

CONCORDIA UNIVERSITY

**A GIS BASED MODELLING APPROACH TO ASSESS LAKE
EUTROPHICATION**

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ABSTRACT

A GIS Based Modeling Approach to Assess Lake Eutrophication

Linda El Farra

Large proportion of the world's readily available water supply is at risk due to the rapidly increasing populations of certain types of harmful algae. During the photosynthesis, species like blue-green algae and cyanobacteria consume nutrients and produce toxins that have potential adverse effects to humans and animals.

This thesis focuses on developing a GIS-based statistical approach to explore the water quality parameters facilitating the algae bloom, and to geographically map the extent and spread of these parameters to enable tracking and prediction of potential algae outbreaks.

The relationship between Chlorophyll-a, which represents the concentration of algae biomass, and the water quality parameters such as depth, phosphorus, nitrogen, alkalinity, suspended solids, pH, temperature, electrical conductivity, dissolved oxygen and secchi depth is analyzed through correlation matrix then by utilizing modeling techniques including multiple linear, nonlinear regression, neural network and data mining prediction models are developed to quantify the contribution from essential water quality parameters to eutrophication.

The developed GIS and statistical analysis approaches have been applied to the Lake Champlain. The performance for the developed statistical, neural network and data mining chlorophyll-a models has been examined through the comparison with the observed field data and through statistical error analysis. Two new techniques have been examined in this thesis study. First, data mining has helped to reveal the nonlinear behavior of algae growth in some parts of the case study area. Second, the GIS spatial analysis is employed to visualize the spread and extent of the water quality parameters and the algae chlorophyll-a, which graphically present

the location-based impact of eutrophication on important lake water resources. For example, the analysis of the GIS-based impact maps suggests that the algae is affecting the Vermont section of Lake Champlain mainly the Northern and Southern section. The developed models suggest that algae production is affected by nutrients particularly phosphorus. When phosphorus is encountered at low to mild concentrations, the nutrient is linearly affecting algae production, however, at extreme concentrations of the nutrient the relationship between nutrient and algae production become nonlinear. The developed GIS model along with the statistical analysis applied on lake Champlain suggest that Extreme levels of Nitrogen in north and Chloride in the South caused deviations in the models prediction accuracy

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TABLE OF CONTENTS

LIST OF TABLES	ix
LIST OF FIGURES	x
LIST OF SYMBOLS	xiii
LIST OF ABBREVIATIONS	xiv
CHAPTER 1: INTRODUCTION	1
1.1 Background	2
1.2 Thesis Objective	4
1.3 Organization of the Thesis	5
CHAPTER 2: LITERATURE REVIEW	6
2.1 Lake Eutrophication	7
2.1.1 Phosphorus cycle.....	7
2.1.2 Nitrogen cycle.	8
2.2 Review of Lake Eutrophication Models.	9
2.3 GIS- Based Lake Assessment and Management.....	11
CHAPTER 3: METHODOLOGIES	12
3.1 Lake Nutrient Level Standards	13
3.2 Chlorophyll-a Lake Eutrophication Statistical Models that Use Multiple Linear Regression (MLR)	13
3.3 Chlorophyll-a Lake Eutrophication Models that Use Multiple Nonlinear Regression (MNR)	15
3.4 Chlorophyll-a Models that Use Data Mining (DM)	15
3.5 Chlorophyll-a Model Evaluation Techniques	16
3.5.1 Determination of coefficient R^2	16
3.5.2 Standard error of the estimate	17
3.5.3 Confidence interval and critical value	18
3.6 GIS Based Modeling and Assessment	19

CHAPTER 4 CASE STUDY: LAKE CHAMPLAIN EUTROPHICATION	22
4.1 An Overview of Lake Champlain	23
4.2 Raw Data and Variables for the Lake Champlain Case Study	25
4.3 Lake Quality Criteria	25
4.4 Data Collection and Quality Analysis	30
A-Data source, format and units	30
B- Data quality analysis	30
C- Monitoring frequency	30
D-Gaps and range	33
4.5 Data Preparation	35
A-Linear and nonlinear interpolation	35
B-Extreme and outliers detection	40
C-Selecting data range and variables	43
4.6 Modeling Steps	44
4.6.1 Multiple linear regression	45
4.6.2 Neural network analysis	48
4.6.3 Data mining	49
4.6.4 Geostatistical analysis	49
 CHAPTER 5: LAKE CHAMPLAIN CHLOROPHYLL-a STATISTICAL	
MODELING RESULTS	51
5.1 Correlation Matrix Analysis Results	52
5.2 Determination of Analysis Data Set	55
5.3 Chlorophyll-a Modeling Using Multiple Linear Regression (MLR)	55
5.3.1 SPSS statistical analysis	55
5.3.2 ANOVA analysis of the variance of the MLR models	56
5.3.3 Multiple linear regression (MLR) results	56
5.3.4 Discussion of MLR model # 6	59
5.4 Lake Champlain Chlorophyll-a Modeling Using Multiple Nonlinear Regression (MNR)	64
5.5 Lake Champlain Chlorophyll-a Modeling Using Neural Networks NN	64

5.5.1 NN model #8 verification	69
5.6 Lake Champlain Chlorophyll-a Modeling Using Data Mining (DM)	71
5.6.1 DM modeling and water quality variables	71
5.6.2 Lake Champlain DM model #1 verification and comparison with MLR model #6 and NN model #8	72
5.6.3 Comparison of chlorophyll-a DM, NN, MLR models with actual observations	74
5.7 Discussion of the Results	78
5.7.1 Low to moderate water nutrient conditions	78
5.7.2 High water nutrient conditions.....	78
5.7.3 Causes of the model errors	79
CHAPTER 6: LAKE CHAMPLAIN CHLOROPHYLL- a GIS SPATIAL ANALYSIS	
RESULTS	80
6.1 GIS Based Modeling Results	81
6.2 Determination of the Statistical Model Variables	81
6.3 Model Results and Model Configuration	82
6.3.1 Statistical model with all input variables	82
6.3.2 Statistical model with selected variables	83
6.4 Spatial Trend Analysis	84
6.5 GIS Based Statistical Model Validation and GIS Results for TP and Chla	92
CHAPTER 7 CONCLUSION AND CONTRIBUTION	96
7.1 Conclusion	97
7.2 Contributions of the Research	98
7.3 Future Studies	100
REFERENCES	102
APPENDICES	114
Appendix A: Lake Champlain Outliers.....	115
Appendix B: Multiple Linear Regression Matlab Code	117
Appendix C: Multiple Nonlinear Regressions	121
Appendix D: Data Mining Results	123

LIST OF TABLES

Table 4.1 Names, abbreviations and definition of water quality monitoring parameters (variables) used in the LEF modeling studies, using lake Champlain data.....	23
Table 4.2 Lake Champlain phosphorus criteria targets (2011) vs. observed values.....	26
Table 4.3 Lake trophic criteria.....	27
Table 4.4 Lake Champlain variables and their monitoring range and frequency	31
Table 4.5 Port Henry segment (07) of lake Champlain observed data.....	33
Table 4.6 Lake Champlain variables monitoring range and frequency	43
Table 4.7 Lake Champlain yearly data for (1993-2011).....	46
Table 5.1 Pearson’s correlation matrix results	52
Table 5.2 Lake Champlain MLR modeling results for (2003-2011).....	57
Table 5.3 Chlorophyll-a (Chla) MLR coefficients of the six lake Champlain MLR models.....	58
Table 5.4 ANOVA analysis of the six lake Champlain MLR models.....	59
Table 5.5 Lake Champlain early years data, bootstrapping model results.....	63
Table 5.6 Results of lake Champlain DM model #1 for (1992-2011).....	71
Table 5.7 Summary of chlorophyll-a models described in this thesis.	78
Table 6.1 GIS based model #1(OLS) results.	82
Table 6.2 GIS based model #2 (OLS) results.....	83

LIST OF FIGURES

Figure 2.1 Phosphorus cycle in lake Champlain.....	7
Figure 2.2 Nitrogen cycle in lake Champlain.	9
Figure 3.1 R ² for unfit models	17
Figure 3.2 Error distributions.....	18
Figure 3.3 Bell shape error distribution	18
Figure 3.4 GIS hierarchy	20
Figure 3.5 Lake Champlain eutrophication modeling using the GIS	21
Figure 4.1 Lake Champlain watershed	24
Figure 4.2 Phosphorus levels in Lake Champlain and water quality criteria	29
Figure 4.3 Lake Champlain monitoring stations.....	32
Figure 4.4 Nonlinear curve types	34
Figure 4.5 Yearly calcium data for lake Champlain station 02.....	35
Figure 4.6 The Mann–Kendall test and the interpolation	36
Figure 4.7 Yearly TP, Cl and minerals chart for lake Champlain Port Henry.....	37
Figure 4.8 Data mining (FindGraph) analysis	38
Figure 4.9 Data mining (FindGraph) results.....	39
Figure 4.10 Minerals Fourier prediction for station 02	39
Figure 4.11 Screening Outlier daily data of TP for station 02.....	42
Figure 4.12 Model flowchart verification.....	45
Figure 4.13 Neuron in a neural network	48
Figure 4.14 Lake Champlain polygon creation.....	50
Figure 5.1 Cross correlation scatter plots for 8 independent water quality variables and the dependent variable chlorophyll-a.....	53
Figure 5.2 MLR model #6 standard error distribution.....	60
Figure 5.3 Lake Champlain chlorophyll-a levels by years (2003-2011) with MLR.....	61
Figure 5.4 Lake Champlain chlorophyll-a levels by years (1992-2002) with MLR.....	62
Figure 5.5 NN analysis water quality variables importance chart (top panel) and Chla observed values vs. NN model #8 predicted values for Chla (bottom panel).....	66
Figure 5.6 NN synaptic weight chart for lake Champlain later years data (2003-2011).....	67
Figure 5.7 Lake Champlain chlorophyll-a levels by years (2003-2011) with NN.....	68

Figure 5.8 Lake Champlain chlorophyll-a levels by years (1992-2002) with NN.....	70
Figure 5.9 Observed lake Champlain monitoring data (1992-2003) compared to predictions generated by three chlorophyll a models.....	73
Figure 5.10 Observed lake Champlain monitoring data (2012 and 2013) compared to predictions from MLR model.	75
Figure 5.11 Observed lake Champlain monitoring data (2012 and 2013) compared to predictions from NN model.	76
Figure 5.12 Observed lake Champlain monitoring data (2012 and 2013) compared to predictions from DM model.....	77
Figure 6.1 GIS-ordinary least squares analysis.....	82
Figure 6.2 GIS Kriging inputs	85
Figure 6.3 GIS map showing a summary of lake Champlain total phosphorus levels.....	87
Figure 6.4 GIS map showing a summary of lake Champlain total nitrogen (TN) levels	88
Figure 6.5 GIS map showing a summary of lake Champlain chloride (Cl) levels	89
Figure 6.6 GIS map showing a summary of lake Champlain secchi depths	90
Figure 6.7 GIS map showing a summary of lake Champlain alkalinity levels	91
Figure 6.8 GIS maps comparing lake Champlain chlorophyll-a observed levels with TP observed levels between (2004-2011).....	93
Figure 6.9 Lake Champlain water quality monitoring station observed chlorophyll-a levels compared to GIS model# 2 predicted levels.....	94
Figure 6.10 Lake Champlain monitoring station observed Chlorophyll-a levels vs. MLR model#6 predicted levels.....	95

