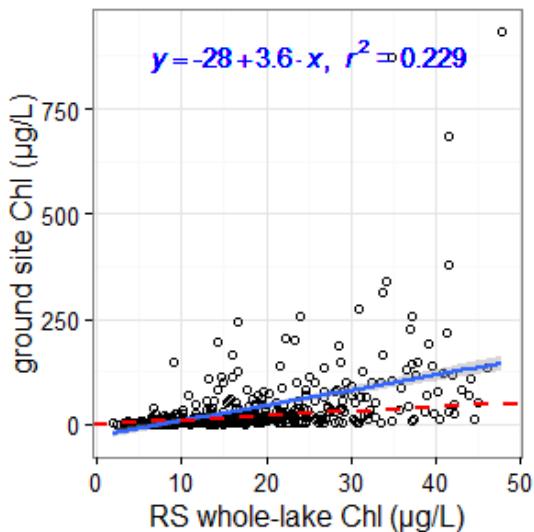


Figure 6-14 Comparison between remotely sensed (RS) whole-lake average summer chlorophyll- α (Chl) with ground-measured Chl from the 2007 National Lake Assessment. Ground-measured Chl was one-time measures in the same summer of RS Chl. The dashed line is a 1:1 ratio line. Solid line is linear regression fit with the function shown on the top and 95% confidence interval in gray. Each point represents one lake ($N = 591$).

The goal of our study was to evaluate general trends of algal biomass with climate change in lakes. We do not suggest paying attention to individual lake biomass predictions. Some lakes had negative predicted changes in Chl. These negative changes could be due to the model uncertainty, or the increase

of total precipitation as well as the decrease of precipitation intensity in those lakes. Note that the negative changes only accounted for 16.7% and 7.4 % of the total 658 lakes in the “low” emission scenario and the “high” emission scenario, respectively. Therefore, the negative changes might not necessarily be interpreted as Chl of some lakes being predicted to decrease in the future climate.

The scenario analyses illustrated that oligotrophic lakes or/and cold lakes were more sensitive to climate change. Oligotrophic lakes with low Chl might be more limited by nutrients or/and temperature than eutrophic lakes, which would explain their greater sensitivity to climate change. In partial analyses of Model 2, the positive effect on temperature on Chl decreased to zero at higher temperatures. The saturation effect was also found in the scenario analyses where Chl barely changed in high temperature lakes (Figure 6-11). This implied that for warm lakes, summer Chl might not respond to temperature increase, but Chl in the other cold seasons might still increase with temperature.

Model 2 suggested that if precipitation intensity increased in the future climate, Chl would increase too. However, if annual total precipitation also increased at the same time and the same place, then the Chl increase would be offset by the possible dilution and rinsing effect of total precipitation. Comparing precipitation of 2099 and 2007, precipitation intensity increased where annual total precipitation increased (Figure 6-15). Therefore, the small predicted Chl changes in the scenarios might be partly due to the opposite effects of precipitation intensity and annual total precipitation. According to the IPCC report (2014), annual total precipitation is predicted to “very likely” increase in most of the United States north of 45°N. Moreover, more precipitation increases will occur in winters and springs, and hot summers will see less precipitation. Therefore, Chl may increase with precipitation intensity while being offset by total precipitation during winters and springs. During summers, Chl may substantially increase with higher precipitation intensity in addition to lower total precipitation. In the other words, summer Chl is likely more sensitive to climate change than the other seasons. The scenario analyses in this study did not take seasonal differences in precipitation into account.

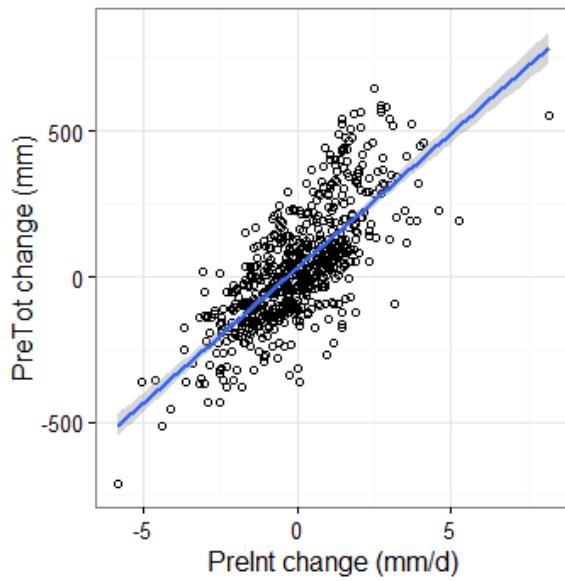


Figure 6-15 Predicted changes in precipitation intensity (PreInt change = Year 2099 – Year 2007), and predicted changes in annual total precipitation (PreTot). 2099 precipitation projections are based on the “high” emission scenario. Solid line is linear regression fit ($r^2 = 0.542$) with 95% confidence interval in gray.

6.4.4 Long-term temperature and precipitation effects

Algal biomass may increase with temperature due to higher growth rate of algae at higher temperatures within a certain range (usually $< 27^\circ\text{C}$) (Lürling et al. 2013). But it is less recognized that temperature may indirectly affect algal biomass by changing nutrient loading. Temperature may change nutrient loading through its effects on watershed evapotranspiration, soil nutrients, and vegetation cover as discussed below. (1) In six watersheds of Susquehanna River (USA), the future nutrient loadings were predicted to decrease in summer for higher temperature using GWLF (Generalized Watershed Loading Function) model, due to higher evapotranspiration and lower stream flow; but to increase during winter for earlier snowmelt. Overall, annual nutrient loadings did not consistently increase or decrease in six watersheds (Chang, Evans, and Easterling 2001). (2) It is still debated whether soil carbon (correlated

with soil nutrients) decreases or not with increasing temperature due to warming-induced acceleration of decomposition and increases of plant nutrient assimilation (Davidson and Janssens 2006).

It is also not clear how soil organic matter changes may affect dissolved organic matter transport to rivers and lakes (Kalbitz et al. 2000). If carbon decomposition does indeed increase more with temperature than carbon assimilation does (Post et al. 1982), then organic nitrogen loadings may decrease due to higher denitrification (Marshall and Randhir 2008). But on the other hand, lower soil pH due to more active decomposition of anaerobic bacteria may provide more bioactive phosphorus available to algae in rivers and lakes. Higher rates of ammonia nitrification especially in fertilized farms with sufficient water may also reduce soil pH and provide more bioactive phosphorus (Stark and Firestone 1995). (3) Vegetation cover may increase with temperature in wet areas (Kardol et al. 2010) but decrease with warmer temperatures and drought in dry areas (Breshears et al. 2005). The former may happen in winter and spring when temperature and precipitation are predicted to increase across most of North America. The latter may happen in summer when temperature is predicted to increase with unchanged or lower precipitation in the future climate according to IPCC (2014). The changes of vegetation cover over space and season may cause changes in soil erosion and thereby lake algal biomass. Inflow nutrient changes due to temperature are short-term processes. However, soil nutrients and vegetation cover may take more than a year to show significant changes. Impacts of temperature on nutrient loadings on a long-term scale are under-researched.

Compared to the short-term effects due to individual precipitation events, the long-term effects of precipitation on algal biomass are also under-researched. The results in this study have revealed a negative correlation between Chl and annual total precipitation. Continuous flushing of rainfall may rinse nutrients from soils. On the other hand, at certain level of precipitation intensity, higher annual total precipitation indicates more wet days, which favor vegetation growth (Ji and Peters 2003; Donohue, McVICAR, and Roderick 2009) and thereby soil stabilization and nutrient accumulation

(Renard et al. 1991). It is unknown whether nutrient loading would increase due to vegetation growth, or decrease due to soil stabilization and rinsing effect. Nonetheless, it may take years of precipitation change to see significant vegetation changes and flushing effects.