LIST OF SYMBOLS

\bar{R}	Adjusted coefficient of determination
RegAlk	Alkalinity
ANOVA	Analysis of the variance
Chl-a	Chlorophyll-a ($\mu\text{g/L}$)
Cl	Chloride ($\mu\text{g/L}$)
R^2	Coefficient of determination
β	Coefficient of lake variables
CI	Confidence interval thresholds
CABs	Cynobacteria algal blooms
DM	Data mining
DO	Dissolved oxygen ($\mu\text{g/L}$)
DIC	Dissolve inorganic carbon ($\mu\text{g/L}$)
DOC	Dissolve organic carbon ($\mu\text{g/L}$)
ε	Error
TF_e	Iron ($\mu\text{g/L}$)
TKN	Kjldahl nitrogen ($\mu\text{g/L}$)
TPb	Lead ($\mu\text{g/L}$)
Y	Model output (Dependent variable)
Z	Model Inputs (independent variables)
TK	Potassium ($\mu\text{g/L}$)
\hat{Y}	Predicted value
Secchi	Secchi depth (m)
TNa	Sodium ($\mu\text{g/L}$)

TempC	Temperature (deg C)
TNH ₃	Total ammonia (µg/L)
TCa	Total calcium (µg/L)
TMg	Total magnesium (µg/L)
TMDLs	Total maximum daily loads
TNOX	Total nitrate nitrate (µg/L)
TN	Total nitrogen (µg/L)
TOC	Total organic carbon (µg/L)
TP	Total phosphorus (µg/L)
TSS	Total suspended solids

LIST OF ABBREVIATIONS

DEC	Department of environmental conservation
EBK	Empirical Bayesian Kriging
EPA	Environmental protection agency
ESRI	Environmental systems research institute
GIS	Geographic information system
GWR	Geographically weighted regression
IWRM	Integrated water resource management
IDW	Inverse distance weighted
MK	Mann–Kendall test
MLR	Multiple linear regression
MNR	Multiple non linear regression
NN	Neural network
OLS	Ordinary least square
SR	Symbolic Regression
THMs	Trihalomethanes
TSI	Trophic state index
USGS	US Geological survey
VIF	Variance inflation factor
WHO	World health organization

CHAPTER 1

INTRODUCTION

INTRODUCTION

Water bodies respond differently to increased amounts of nutrients (Correll, 1998). Many factors contribute to eutrophication, including: hydrologic conditions, ecosystems, geology (Correll, 1998), sediment loading capacity (Froelich, 1988), and both urban and agricultural land use (Short et al., 1996).

1.1 Background

The 2014 US Geological survey (USGS) report indicated that of the 1.386 km^3 of total water on earth, only 0.77% (10.7 km^3) is usable fresh water and 1.74% is unusable fresh water present in ice caps, frozen glaciers and permanent snow. Unfortunately, a large proportion (70%) of the world's usable water supply is at risk due to contamination by environmentally harmful Cyanobacteria (also called blue-green algae). Cyanobacteria range in colour from green to red, and form large masses (called algal blooms) in warm shallow water that is slow moving or still.

During photosynthesis, cyanobacteria blooms consume nutrients essential for lake biome survival and produce toxins that are poisonous to the humans and wildlife living in the lake environment. These toxins include neurotoxins (affect the nervous system), and hepatotoxins (affect the liver), as well as those that irritate the skin and eyes.

The microcystins are a group of approximately 50 toxins produced by the cyanobacterium *microcystis aeruginosa*. These are important because they are chemically extremely stable in water of widely varying temperature and pH. Microcystin-LR is the most widely studied because it is found in fresh water supplies worldwide, and is undetectable by odor, taste or appearance. Symptoms of microcystin poisoning include diarrhea, abdominal pain, nausea, vomiting, headache, fever, irritated eyes and skin, and allergic reactions. Unfortunately, boiling microcystin-contaminated water does not remove the toxins or destroy their activity.

Chlorophyll-a (also called chlorophyll a) is a plant pigment that is a primary electron donor in the electron transport chain and essential for photosynthesis. Chlorophyll-a can be used as a biomarker for the presence of cyanobacteria, as there is a direct relationship between the mass of the cyanobacterial algal bloom and the concentration of chlorophyll-a in fresh water.

These include the following physicochemical parameters of water: 1) temperature; 2) pH; 3) electrical conductivity; 4)-6) concentration of phosphorus, nitrogen, and dissolved oxygen; 7) secchi depth (a measure of water clarity, inversely proportional to CAB growth). Secchi depth is measured using a circular secchi disk lowered into the water until it is not visible. Suspended solids, including CABs reduce water clarity.

Eutrophication is the oversupply of artificial or natural substances, mainly phosphates (e.g. pollution from fertilizers, sewage and detergents) to an aquatic system, which promotes the excessive growth and decay of plants and bacteria, including algal blooms. After these organisms die, oxygen depletion (hypoxia) occurs, which then inhibits the growth of fish and other organisms in the environment. Eutrophication decreases the value of lakes and rivers and impairs drinking water treatment. Eutrophication is one of most significant and widespread water quality concerns in the global environment. It causes premature ageing of lakes and other water bodies. The estimated damage cost of cultural eutrophication (from human activities) in the U.S alone exceeds \$2.2 billion annually (Dodds et al., 2009). The ability of a lake to recover from eutrophication depends on the quantity of phosphorus in the lake sediment and in the volume of water in contact with the sediment. It may take decades before nutrients are naturally flushed out of lakes (Chambers et al., 2001; Hiscock et al., 2003).

Several studies have been published around lake Champlain, for example in 1989 a group of scientists from the Vermont Department of Environmental Conservation published a comprehensive study on lake Champlain, and concluded that it would be unrealistic to use daily data for lake Champlain to detect emerging lake eutrophication problems (Smeltzer et al., 1989), then in 1997 satellite images for the watershed was used to estimate the proportions of the baseline nonpoint source loads attributed (Millette, 1997), and in 2009 a Danish study suggested that eutrophication in lake Champlain is affected by the climate changes (Jeppesen ,2009). Many other studies around eutrophication are found and reviewed in section 2.2 and 2.3, and only a handful of these studies dealt with the GIS location characterization of water bodies (Aaby, 2005), and barely few studies exist that used data mining and computing power to reveal hidden pattern and information within the waterbodies data different timeframes (Petersen et al., 2001; Chen et al., 2003 and Chau et al., 2007).

This study presents a new approach for exploding algae and eutrophication models by searching for linear and nonlinear models using data mining, neural network and multiple

linear regression model throughout the different lake data timeframes, and by utilizing GIS location information to investigate the location impact on the lake eutrophication and algae spread.

1.2 Thesis Objective

Few large-scale watershed eutrophication studies have been reported, and these have primarily focused on marine and coastal waters rather than on fresh water lakes, streams, rivers and reservoirs (Arheimer et al., 2000; Nixon et al., 2002). Objectives of this thesis study include:

- A. To quantify the environmental variables associated with lake water quality such as: depth, phosphorus, nitrogen, alkalinity, suspended solids, pH, temperature, electrical conductivity, dissolved oxygen concentration and secchi depth contributions to algae bloom.
- B. To develop new statistical and generic algorithm based water quality models including data mining, nonlinear regression, and neural networks to assess and help to manage lake eutrophication
- C. To couple the developed lake eutrophication models with geographical information systems (GIS) to examine the location importance and impact on algae spread.
- D. To apply the developed methodology to the lake Champlain to further develop and validate field scale statistical linear and nonlinear chlorophyll-a models using data mining, neural network and multiple regression modeling techniques.

1.3 Organization of the Thesis

This thesis is organized in the following seven chapters

Chapter 1 defines the scope of the thesis, and introduces eutrophication and its impact on cyanobacterial algal bloom (CABs). Chapter 2 presents reviews of related literatures on eutrophication statistical studies, data mining and GIS-based studies on eutrophication. Chapter 3 summarizes the analyses used to create the chlorophyll-a models and the techniques used to evaluate the models. Chapter 4 presents the Lake Champlain case study data and discusses the methods used to prepare the raw data for the analysis. In Chapter 5 data for the water quality parameters that contribute to CAB are analyzed using various techniques, the analyses are verified, and the results are compared to find the optimal set of prediction models. Chapter 6 shows how ArcGIS was incorporated to generate maps that illustrate the extent and spread of the CABs. Finally, Chapter 7 summarizes the results and provides suggestions and recommendations for future research.

CHAPTER 2

LITERATURE REVIEW

2.1 Lake Eutrophication

Eutrophication is the process where a waterbody progresses from its current state to its extinction by gradual accumulation of nutrients and organic biomass (Das, 2003). Nutrients generally enter aquatic ecosystems sorbed to soil particles that are eroded into lakes, streams, and rivers (Sharpley et al., 1994). Human activities, excess use of fertilizers, mining phosphorus, animal feeds, agricultural crops, and other products, causing excess amount of nutrients to accumulate in soil thus altering the global phosphorus cycle (Schindler, 1977). The increasing nutrients levels in the soil elevate the potential amount that carried by runoff water to the aquatic ecosystems (Fluck et al., 1992).

2.1.1 Phosphorus cycle

Usually external loading is the main factor determining the lake's trophic status because of its large scale (Horne 1998); In 2005 a study published by the European Environmental Agency (EEA) suggested that: although phosphorus and nitrate concentrations in inland freshwater systems declined, eutrophication continued and haven't stopped, the continuation of the eutrophication was due to internal loading, therefore nutrients released to the water column from the sediment is a factor to be considered in lake eutrophication (Bostrom et al., 1988) and (Elwood et al., 1983).

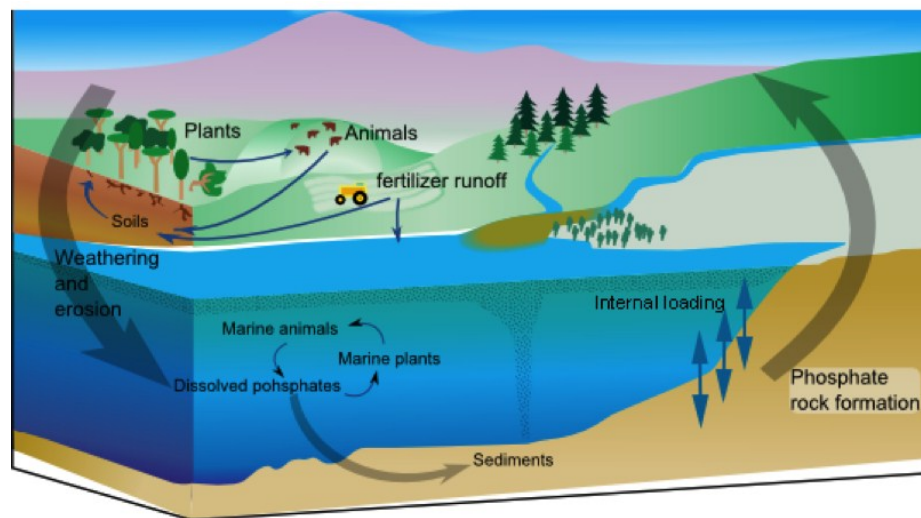


Figure 2.1 Phosphorus cycle in lake Champlain. Source: <http://prezi.com> accessed on August 2014

Internal and external loading of phosphorus into a lake body is referred to as phosphorus cycle, and this loading is the results of phosphorus being very biologically active elements. Figure 2.1 shows the phosphorus cycle in Lake Champlain, where phosphorus arrives into the lake through runoff water or sorbed through soil particles. The phosphorus compounds are then hydrolyzed either chemically or enzymatically to orthophosphate which is the only form of phosphorus that can be digested by algae or microbial (Smith et al., 2009). Excess and heavy particulates of phosphorus are deposited to the bottom and gradually form the sediment part of sediment phosphorus is released back into the water column as orthophosphate or it stays in the sediment and forms phosphate rock formation, which later on is dissolved by rain, snowmelt, irrigation or runoff water and is deposited back into the soil, rivers and lakes to eventually makes sediments rock formation (Goodwin, 2011).

2.1.2 Nitrogen cycle

When 71% of the earth surface is water, and 80% of the atmosphere is Nitrogen gas N_2 , and when it takes millions of years for the rock sediment carrying phosphorus to raise up to the surface then moved by runoff water or sorbed through soil particle for the phosphorus to complete its cycle, while it may only takes days or even less for the nitrogen to complete its cycle, then it becomes clear why nitrogen concentration is 16 times higher phosphorus in open waters (Rydin and Rast, 1992).