Additionally, after nutrient loadings are changed by vegetation and soil nutrients, it may take years (*e.g.*, 10-15 years for total phosphorus, and < 5 years for total nitrogen based on a study of 35 cases) for lakes to reach a new nutrient equilibrium, considering internal nutrient legacies (Jeppesen et al. 2005). The internal nutrients might have caused the 2007 precipitation to have a lower contribution in Model 2 than slope and soil properties. Specifically, 2007 precipitation might be related more to 2007 nutrient loadings while slope and soil properties might be more related to internal nutrients. A greater importance of internal nutrient sources might cause more contributions of slope and soil properties in Model 2. With all considerations of long-term terrestrial processes and in-lake nutrient legacies, the time lag of temperature and precipitation effects on algal biomass may be longer than anticipated.

In Model 2, slope and soil properties explained much more annual Chl spatial variation than the 2007 precipitation. Slope and soil properties were the most important variables. Overall evidence suggested that lake algal biomass might depend more on internal nutrients than yearly nutrient loadings. In other words, short-term changes in precipitation patterns may not be as important as we think. This finding agrees with some studies in individual lakes, which indicated that internal bioactive phosphorus was as important as new inputs (Auer et al. 1993; Nowlin, Evarts, and Vanni 2005).

In summary, climate change may affect algal biomass through both short-term or long-term mechanisms, which were not discriminated in our models. This study used the method of space as substitution of time, assuming each lake was in an equilibrium status under the influence of temperature and precipitation. These levels could reflect long- or short-term responses depending on local variations. Therefore, the sensitivity results only suggested how much algal biomass might change

with climate change, but did not provide information about how soon the change would happen after climate change.

6.4.5 Climate change mitigation

From a climate change mitigation point of view, the Chl partial analyses in Model 2 (Figure 6-6) suggest that reducing human disturbance (indicated by urban and agricultural lands) might offset Chl increases due to temperature or precipitation. Chl decreased with less disturbance in Model 2. In Model 1, Chl also decreased with TN and TP, which is related to human disturbance. How much change in human disturbance would be enough to counterweight temperature rise? Taking 2 µg/L of annual average Chl increase for example, it may require the percentage of urban and agricultural lands to decrease from 100% to 0% to neutralize the temperature effect (Figure 6-6). It seems impractical to solely rely on controlling urbanization and agricultural activities to mitigate the risk of algal blooms due to climate change.

6.5 Conclusion

Algal biomass in lakes across the US increases with temperature. Chl sensitivity to temperature increases with increasing nutrient availability (*i.e.*, TN and TP). Thus, the regulation of Chl sensitivity to temperature by nutrients is most important when nutrients are limiting.

Algal biomass increases with higher precipitation intensity, but it decreases with higher annual total precipitation (or precipitation frequency). Precipitation effects are mediated by soil properties including soil erodibility, soil hydraulic conductivity, and perhaps soil nutrient content as well.

Algal biomass will increase with the future climate change. More Chl increase is expected in the “high” CO₂ emission scenario than the “low” scenario. Lakes with low Chl or/and low temperature are more sensitive to climate change.

Acknowledgement

This work was supported by the U.S. Environmental Protection Agency (EPA) under Grant R835203. The views and opinions expressed in this article are those of the authors and do not necessarily reflect the official policy or position of U.S. EPA, or any other agency of the U.S. government.

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7 SUMMARY

7.1 Dissertation summary

Harmful algal blooms are emerging hazards with a dramatic increase of public attention in recent years.

Climate change is projected to increase temperature, change seasonal distribution of precipitation, increase frequency and intensity of droughts and floods, and increase annual precipitation in most areas in the United States. The overarching goal of this dissertation research was to advance our knowledge of the relationship between climate change and algal blooms. I hypothesized that the probability of algal blooms will increase with climate change, because of rising temperature and higher nutrient loads to lakes carried by runoff from more intense precipitation.

7.1.1 Model development

Historic satellite images can be used to derive long-term records of algal abundance, which provide sufficient duration that they can be related to changes in climate. Most existing algorithms for estimating chlorophyll- α in inland lakes using remote sensing imagery are based on linear regression and are not accurate enough for long-term and large-scale assessment of algal biomass in lakes. Two mature machine-learning algorithms—boosted regression trees (BRT) and random forest (RF)—were tested using 383 Landsat TM/ETM+ images that covered 483 lakes across the continental United States. Both algorithms showed significant improvements over traditional linear regression. Specifically, the BRT model explained 46% of the total variance in ground-measured chlorophyll- α in lakes measured by 10-fold cross validation, but the linear regression model only explained 40%. The RF model had similar performance to the BRT model, explaining 45% of the total variance. Chlorophyll- α measures based on the machine-learning algorithms were tested in western Lake Erie and the results indicated that these measures are good enough to identify spatial distribution and temporal duration of the algal blooms. Moreover, the correlation between remotely sensed chlorophyll- α and total phosphorus was as strong as the correlation between ground-measured chlorophyll- α and total phosphorus, especially when

remote sensing chlorophyll- α was the average of multiple measures. These assessment results imply that Landsat TM/ETM+ with machine-learning algorithms can be used to evaluate the historic conditions of algal abundance in lakes across the continental United States, and relate those conditions to climate change. The RF algorithm has been applied in Google Earth Engine—which has stored all Landsat data and is fast in data processing by using cloud calculation—to automatically and rapidly produce long-term whole-lake algal biomass for any lake of interest that is covered by Landsat TM/ETM+ images.

Applications outside the continental United States need to be further verified and lake areas measured should be larger than one image pixel (30 m × 30 m) at least.

7.1.2 Interference from optically active agents in water

One of the greatest concerns about using remote sensing to measure chlorophyll- α in lakes is the variable optical interference from combinations of algae, suspended sediments, and colored dissolved organic matter (CDOM). Machine-learning algorithms are new in remote sensing of chlorophyll- α . The effects of sediments and CDOM on chlorophyll- α in empirical models using remote sensing imagery in inland waters have rarely been determined on a broad spatial and temporal scale, where sediments and CDOM conditions greatly vary across lakes and seasons. The results based on a 24-year (1989–2012) *in-situ* dataset in 39 reservoirs across Missouri (USA) showed that modeled chlorophyll- α based on BRT had systematic bias *related* to sediments or CDOM. However, sediments and CDOM only explained respectively 6.7% and 4.6% of the total residual variance. What's more, the errors were unlikely *caused* by sediments or CDOM, because the errors did not increase with higher concentrations of sediments or CDOM as was expected in the theoretical simulations. There are two possible explanations for the model insensitivity to sediments and CDOM. First, the machine-learning algorithm (*i.e.*, BRT) may have discriminated the sediments and CDOM effects on chlorophyll- α measurements by using band and band ratios and considering the interactions between algae, sediments and CDOM. Second, the BRT model explained 35% of the total variance in the measured chlorophyll- α , so the accuracy might not be high

enough to capture the effects of sediments or CDOM on the remote sensing signal. These results indicate that sediments and CDOM should not introduce systematic bias in using remote sensing chlorophyll-*a* to relate climate change to algal blooms.