Nitrogen exists in many forms, one of its form is ammonia NH_3 ; Ammonia comes from plant, animal wastes, decomposition of organic nitrogen and is used extensively in fermentation (Luvall et al., 1999) and as a cleaning agents; Ammonia has a deadly effect on fish and plant and it encourages algae growth.

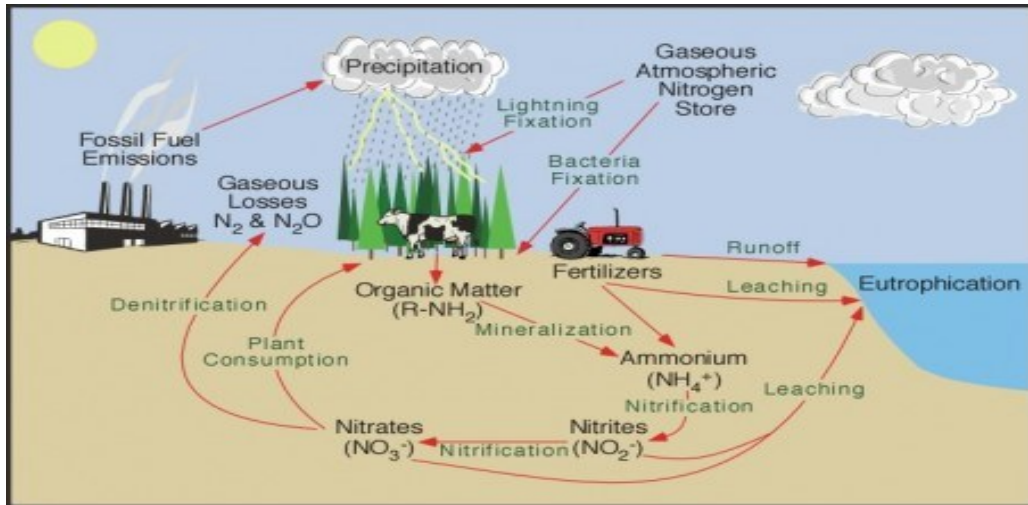


Figure 2.2 Nitrogen cycle in lake Champlain; Source: <http://image.frompo.com/w/peerless-travels> accessed on August 2014

2.2 Review of Lake Eutrophication Models

The German agricultural chemist Justus von Liebig conducted the first eutrophication study in 1950. Prior to this, Weber (1907) and Johnstone (1908) found a link between nutrients and aquatic productivity (reviewed in Smith et.al, 1999). In the years that followed several eutrophication studies were conducted; the majority of those studies focused on statistical analytical techniques.

Due to the widespread of the eutrophication problems in fresh water supplies, many studies were made in attempt to find the cause and solution, and in this section I presented the different unique approaches I found related to topic, however it is worth to mention that the sequence of studies is not necessary in a historical essay.

In 1973, Dieter Imboden developed a phosphorus model for Lake Lucerne eutrophication using oxygen consumption as a function of phosphorus loading. Dieter's model calculates the mean Oxygen O_2 consumption in water as a function of phosphorus loading and gives the critical P-loading values above which the lake turns eutrophic for changing mean depth of the Lake and hydraulic loading factor. The model produces a general rough behavior for lakes categorization by elements and was not able to explain the cause behind the CABs in the lake. Another different approach to instigate lake eutrophication was made by Lotter, who used the annual layer of

sediment in rocks (varve) to model the historical eutrophication of Lake Baldeggersee in (Switzerland), and although eutrophication is suggested to be highly correlated with sediment (Lijklema, 1980), however Lotter's climate and trophic state models were only able to justify one third of the variance data. (Lotter et al., 1997).

Many of the analytical eutrophication studies simplify the complexity between the lake variables and eutrophication, and use multiple linear regression MLR which is technique that attempts to find the relationship between several explanatory variables and a response variable by fitting a linear equation to the training data. (Cüneyt, 1999; Xia et al., 2011), while other eutrophication studies use more complex technique such as fuzzy logic to study eutrophication (Selçuk et al., 2004).

In recent years with the availability of computing power there was a growing tendency to use neural network to create eutrophication models (Recknagel et al., 1997). Some of those studies used artificial neural networks (Yabunaka et al., 1997; Scardi et al., 1999; Jeong et al., 2001 and Xia et al., 2011), while other used fuzzy and neuro-fuzzy techniques (Maier et al., 2001); and most recently with the advances in software development, DM techniques started to show in eutrophication studies (Petersen et al., 2001; Chen et al., 2003).

Although many advances were made, the wide variation in water body scenarios (e.g. naturally occurring seasonal and annual variations in water quality parameters), and the complexity between nutrients and eutrophication in a dynamic ecosystem made it a challenge to develop a defined standard that defines water eutrophication (Correll, 1998). Different studies provided distinctive eutrophication model.

In summary, the literature review showed:

- 1) There are many different analysis methods available to predict freshwater lake eutrophication and CABs mass growth.
- 2) Several models are required to accurately deal with all lake scenarios (low vs. high nutrient concentrations).
- 3) The most important predictive parameters for lake eutrophication and CABs mass growth were total nitrogen (TN) and total phosphorus (TP) in the water.
- 4) Most studies focused on solving the eutrophication problem using standard analysis techniques that do not address the nonlinearly problem of lake eutrophication at extreme concentrations.

5) None of the studies utilized data mining techniques to model eutrophication problem in the lakes, and there is a lack of comprehensive research to formalize the relation between water variables and algae bloom.

2.3 GIS- Based Lake Assessment and Management

In 1973, ESRI developed the first commercial GIS system, the Maryland Automated Geographic Information System (ESRI, 2006). They subsequently developed individual tools (e.g. ArcInfo workstation, ArcView GIS 3.x, MapObjects, ArcSDE), which were integrated as ArcGIS in 1999. Hiscock and coworkers utilized GIS to study phosphorus loading with land use, soil type and rainfall in the Florida basins (Hiscock et al., 2003). Their results indicated that the amount of developed land and the phosphorus loading have a strong correlation with lake eutrophication.

In 2008, Dirk Craigie suggested using GIS as a resource to incorporate geographically linked data used in the Integrated Water Resource Management (IWRM) system (Dirk, 2008). Hameed's group used GIS analysis to classify 50 inland lakes in Sweden according to their degree of eutrophication and acidity, based on water pH and/or alkalinity monitoring data (Hameed, 2010).

In 2011 Gupta used GIS to evaluate nitrogen and phosphorus levels in the Rönneå River drainage basin in Sweden, and to estimate future discharge into the basin (Gupta et al., 2011). Akdeniz used the inverse distance weighted (IDW) method of ArcGIS to create trophic state index (TSI) maps for the shallow Uluabat Lake in Turkey (Akdeniz et al., 2011). Anoh used GIS to study eutrophication in the Taabo River (Ivory Coast) using multi criteria analysis of water quality parameters, which highlighted the areas in the watershed that required protection (Anoh et al., 2012). Lake Michigan was studied using satellite images from MODIS to predict chlorophyll-a concentration, the results showed the possibility of using satellite images effectively to track algae (Huang, Deng, 2013).

In conclusion, GIS provides a powerful method to analyze lake eutrophication and the growth of cyanobacteria algal blooms (CABs) spatially and to help effectively manage large-scale lake eutrophication in countries worldwide.

CHAPTER 3

METHODOLOGIES

3.1 Lake Nutrient Level Standards

There is currently no world standard for acceptable nutrient levels in lakes, because each presents a unique ecosystem, which is highly variable due to natural seasonal variations and also natural and man-made changes in the environment. For this reason, in order to study eutrophication in a particular lake, one needs to examine parameters that affect the entire geographical region (Nixon, 2009).

3.2 Chlorophyll-a Lake Eutrophication Statistical Models that Use Multiple Linear Regression (MLR)

Some of the published chlorophyll-a models used the statistical method of multiple linear regression (MLR) to investigate multiple scalar dependent variables (Z = water quality parameters) that are hypothesized to be linearly related to the explanatory variable (Y = chlorophyll-a, a biomarker for the growth of cyanobacteria algal blooms (CABs) which cause eutrophication in lakes). This is described below in the general matrix format for the MLR equation (John et.al, 1996; see Introduction to Linear Regression Analysis by Douglas C. Montgomery - Statistics reference textbook for MLR method, 2012; Handan Çamdevyren et al., 2005, a review of chlorophyll-a MLR models).

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} \beta_0 + \beta_1 z_{11} + \beta_r z_{1r} + \varepsilon_1 \\ \beta_0 + \beta_1 z_{21} + \beta_r z_{2r} + \varepsilon_2 \\ \vdots \\ \beta_0 + \beta_1 z_{n1} + \beta_r z_{nr} + \varepsilon_n \end{bmatrix} = \begin{bmatrix} \beta_0 + \beta_1 z_{11} + \beta_r z_{1r} \\ \beta_0 + \beta_1 z_{21} + \beta_r z_{2r} \\ \vdots \\ \beta_0 + \beta_1 z_{n1} + \beta_r z_{nr} \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix} \quad \text{Eq. 3.1}$$

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}, Z = \begin{bmatrix} 1 & z_{11} & z_{1r} \\ 1 & z_{21} & z_{2r} \\ \vdots & \vdots & \vdots \\ 1 & z_{n1} & z_{nr} \end{bmatrix}, \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}, \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_r \end{bmatrix}$$

Rearranging equation 3.1, we obtain the following:

$$Y = \begin{bmatrix} 1 & z_{11} & z_{1r} \\ 1 & z_{21} & z_{2r} \\ \vdots & \vdots & \vdots \\ 1 & z_{n1} & z_{nr} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_r \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix} = Z\beta + \varepsilon \quad \text{Eq. 3.2}$$

Where, Y is an n -by- 1 vector of responses, β is a m -by- 1 vector of coefficients, Z is the n -by- r design matrix for the model, ε is an n -by- 1 vector of errors, is the output or dependent variable, and $z_{11} \dots z_{nr}$ are the independent or input variables. The short version of the general MLR format is written as follows:

$$Y_i = \beta_0 + \beta_1 z_{1i} + \beta_2 z_{2i} + \dots + \beta_j z_{ji} + \varepsilon \quad \text{for } i = 1, \dots, n \text{ and } j = 0, \dots, n \quad \text{Eq. 3.3}$$

In this type of chlorophyll-a (MLR) model, chlorophyll- a (Chla) is the dependent variable. $z_1 \dots z_i$ representing: total phosphorus, total nitrogen, chloride, secchi depth, temperature, depth, alkalinity or the independent variables (water quality parameters), while $\beta_0 \dots \beta_j$ represent the coefficients for the independent variables and ε is the error term.

The MLR equation is solved using the least squares method, by estimating the unknown vector of coefficients β of the linear equation, through minimizing the sum of squares of residuals (errors) between the observed data and the predicted data from the linear equation. The coefficients β that produce the best solution are found when the error between the linear equation model and observed data is zero (Kariya et al., 2004). By setting $\varepsilon = 0$ and rearranging the equation, we get $\beta = S_{(\beta)} / Z$, which give the coefficients of matrix β , and the predicted values. By comparing the predicted values to the observed values we can judge the model's accuracy. It is not possible to directly evaluate the coefficients of the matrix β equation since the vector $S_{(\beta)}$ has a different vector size than the matrix Z . Therefore, in appendix B, I wrote a Matlab code called MLR-LEF to work around this problem, and use this code in the Lake Champlain case study.

3.3 Chlorophyll-a Lake Eutrophication Models that Use Multiple Nonlinear Regression (MNR)

Some of the chlorophyll-a models (Handan et al., 2005 and Xia et al., 2011) use multiple nonlinear regression (MNR) to investigate variables (water quality parameters) that are not linearly related to chlorophyll-a and CABs (Nonlinear Regression by G. A. F. SEBER -Statistics textbook ref for MNR; see refs above for chlorophyll-a MLR models). The multiple nonlinear regression model is derived by transforming the nonlinear model to a linear one, the general Nonlinear multivariate power function (Allison, 1999) is written as

$$Y = az_1^{b_1} z_2^{b_2} \dots \dots z_n^{b_n} \quad \text{Eq. 3.4}$$

By taking the natural logarithm for both sides, equation 3.4 is then transformed into a linear function (Allison, 2006)

$$\ln Y = \ln(a) + b_1 \ln(z_1) + +b_2 \ln(z_2) \dots \dots \dots + b_n \ln(z_n) \quad \text{Eq. 3.5}$$

Comparing Eq. 3.3 to Eq. 3.5 we get

$$Y_i = \ln Y \quad , \quad z_i = \ln(z_i) \quad , \quad \beta_i = b_i \quad , \quad \beta_o = \ln(a) \quad \text{Eq.3.6}$$

Equations 3.5 and 3.6 can be used to derive the chlorophyll-a MNR model (Handan et al., 2005 and Xia et al., 2011).

3.4 Chlorophyll-a Models that Use Data Mining (DM)

Data mining (DM) is used to discover patterns within a data set (Weiss et al., 1999; Malek et al., 2011). A number of published chlorophyll-a models use DM to discover patterns in data sets of water quality parameters (independent variables) that are related to chlorophyll-a levels (dependent variable), a biomarker for CABs growth. For example DM was used in a chlorophyll-a model to examine habitat utilization patterns of reef fish along the West coast of Hawaii (Kleiner et al., 2000; Bailey et al., 1994). The software used in this study for data mining

is Eureka 1.12.1 Beta from Nutonian. Eureka software derives the equations by searching the space of mathematical expressions to find the model that best fits a given dataset, both in terms of accuracy and simplicity, this process is known as Symbolic Regression (SR), and unlike multiple nonlinear regression MNR where a specific equation is need to start with the analysis, in Symbolic Regression no particular model is needed to start with the analysis and the initial expressions are formed randomly by combining mathematical building blocks such as mathematical operators, analytic functions, constants, and state variables. Equations are then build by recombining previous equations, using genetic programming, by letting the patterns in the data reveal the suitable models, rather than imposing a model to avoid human bias, or unknown gaps in domain knowledge.

3.5 Chlorophyll-a Model Evaluation Techniques

To find the best chlorophyll-a model for the Lake Champlain case study, I used three published methods to evaluate chlorophyll-a models, and these are described in detail below.

3.5.1 Determination of coefficient R^2

This method was used to evaluate most chlorophyll-a models used in lake eutrophication studies, (e.g. Handan et al., 2005; Xia et al., 2012). The Pearson R correlation coefficient measures the linear correlation between two variables (value between +1 and -1). R^2 (the square of the Pearson R) indicates how close the regression model fits to the observed data (value between 0 and 1).

$$R^2 = \frac{\sum_{i=1}^n (\hat{Y} - \bar{Y})^2}{\sum_{i=1}^n (Y - \bar{Y})^2} \quad \text{Eq. 3.7}$$

Where, R^2 is the coefficient of determination, \hat{Y} is the predicted value, \bar{Y} is the observed value, Y is the average value, n = the size of the data. The closer the R^2 value is to 1, the better the model fit. Fig. 3.1 shows two examples where this is not the case.

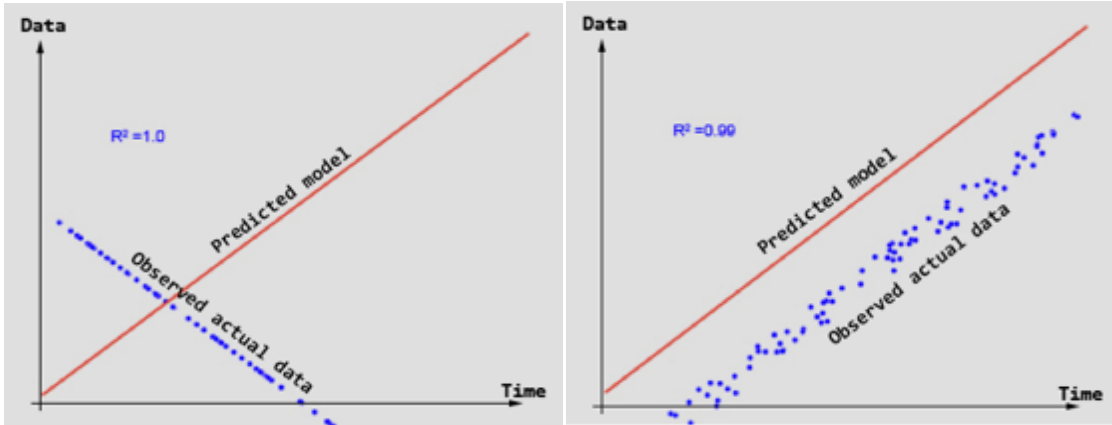


Figure 3.1 R^2 for unfit models (modified from <http://academic.uprm.edu/> accessed on May 2014)

The major problem in calculating R^2 is that its value increases whenever a new variable is added to the model, thus a model with more variables may appear to be a better fit than a model with fewer variables. The adjusted R^2 attempts to compensate for the inaccuracy of R^2 because it increases only if the new variable is statistically significant. The adjusted R^2 is always less than R^2 (Draper et al., 1998).

$$\bar{R} = 1 - \left(\frac{(1 - R^2)(n - 1)}{n - k - 1} \right) \quad \text{Eq. 3.8}$$

Where \bar{R} is the adjusted coefficient of determination, R^2 is the coefficient of determination, n is the total sample size, k is the number of predictors (variables).

3.5.2 Standard error of the estimate

This method was used in the verification analysis of Lake Ontario (Thomann et al., 1979). The standard error of the estimate is an estimate of the average squared error and is calculated as follows (Kenney et al., 1963).

$$\begin{aligned} \text{Std. Error} &= \sqrt{\text{Mean Square of residuals}} = \sqrt{\frac{\text{Sum of Squares residuals}}{df \text{ degree of freedom}}} \\ &= \sqrt{\frac{\sum_{i=1}^n (Y_i - \hat{Y}_i)^2}{df}} \end{aligned} \quad \text{Eq. 3.9}$$

3.5.3 Confidence interval and critical value

A good model should have the smallest errors, and these should be distributed evenly above and below the regression line (Fig. 3.2).

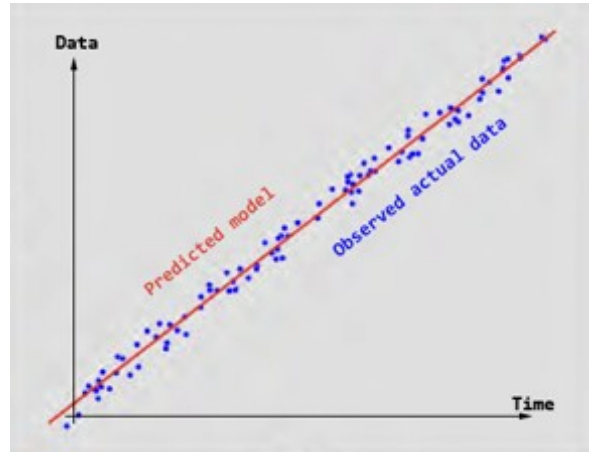


Figure 3.2 Error distributions (modified from <http://academic.uprm.edu/> accessed on May 2014)

Confidence interval (CI) thresholds are used to maintain small and evenly distributed errors, and error values outside the threshold (also called limit) values are ignored. The lower the CI threshold value, the better the model. Critical values are the boundaries of the CI, found by using the z score table (the lower critical value = $-z^{\alpha/2}$; the upper critical value = $z^{\alpha/2}$). The critical values in most data analysis software packages are a user-defined input that is set manually before data processing.

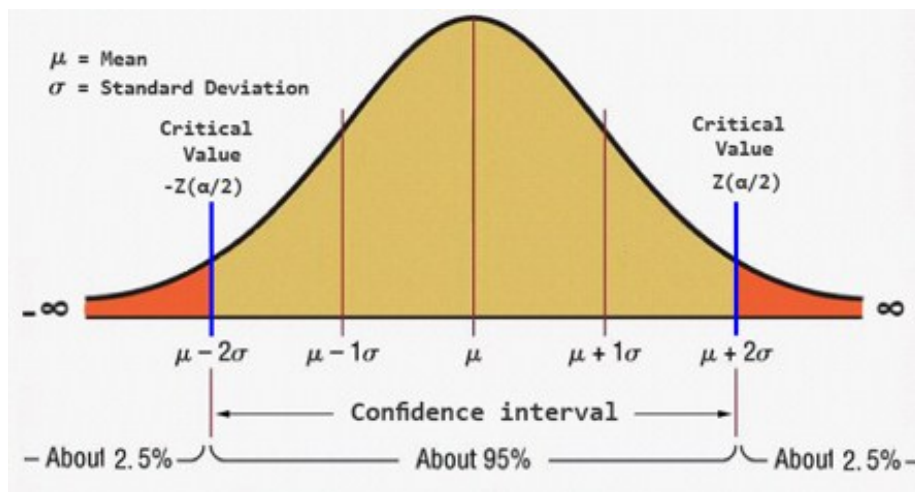


Figure 3.3 Bell shape error distribution (modified from Kendall et al., 1968).

An alternative method to find z score is to use MS excel command line to calculate the z value, which can be calculated using the following command

=NORMSINV(x)

Where x is the value that we want to find its z score

3.6 GIS Based Modeling and Assessment

The Geographical Information System (GIS) is combination of software, data and hardware that allow the user to query, visualize, and interpret spatial information to disclose relationships, trends, and patterns within a data set. ArcGIS, developed by Environmental Systems Research Institute (ESRI) is the most commonly used GIS package utilized by researchers community for business analysis, planning, environmental applications and geostatistical analysis. (See GIS Software - a description in 1000 words by Stefan Steiniger, 2009). The components (objects) in ArcGIS represent water quality monitoring stations and other real world objects. The objects used in the Lake Champlain case study were the over 50 water quality monitoring stations located throughout the lake. The objects are stored in the ArcGIS Geodatabase, which is the top-level element in the ArcGIS hierarchy, shown in figure 3.4. The hierarchical data structure allows feature classes to inherit the attributes and behaviors of the object above while retaining its spatial properties (Zeiler, 1999).

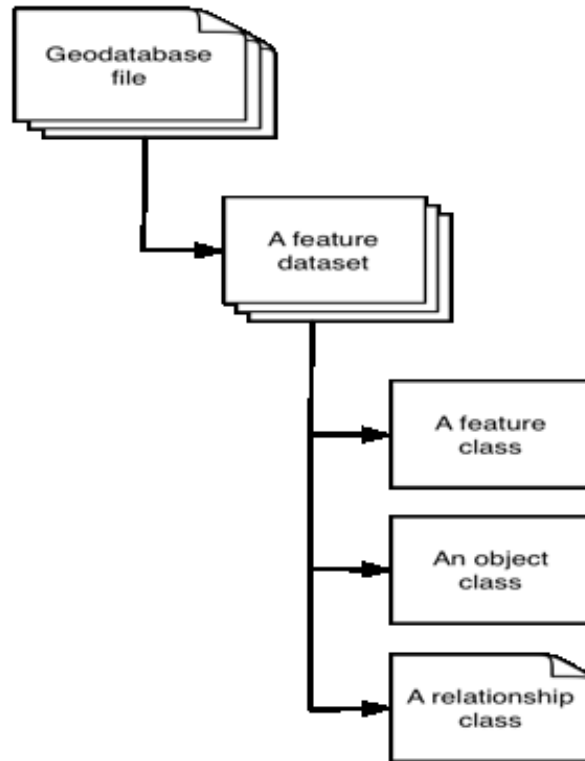


Figure 3.4 GIS hierarchy (modified from <http://webhelp.esri.com>; accessed on Jan 2014).