7.1.3 Interference from the atmosphere

Another major concern about using remote sensing to measure chlorophyll-*a* in lakes is the interference by atmospheric effects. The atmospheric signal may account for as much as 90% of at-sensor radiance over waters, so the atmospheric interference on remote sensing of algal abundance is expected to be substantial in lakes where atmospheric conditions greatly vary over time and space. Landsat surface reflectance products corrected for atmospheric effects are new and have recently been made freely available. The products are provisional and the atmospheric correction method was designed to meet the needed accuracy for land (not water) surface reflectance. To test whether the atmospheric corrections had improved the quality of Landsat TM/ETM+ images for remote sensing of inland water, these products were examined by using ground-measured water samples during 1989-2012 in 39 reservoirs of Missouri (USA). Except for the thermal band (Band 6), all bands and band ratios were investigated separately by using the model: $B_i = RF$ (chlorophyll-*a*, sediments, and CDOM), where B_i is the band or band ratio, RF is random forest, and the dependent variables are three optically active agents in water. The model validation R^2 for bands and band ratios *without* the correction ranged from 0 to 0.633 (mean = 0.271). The model validation R^2 for bands and band ratios *with* the atmospheric corrections ranged from 0 to 0.577 (mean = 0.226), which was not better than the models *without* the atmospheric corrections, indicating the atmospheric corrections did not improve the imagery signals related to chlorophyll-*a*, sediments, and CDOM. As a result, there was no significant difference in estimates of chlorophyll-*a*, sediments, or CDOM concentrations using the corrected or uncorrected Landsat TM/ETM+ images. Specifically, the optical agents—chlorophyll-*a*, sediments, and CDOM—were measured by using the model: Optical agent = RF (bands, band ratios), where the agent is chlorophyll-*a*,

sediments, or CDOM. The model validation R^2 was 0.312 (chlorophyll- a), 0.505 (sediments), and 0.731 (CDOM) with the *uncorrected* bands and band ratios. The model validation R^2 was 0.329 (chlorophyll- a), 0.508 (sediments), and 0.733 (CDOM) with the *corrected* bands and band ratios. The atmospheric correction method that was applied in the new Landsat TM/ETM+ products may be an improvement for land applications but not for remote sensing of the optical characteristics of water, where radiance signals are much weaker than those from land surfaces.

7.1.4 Time series analyses

The relationship between climate change and algal blooms was evaluated in four reservoirs in Missouri (USA), where 28 years (1984-2011) of algal biomass data were generated from Landsat TM images. Both changes in land use/cover and climate can affect algal biomass in lakes. Land use/cover barely changed over the 28 years in the study watersheds, providing an opportunity to relate climate to algal biomass given the minor effects from changes in land use/cover. Algal biomass was studied on four temporal scales: 28-years, yearly, seasonal, and daily. Four of 13 reservoir zones had significant increases in annual temperature (lake surface) during the 28 years, but only one of them (1/4) had significant increases in annual algal biomass. All 13 reservoir zones had significant increases in annual precipitation intensity (mm/d), but only four of them (4/13) had significant increases in annual algal biomass. Annual total precipitation did not show significant increases or decreases over the years. The trend of annual algal biomass did not necessarily agree with the trend of annual temperature or annual precipitation (sum or intensity) during the 28 years, indicating that the trend of annual algal biomass was not determined by only one factor, *i.e.*, annual temperature, annual total precipitation, or annual precipitation intensity. During the 28 years, algal biomass peaked usually in summers and was low in the other cold months. Summer algal biomass significantly increased with summer temperature in only one of 13 reservoir zones, indicated by univariate linear regression. However, annual algal biomass significantly increased with annual temperature in six of 13 reservoir zones. It implies summer algal

biomass may saturate with rising temperature but the algal growth season may expand resulting in an increase in mean annual algal biomass. Summer algal biomass had a mixed response (positive, negative, or insignificant) to summer precipitation (sum and intensity). Summer algal biomass significantly increased with spring precipitation intensity in four of 13 reservoir zones, and significantly increased with spring total precipitation in five of 13 reservoir zones, indicating that summer algal biomass may increase with climate change where more spring precipitation is predicted. Annual algal biomass significantly increased with annual total precipitation in four of 13 reservoir zones, and significantly increased with annual precipitation intensity in four of 13 reservoir zones, indicating that annual algal biomass may increase with climate change where precipitation is predicted to be wetter and extremer.