Geostatistics analysis will produce the same modeling results as MLR if location has no impact on the lake dataset. The ordinary least square (OLS) regression method, which is the multi linear regression method used in ArcGIS, was used to test the significance of the location of the lake variables. If location is an important independent variable for the Lake Champlain study, then geographically weighted regression (GWR) tool from ArcGIS is used where location is considered as an independent input variable that affects the model. In the final stage of the analysis, the spread and distribution of the pollutant (chlorophyll-a) and of the variables (water quality parameters) was determined by creating maps using the Empirical Bayesian Kriging (EBK) method.

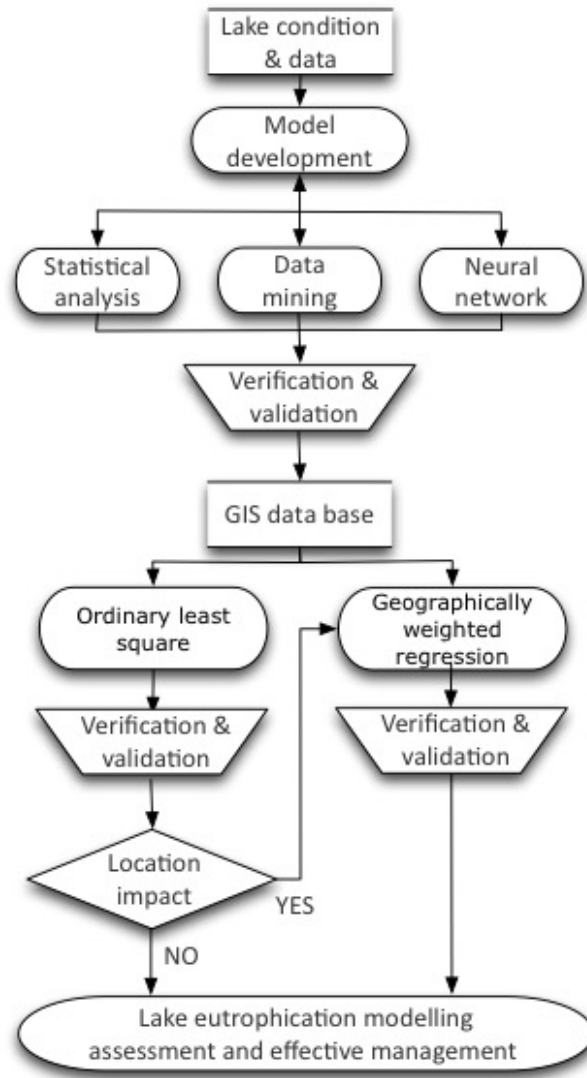


Figure 3.5 Lake Champlain eutrophication modeling using the GIS integrated analysis approach

CHAPTER 4

CASE STUDY: LAKE CHAMPLAIN

4.1 An Overview of Lake Champlain

This lake is one of the largest glacially formed lakes in North America (see figure 4.1). It is situated partially in Vermont and NY states, USA, and partially in Quebec, Canada. Its approximate dimensions are: L=193 km, maximum width =30 km, watershed =21 km², surface area =1100 km², maximum depth =122 m (most is shallow =1.5 m), mean depth =19 m. The lake has 5 different environmental zones (<http://www.lakechamplaincommittee.org/learn/natural-history-lake-champlain>, accessed on Dec 2014). The five major segments of the lake are:

- The South Lake, which is long skinny and shallow.
- The Main Lake, which is the deepest and widest section of the lake.
- Malletts Bay circumscribed by historical railroad and road causeways.
- The Inland Sea, which lies to the east of the Hero Islands.
- The Missisquoi Bay and is a large and discrete bay rich with wildlife.

This geography was used in the case study to improve the results of the multiple linear regression and in data mining classification analysis.

No.	Variables	Definition	
1	Chlorophyll-a (Chla) (µg/L)	Biomarker for Cyanobacteria algal blooms (CABs)	Lake Champlain watershed management 2013
2	Total Phosphorus (TP) (µg/L)	Pollutant from agriculture and industry, a nutrient for CABs growth	
3	Chloride (Cl) (µg/L)	A highly reactive gas, used as a disinfectant in water Treatment	
4	Secchi Depth (Secchi) (m)	Measure of water clarity/turbidity, a physical indicator of bacterial growth	
5	Total Nitrogen (TN) (µg/L)	Pollutant from wastewater from agriculture and industry, a nutrient for CABs growth.	
6	Temperature (T)(°C)	Surface temperature	
7	RegAlk	The quantitative capacity of an aqueous solution to neutralize an acid	
8	Depth (m)	Monitoring stations sampling depth	

Table 4.1 Names, abbreviations and definition of water quality monitoring parameters (variables) used in the LEF modeling studies, using Lake Champlain data.

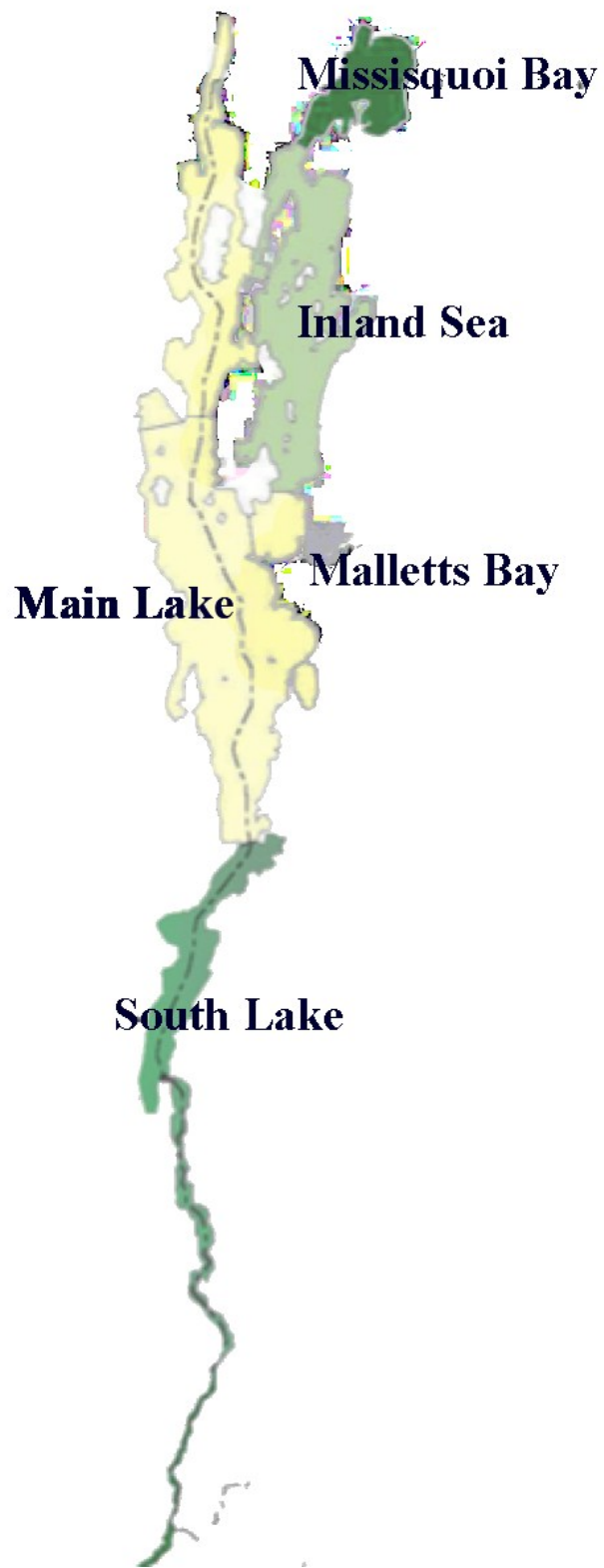


Figure 4.1 Lake Champlain watershed (modified from Hegman et al., 1999).

4.2 Raw Data and Variables for the Lake Champlain Case Study

Environmental stress on Lake Champlain started in the early 1980s when phosphorous levels from agricultural runoff and municipal sewage treatment plants caused excessive cyanobacteria algal blooms (CABs), which resulted in drinking water contaminated by trihalomethanes (THMs) produced by the CABs, and the presence of nuisance plant species such as the genus *Salvinia* and a wide range of Cyanobacteria algae (Amsterdam et al., 2005). The water quality parameters (variables) used in my modeling studies are shown in Table 4.1 above, together with their abbreviations and definitions. The source of the data on water quality parameters (including chlorophyll-a concentrations) used in the present study was from the state of Vermont, which decided to share Lake Champlain's environmental data with the public to help researchers conduct studies that could provide solutions for the lake's problems (Vermont Agency of Natural Resources, 2011). This data included information on total maximum daily loads of pollutants, available to the public and researchers via the Lake Champlain watershed management web site (www.watershedmanagement.vt.gov), accessed for this thesis project on Dec 2012.

Section 303(d) of the Federal Clean Water Act 1972 obligated all states in USA to identify waters for which wastewater effluent did not attain water quality standards. In 1998, the US Environmental Protection Agency (USEPA) defined the total maximum daily loads (TMDLs) framework for determining acceptable levels of nutrients in fresh water lakes. According to the 2001 Clean Water Action Plan, Vermont had to determine the TMDLs for the pollutants causing water problems in Lake Champlain and present a study with proposed solutions (Lake Champlain Phosphorus TMDL, 2002).

4.3 Lake Quality Criteria

Global drinking water guidelines are based on the world health organization (WHO). According to WHO, the provisional value for cyanobacteria concentration in drinking waters is 1.0 µg/L. However, WHO does not provide any criteria for the acceptable levels of total phosphorus or nitrogen concentration within lakes, rivers or reservoirs.

In the United States, there are no federal regulatory guidelines for cyanobacteria (algae) concentrations in water (EPA-810F11001, 2012). However, section 303(d) of the Federal Clean Water Act obliges each state to distinguish waters for which wastewater effluent limitations are not sufficient to attain the quality standards, and to suggest solutions based on studies and filed data analysis to obtain the required funding to solve the water problem. The water quality standards and criteria change from one lake to another, even within a single lake we may see different criteria, and a good example for that is lake Champlain, where there are various criteria within lake Champlain due the difference in the hydraulic retention time between the lake segments where the time varies from two months to three years, resulting in significant difference in the nutrient distribution within the lake basin. The standards and criteria set for Lake Champlain were derived from: 1) Trophic categorization schemes for lakes (e.g. Table 4.2); 2) Lake user survey and analyses between predicted and recorded values for total phosphorus (TP) concentrations (Smeltzer, 1999); 3) The 1993 Water Quality Agreement, which establish TP targets for 13 segments of Lake Champlain.

Selected Lake Champlain Water Quality Monitoring Stations	Depth (m)	Current Level (2011)		Criteria Targets	
		TP µg/L	Chla µg/L	TP µg/L	Chla µg/L
02 - South Lake B	5	52	10557	25	No defined criteria
04 - South Lake A	10	47	16677	25	
07 - Port henry Segment	50	21	6374	14	
09 - Otter Creek Segment	97	18	6177	14	
16 - Selburne Bay	25	16	5830	14	
19 - Main Lake	100	16	4836	10	
21 - Burlington Bay	15	16	4961	14	
25 - Malletts Bay	32	15	2928	10	
33 - Cumberland Bay	11	20	4568	14	
34 - Northeast Arm	50	23	4250	14	
36 - Isle LaMotte (off Grand Isle)	50	18	3043	14	
40 - St. Albans Bay	7	31	5770	17	
46 - Isle LaMotte (off Rouses Pt)	7	21	3941	14	
50 - Missisquoi Bay	4	50	10658	25	
51 - Missisquoi Bay Central	5	53	16196	25	

Table 4.2 Lake Champlain phosphorus criteria targets 2011 vs. observed values for the same year (updated and modified from Lake Champlain Phosphorus TMDL, 2002).

Variable	Ultraoligotrophic	Oligotrophic	Oligomesotrophic	Mesotrophic	Mesotrophic	Eutrophic	Hypereutrophic	Reference
Total Phosphorus (µg/L)	-	<10	-	10-35		35-100	>100	OECD 1982 CCME 2004 Thomann and Mueller 1987 Chambers et al 2001 Wetzel 1983
	<4	4-10	-	10-20	20-35	35-100	>100	
	-	<10	-	10-20	-	>20	-	
	-	<5	-	10-30	-		>100	
	<5	-	5-10	-	10-30-	30-100	>100	
Chlorophyll a (µg/L)	-	<10	-	10-30	-	-	>100	Nürnberg 1996 ECD 1982 Thomann and Mueller 1987 Wetzel 1983
	-	<2.5	-	2.5-8		8-25	>25	
	-	<4	-	4-10	-	>10	-	
	0.01-0.5	0.3-3	-	2-15	-	10-500	-	
	-	<3.5	-	3.5-9	-	9.1-25	>25	
Secchi Depth (m)	-	>6	-	3-6	-	<1.5	-	Nürnberg 1996 Thomann and Mueller 1987
	-	>4	-	2-4	-	<2	-	
	-	>4	-	2-4	-	1-2.1	<1	
	-	<350		350-650	-	651-1200	>1200	
	<1-250	-	250-600	-	500-1100	-	500-15000	
TN (µg/L)	<200	-	200-400	-	300-650	500-1500	>1500	Wetzel 1983
	<200	-	200-400	-	400-700	700-1200	>1200	
Hypolimnetic oxygen saturation (% saturation)	-	>80	-	10-80	-	<10	-	Thomann and Mueller 1987
TOC (mg/L)	-	<1-3	-	<1-5	-	5-30	-	Wetzel 1983
DOC (mg C/L)	-	2	-	3	-	10	-	Kliff 2002

Table 4.3 Lake trophic criteria, Source: (Literature review related to setting nutrient objectives for lake Winnipeg, 2006)

The way criteria levels were decided for Lake Champlain segments was explained in the Vermont DEC (1990) as well as in Lake Champlain basin program (1996), and is summarized as follows:

- Main Lake and Mallets Bay segments are large central broad areas with low nutrient level; therefore an oligotrophic standard of 0.010 mg/L phosphorus is desirable for these two segments.
- In the remaining parts of the lake, the phosphorus concentrations are significantly higher than 0.010 mg/L, consequently the attainability for these segments to oligotrophic criterion is doubtful. Therefore, higher criteria level of 0.014 mg/l was chosen for the rest of the lake (except for St. Albans Bay, Missisquoi Bay, and the South Lake). The mean value of 0.014 mg/L represents a phosphorus level at which an algae nuisance condition would be present only 1% of the time during the summer.
- St. Albans Bay, Missisquoi Bay, and the South part of the lake are highly eutrophic segments; therefore the target of 0.014 mg/l criteria would not be realistically attainable. There have been many attempts in St. Albans to reduce phosphorus levels including treatment plant upgrades and nonpoint source controls. The water quality set by the Vermont department of environmental conservation (DEC) in the St. Albans Bay aim is to reduce the phosphorus in the center bay area to a concentration of about 0.003 mg/l above the level outside the bay in the Northeast arm. Thus, a phosphorus criterion of 0.017 mg/l was selected for St. Albans Bay.
- Missisquoi Bay and the South lake segments are shallow depth and have wetland like characteristics therefore, they are considered as naturally eutrophic (high nutrient) areas. The high eutrophic state in Missisquoi Bay area has beneficial values for productive warm-water fisheries and wildlife habitats. Therefore, a phosphorus criterion of 0.025 mg/l reflecting a moderate level of eutrophication was selected for these segments.

Recent and historical phosphorus and cyanobacteria concentrations in lake Champlain have exceeded the desired criteria levels. In many cases the recorded values were more than double of the desired criteria. Figure 4.2 shows the phosphorus levels in Lake Champlain compared with water quality criteria.

Phosphorus Levels in Lake Champlain 1990-2003 Compared with Water Quality Criteria (red lines)

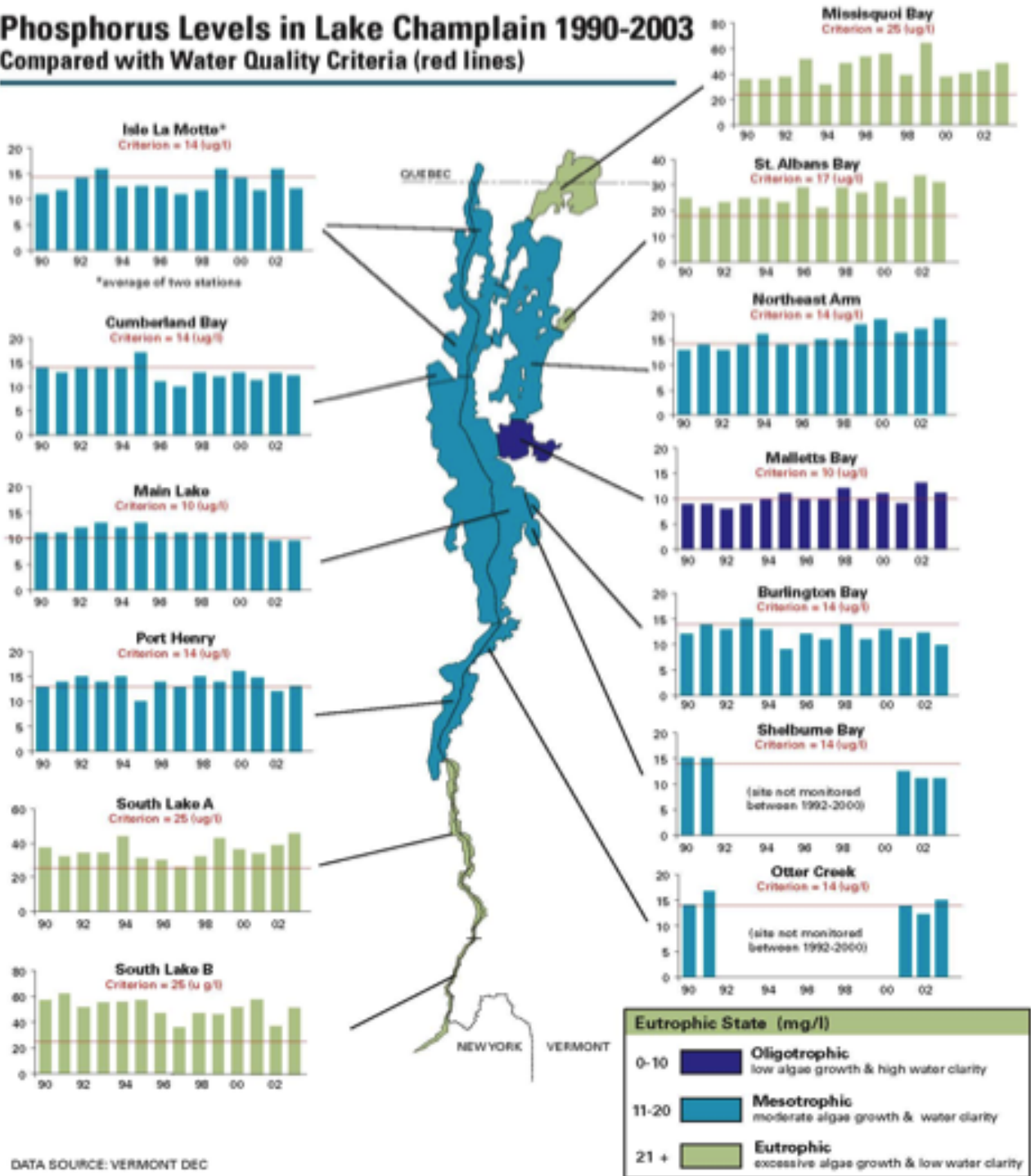


Figure 4.2 Phosphorus levels in Lake Champlain and water quality criteria (Lake Champlain Phosphorus TMDL, 2002).

4.4 Data Collection and Quality Analysis

The process of data entry and acquisition is inherently prone to errors and the raw data from the Lake Champlain monitoring stations did not reveal much information. A thorough data preparation and cleansing was required before starting with modeling and statistical analysis.

A -Data source, format and units

The process of Lake Champlain monitoring station data entry and acquisition is inherently prone to errors; lake Champlain's data is available in its raw format through the lake Champlain long-term water quality program. After downloading the data, it is then sorted and transformed into one file of MS excel. To simplify the analysis all the concentrations for the different water quality parameters are unified and converted to $\mu\text{g/L}$.

B -Data quality analysis

For Lake Champlain, data quality control is implemented through the Vermont department of environmental conservation (DEC), while for this research data quality control is implemented through filtration of outliers and working with averages.

C -Monitoring frequency

Since 1992 volunteers helped collecting the data for Lake Champlain between 1992 and 2011. The database contained 12,994 records for 33 variables. Table 4.4 lists the variables, their monitoring range and frequency while figure 4.3 shows the location of the monitoring stations.

Variables	Code	Units	Date Range	Lab	Sampling Frequency
Total Phosphorus	TP	µg/L	1992 - 2011	VT and NY	10/year
Dissolved Phosphorus	DP	µg/L	1992 - 2011	VT and NY	10/year
Ortho-Phosphorus	DOP	µg/L	1992 - 1994	VT and NY	-
Chloride	Cl	mg/L	1992 - 2011	VT and NY	10/year
Dissolved Silica	DSi	mg/L	1992 - 2011	VT and NY	10/year on a 5 yr cycle
Total Nitrogen	TN	mg/L	1992 - 2011	VT	10/year
Total Kjeldahl Nitrogen	TKN	mg/L	1992 - 1996	NY	-
Total Nitrate-Nitrite	TNOX	mg/L	1992 - 1996	VT and NY	-
Total Ammonia	TNH3	mg/L	1992 - 1996	VT and NY	-
Calcium	TCa	mg/L	1992 - 2011	VT and NY	3/year on a 5yr cycle
Magnesium	TMg	mg/L	1992 - 2011	VT and NY	3/year on a 5yr cycle
Sodium	TNa	mg/L	1992 - 2011	VT and NY	3/year on a 5yr cycle
Potassium	TK	mg/L	1992 - 2011	VT and NY	3/year on a 5yr cycle
Iron	TFe	µg/L	1992 - 2010	VT and NY	3/year on a 5yr cycle
Lead	TPb	µg/L	1992 - 1998	NY	-
Total Organic Carbon	TOC	mg/L	1992 - 1999	NY	-
Dissolved Organic Carbon	DOC	g/L	1992 - 1999	NY	-
Dissolved Inorganic Carbon	DIC	mg/L	1992 - 1996	NY	-
Temperature	TempC	deg C	1992 - 2011	VT	10/year
Dissolved Oxygen	DO	mg/L	1992 - 2011	VT	10/year
Conductivity	Cond	µS/cm	1992 - 2005	VT	10/year
pH	pH	-	1992 - 2005	VT	10/year
Alkalinity	RegAlk	mg/L	1992 - 2011	VT	3/year
Total Suspended Solids	TSS	mg/L	1992 - 2005	VT and NY	-
Chlorophyll-a	Chla	µg/L	1992 - 2011	VT and NY	10/year
Secchi Depth	Secchi	m	1992 - 2011	VT and NY	10/year

Table 4.4 Lake Champlain variables and their monitoring range and frequency (Lake Champlain Phosphorus TMDL, 2002).