These predicted changes of algal biomass related to climate impacts are based on univariate linear regression, and the uncertainty is high since only 1-6, not all 13, of the models were statistically significant. The multivariate models that considered both temperature and precipitation as well as their time lags at the same time further revealed that daily temperature and daily precipitation together explained 0-51% (varying with reservoir zones) of the total variance in daily chlorophyll-a during the 28 years. The daily temperature contributed more than 90% in the model performance, indicating that the daily precipitation effects on daily algal biomass was relatively small after removing its correlation with daily temperature. This study suggests that climate change impacts on algal biomass may vary with time scale: daily, seasonal, annual, or longer-term. These findings are limited to four Missouri reservoirs and may not be applied to other lakes with different conditions of nutrients, turbidity (light), lake morphology, soil hydraulic condition, soil nutrients, and land use/cover.

7.1.5 Spatial Analyses

Impacts of climate change on algal blooms were evaluated in 1156 lakes in the continental United States, using a space-for-time substitution method. This study assumed that the trajectories of algal biomass changes along temperature and precipitation gradients over space would be the same as the

algal biomass changes with climate over time. Lake algal biomass was characterized by both ground-measured and remotely-sensed algal biomass.

First, a lake model was built with boosted regression trees (BRT) and ground-measured variables: chlorophyll-*a* = BRT (TP, TN, Ts), where TP, TN, and Ts are total phosphorus, total nitrogen, and lake surface temperature, respectively. Each lake was measured once in summer 2007. The lake model explained 41% of the total variance of chlorophyll-*a*. Within the 41% of the total variance, most (91%) of it was explained by nutrients (*i.e.*, TP and TN), and a small amount (9.5%) of it was explained by Ts. The lake model indicated that the spatial variations in algal biomass in lakes were more related to in-lake nutrients than Ts. The lake model showed that algal biomass increased with temperature at a rate of 1.5 µg/(L °C), and more increase occurred in lakes with more nutrients.

Second, a watershed model was built to evaluate the impacts of precipitation changes on algal biomass, because precipitation affects algal biomass in lakes through watershed and in-lake processes with possible time lags. The dependent variables of the watershed model were selected from a large variable pool of climate, soil, ecoregion, geology, hydrology, watershed morphology, lake morphology, and land use/cover. The statistical period of these variables was one year (2007), instead of a shorter period, to consider possible time lags. Algal biomass was measured by using Landsat TM imagery. The watershed model explained 43% of the total variance in annual chlorophyll-*a*. Within the 43% of the total variance, most (72%) of it was explained by watershed slope, soil, and land use/cover, and a small part of it was explained by annual temperature (13%), annual total precipitation (6.7%), and annual precipitation intensity (mm/d, 2.7%). The watershed model indicated that watershed characteristics were more important than climate in predicting the spatial variation of annual algal biomass. The watershed model showed that mean annual algal biomass decreased with annual total precipitation, but increased with annual precipitation intensity. Algal biomass sensitivity to precipitation intensity increased with soil erodibility. The assessment of precipitation effects on algal biomass has a high uncertainty because the

precipitation variables explained a very small amount of the total algal biomass variance in the watershed model. Finally, the watershed model predicted that algal biomass would increase in both the “low” and the “high” CO₂ emission scenarios, and the increase in the high scenario is more than the increase in the low one. Note that the impacts of climate change on algal biomass are aggregated results for all study lakes. The findings show general trends when all lakes were treated as a whole. Differences in magnitude or even opposite effects are expected for some individual lakes.