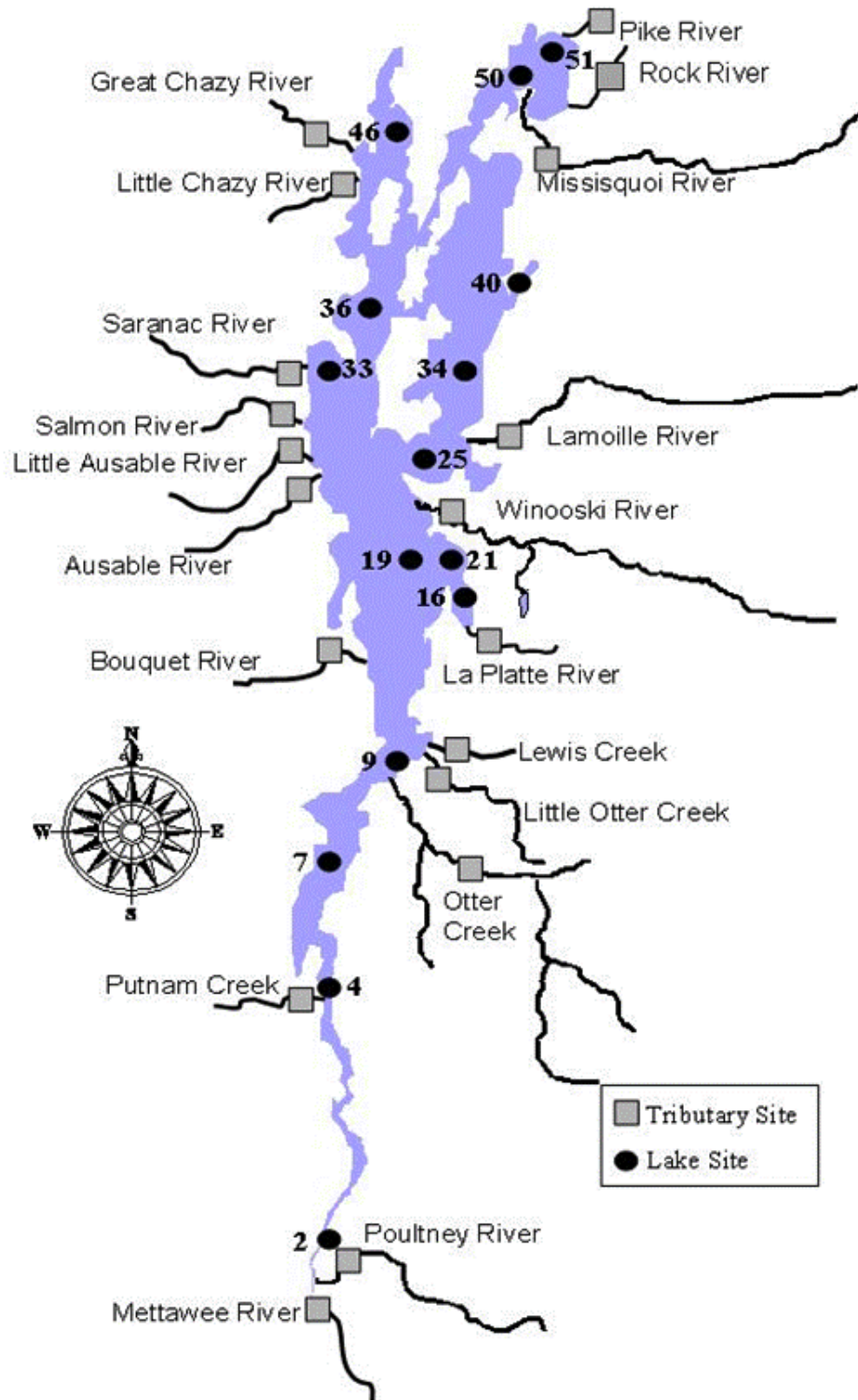


Figure 4.3 Lake Champlain monitoring stations (www.vtwaterquality.org; accessed on Jan 2014)

D -Gaps and range

Some of the reasons that contributed to problems within the lake data were:

- Monitoring stations for Lake Champlain were introduced over different periods of time.
- New variables are being introduced while others were dropped.
- The collection of the variables was not made concurrently as would be desirable for the purpose of analyzing ecological interrelationships.

As a result, the monitoring periods vary between the lake variables and between one station and another, therefore the lake daily data is full of gaps and missing ranges. For example out of the 12,994 data records for lake Champlain, not a single row contained a complete set of concurrent reading for a set of variables. This was a major setback, since empty cells typically are dropped or interpolated during analysis, another challenge is that : the gaps and missing ranges for several variables exceeded 20 months, thus making interpolation, or exploration a difficult task. Table 4.5.of the yearly data for station 07 Port Henry of Lake Champlain, illustrate the extent of the gaps problem.

Year	Depth	TP	CI	TN	TCa	Minerals	Toxic	TOC	TempC	DO	pH	Secchi	RegAlk	Chla
1992	50	13.58	11742	509.58		13847.44	22	4.3	16.54		7.98	4.33	53.91	5.63
1993	50	18.25	11501	456.79		12804.96	15.75	3.95	23.5		7.67	3.63	54.3	5.25
1994	50	15.78	11987	460.9		12608.9	22.72	8.84	22.16		7.21	3.68	53.55	5.27
1995	50	10.33	13175	384.44		11718.8	5.2	15.3	15.75	10.18	7.54	5.23	53.02	3.05
1996	50	13.88	12524	445.33		12156	5	4.75	16.48	9.96	7.91	4.06	51.1	4.44
1997	50	13.23	12184	454.4		13140.5	5.13	3.33	24.02	10.53	7.8	4.27	53.9	4.78
1998	50	13.75	12076	438.5		10367.67	5	4.86	17.12	10.28	7.77	3.96	54.6	4.72
1999	50	13.39	12641	460.33		14121		3.56	19	10.39	7.82	4.92	50.41	6.83
2000	50	15.31	12575	451.25		14322.13			25.86	10.32	7.72	4.22	51.62	5.98
2001	50	12.93	13163	479.83		14695.25			23.18	10.54	7.74	4.47	53.23	3.49
2002	50	10.59	13979	400.6		15113			17.84	10.15	7.78	5.03	51.63	1.82
2003	50	12.92	15093	433.39		15717.7			25	10.42	7.84	4.95	51.23	5.46
2004	50	16.44	14981	412.08		16243.6			23.68	10.2	7.91	4.4	51.95	5.45
2005	50	16.36	15344	410.54		14793.88			12.18	10.41	7.84	3.1	52.6	10.34
2006	50	17.13	14582	438.3					20.54	10.06		3.46	54.53	6.17
2007	50	14.61	13843	438.02					18.43	10.34		4.05	51.91	4.92
2008	50	18.69	14720	444.25					8.7	10.22		3.6	53.36	4.8
2009	50	16.64	14583	407.57					22.9	10.8		3.47	55.5	4.9
2010	50	16.5	14155	363.72		15286.75			13.1	10.29		3.55	57.13	4.87
2011	50	22.12	12926	405.12		15466.67			21.98	10.21		2.66	55.32	6.25

Table 4.5 Port Henry segment (07) of lake Champlain observed data.

I presented table 4.5 with the yearly data since it was easier to show the extent of the problem, however, I started the analysis using the daily data, where the problem is greater. The biggest challenge is that for the Lake Champlain data, each water quality monitoring station exhibits a set of different problems with their variables, and due to the size of the gaps and long missing ranges within the data set, interpolation or extrapolation does not work. As an alternative, I decided to analyze the distribution of the data in order to reveal trends, to make estimating the gaps and missing ranges easier. Trends can be investigated either visually or using statistical tests like Mann–Kendall. Previous studies indicate that this approach is likely to see curves and nonlinear shapes of the data for water quality parameters, rather than straight lines. Figure 4.4 shows the different types of nonlinear curves that we may expect to see in a data set.

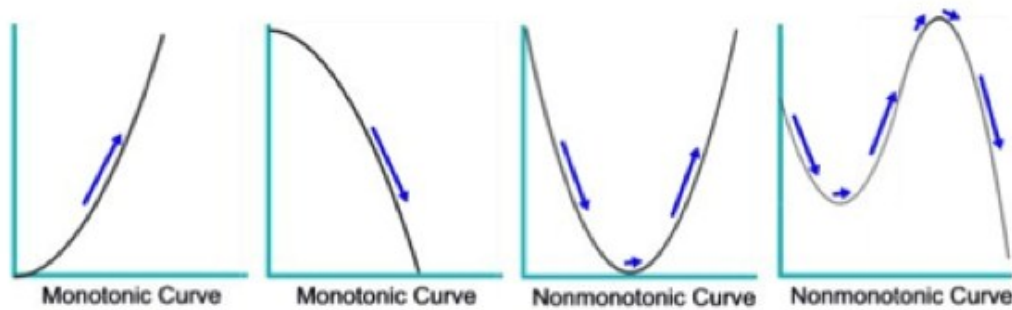


Figure 4.4 Nonlinear curve types (<http://epa.gov/ncct/edr>; accessed in June 2014)

A monotonic curve consistently stays in one direction (either always upwards or always downwards), while a nonmonotonic curve keeps changing its direction (G. Brewka, 1991). Figure 4.5 shows the yearly Calcium observed data for monitoring station 02 (South Lake B); again I used yearly data to show the extent of the problem. Within the data there is 36 months gap between 1992 and 1995, such gap can be clearly seen on the graph, at the same time the data seems to take a non-monotonic distribution throughout the recorded range.

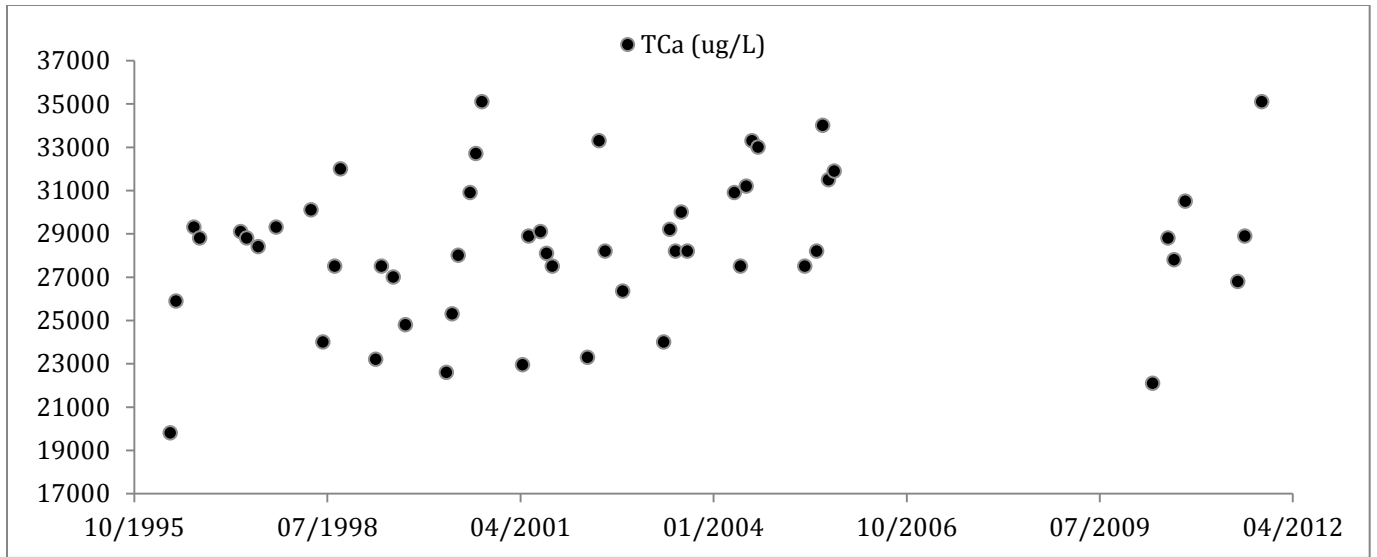


Figure 4.5 Yearly calcium data for lake Champlain water quality monitoring station 02.

4.5 Data Preparation

Visual inspection of the daily, monthly and yearly lake data distribution didn't reveal any obvious trend, thus making it difficult to fill in the gaps within the lake data. Therefore, I used the following analysis approaches to fill in the gaps within the data.