7.2 Future directions

This research is the first attempt to quantify how algal abundance in lakes responds to rising temperature and more extreme precipitation in future climate on a large continental scale. It was made possible by the improvement in remote sensing of algal biomass in lakes with machine-learning algorithms and Landsat TM/ETM+ imagery. Algal biomass in lakes across the continental United States will generally increase with climate change. This conclusion is supported by the findings of this study. However, to explain how climate change affects algal biomass in lakes requires more research. Moreover, this study has not related algal biomass to harmful algal blooms that are dominated by cyanobacteria and of more public interest. Below are some research needs based on the findings of this study.

7.2.1 Impacts of temperature increase

The time series analyses in four Missouri reservoirs showed that summer algal did not respond to increasing temperature in some reservoir zones, but *annual* algal biomass responded, suggesting that algal biomass may be saturated in high summer temperature but increase with low temperature in other cold seasons. Ecologically speaking, that could be true because algal growth is less likely limited by temperature in summer than other seasons. However, it also could be just a mathematical phenomenon, because the variance of summer algal biomass is larger than the variance in annual algal biomass. Interestingly, the spatial analyses of a wide range of lakes showed that annual algal biomass

barely increased with high temperature. Therefore, the summer saturation could happen in both summer and annual algal biomass. Algal seasonal succession is controlled not only by temperature, but also other factors including food webs, thermal stratification, nutrients, and light. Will climate change increase the peak algal biomass and expand the algal growth season? This question can be address by analyzing time series of a number of lakes that represent different seasonal patterns of algal biomass. The remote sensing tool developed in this study would be a great help in measuring long-term whole-lake algal abundance.

7.2.2 Impacts of precipitation change

Will summer algal biomass increase with more spring precipitation that is predicted by the climate change models? The univariate regression in four Missouri reservoirs showed that it was likely to be true. However, the significance of the models varied reservoir by reservoir, and even varied between zones in the same reservoir. Time lags may be related to traveling time of sediments that are brought by precipitation events, and the mixing current characters that change with lake morphology. The first step of future studies should be an analysis of lakes that may have time lags. Then a follow-up quantification study should evaluate how much algal abundance will change due to more spring precipitation. The assessment based on the watershed model in this study did not consider the seasonal changes of precipitation. Therefore, the precipitation impacts may have been underestimated.

An interesting finding in the spatial analyses is annual algal biomass decreased with annual total precipitation (“rinsing effect”). However, this effect was not found in the time series analyses in four Missouri reservoirs, where annual algal biomass significantly increased with annual total precipitation in four of 13 reservoir zones. There are at least two possible explanations for these controversial findings. First, the rinsing effect may not exist, and the decrease of algal biomass in the watershed model was the result of covariation with unexplained errors. The model only explained 42.8% of the total variance in annual algal biomass in the watershed model. Second, the rinsing effect does exist in some lakes, but

not the others such as the study Missouri reservoirs. A time series inventory of lakes regarding this effect is suggested for future research. The remote sensing tool developed in this study based on Google Earth Engine has made future large-scale and long-term ecological studies practical, like the ones suggested here.

7.2.3 Remote sensing of algal species

This study used chlorophyll- α as a proxy of algal biomass. Even though chlorophyll- α is a common pigment of all algae, the pigment composition and the concentration of chlorophyll- α is different in different algal species. That may introduce systematic bias in remote sensing of algal abundance. For example, the spring blooms that are dominated by diatoms may be underestimated and summer blooms that are dominated by green algae may be overestimated. The magnitude of this possible bias should be the subject of future evaluation.

Can machine-learning algorithms discriminate cyanobacteria blooms from the blooms that are dominated by other species? Since most harmful algal blooms in freshwater are cyanobacteria blooms, answering this question if of great interest of the public. cyanobacteria blooms are usually featured with accumulated surface algae and hence higher reflectance and land-vegetable-like spectrum characters. Machine-learning algorithms may be sophisticated enough to discriminate cyanobacteria blooms from the others. It is suggested to test this hypothesis in the National Lake Assessment data with algae taxonomy measures. Finally, it may be possible to directly relate climate change to cyanobacteria blooms after addressing the problems in remote sensing of algal species.