A -Linear and nonlinear interpolation

Mann-Kendall (MK) test, also known as the “Kendall’s tau” test, is a rank based non-parametric test used to assess the significance or existence of a trend within a data series. The probability value P for the MK statistical test for a dataset is (Kendall MG. 1975):

$$P = \begin{cases} 0.5 & \text{When there is no trend} \\ \text{Close to 1} & \text{When there is a strong negative trend} \\ \text{Close to 0} & \text{When there is a strong positive trend} \end{cases} \quad \text{Eq. 4.1}$$

Due to the size of the Lake Champlain dataset, statistical analysis software package Systat 13 was used to run the MK test on the daily, monthly and yearly data.

The MK test for the variable minerals for the daily and monthly data did not provide any significant results; however, for the yearly data presented in table 4.5, the results indicated a

significant P value for both upward and downward trends, indicating a two-sided trend. The MK test also indicated that the upward trend better describes the general data distribution.

The Systat 13 software detected the gaps within the data using the MK test: the gap in the middle of the series from 2005 till 2010, and the missing values for the years of (2006, 2007, 2008 and 2009). Systat 13 automatically interpolated these gaps, and the interpolation was completed using local quadratic smoothing as shown in figure 4.6.

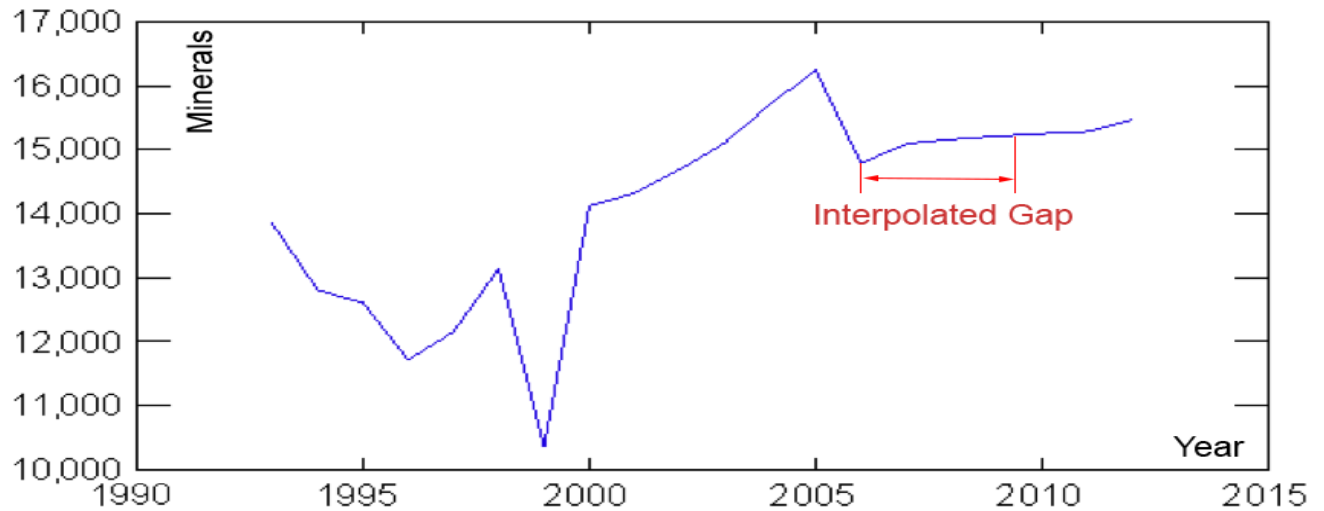


Figure 4.6 The Mann–Kendall test and the interpolation.

This interpolated gap approach is typical of many software packages; they either fill the gaps or completely ignore the missing range. The gap in the mineral variables yearly data was common across all the monitoring stations; hence it wasn't possible to verify the results. I compared the minerals data distribution against other variables, which did have a complete data range. I scaled the TP and Cl variables data records up to fit within the same range as the minerals dataset, and the results are plotted in figure 4.7. I noticed that in the gap period, the datasets for both TP and Cl exhibited a non-monotonic behavior, while the interpolated data range for minerals, which was done using the MK test, was a straight line. Additionally, before and after the range, the datasets for all three variables had non-monotonic behavior. This provided enough evidence to raise doubts about the interpolated results and to stop the investigation using MK trend analysis as a tool to fill in the gaps and to predict the missing data ranges.

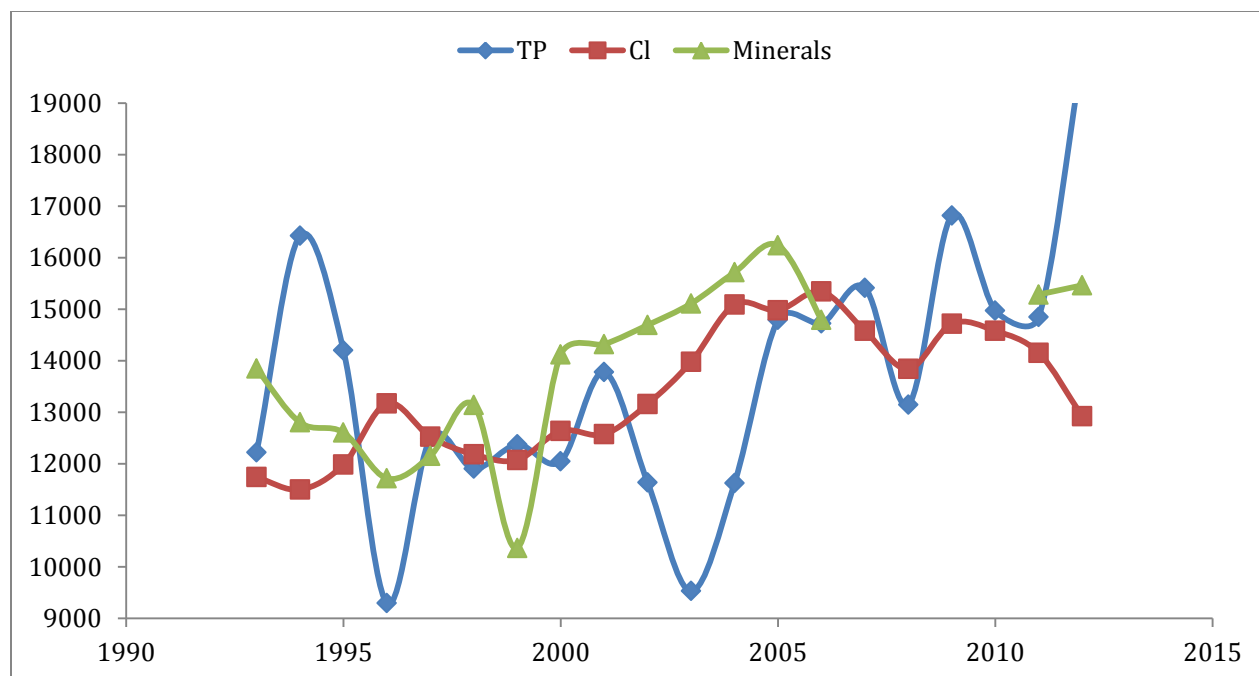


Figure 4.7 Yearly TP, Cl and minerals chart for lake Champlain Port Henry

Further investigation of the lake data shows that the lake variables have a non-monotonic data distribution therefore; linear interpolation or extrapolation was not an option.

An earlier study of Lake Champlain suggests that using mean values of water quality parameters produced a relatively high degree of statistical precision (Smeltzer, et al., 1989). By using the mean values we remove many of the unwanted gaps, therefore daily data for Lake Champlain was averaged to produce monthly data, however the monthly data also had several gaps and missing range, so the investigation and the data cleansing process continued on the monthly data. To avoid presenting redundant results, I skipped presenting the analysis for the daily and monthly data, although I have thoroughly investigated each set, and I directly used the yearly data throughout the rest of the thesis. However, even the yearly data still had gaps and missing ranges, so I used the approach described below to complete the ranges and fill in the gaps for the yearly data of Lake Champlain, in order to avoid dropping a variable from the analysis.

Assuming we manage to get the information about the equation that best describes the data distribution over a significant period, then it is possible to use the function to estimate the gaps and missing range within the data (Zhu et al., 2003). These authors proposed using discrete Fourier transform for time series data, while other studies (Xiang and Gray, 1999) suggested

using Fuzzy logic or recommend neural networks. FindGraph data mining software package is a tool that facilitates the search through 10s of different functions (e.g. Linear Regression, Fourier, Polynomial, Exponential, Logarithm, Power and Waveform) to produce models that fit the data under investigation.

Figure 4.8 is a screen shot of FindGraph software during the setup process; the screen shot reveals the different available time series functions that were used to estimate the Lake Champlain water quality monitoring data distribution.

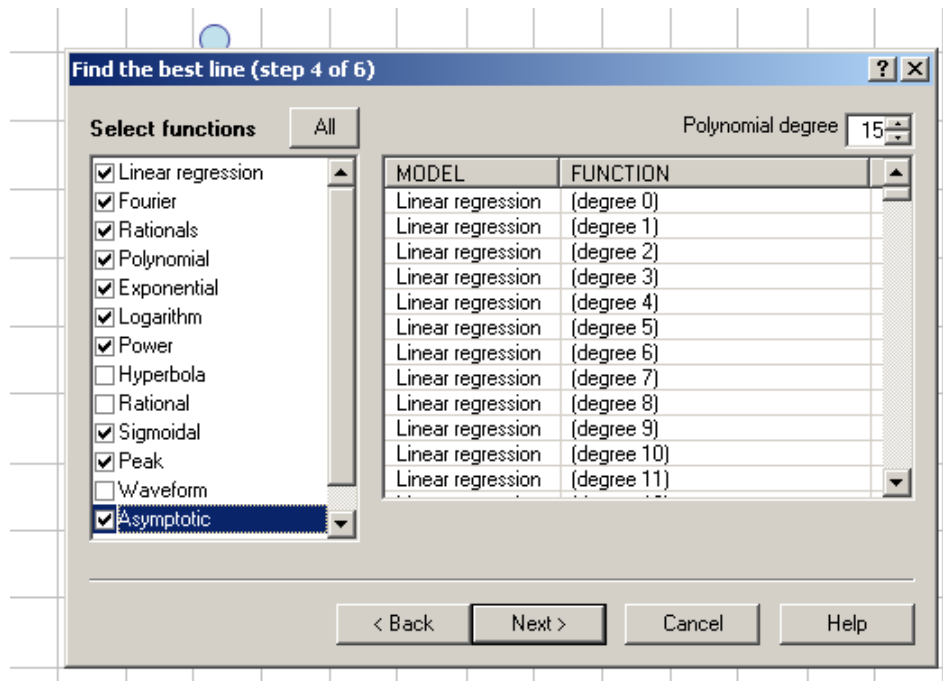


Figure 4.8 Data mining (FindGraph) analysis.

The variable minerals data from table 4.5 was used for the test run, but this time the data was split into two halves: the first half (years 1992 till 2001) was used to generate the time series model; while the second set (between 2002-2011) was used to verify the model. FindGraph software investigated more than 999,999,999 iterations in less than 2 minutes. Several models were generated and were sorted according to their best R^2 . The best curve fit model that represented the minerals data distribution between 1992 till 2001 was a Fourier function with 3 harmonics.

$$\begin{aligned} \text{Minerals}(t) = & 12603.92 + (804.73 \cdot \cos(0.78 \cdot t) + 76.33 \cdot \sin(0.78 \cdot t) \\ & + (773.25 \cdot \cos(1.57 \cdot t) + 26.41 \cdot \sin(1.57 \cdot t)) + (74.06 \cdot \cos(2.35 \cdot t) - \\ & 1044.27 \cdot \sin(2.35 \cdot t)) \end{aligned} \quad \text{Eq. 4.2}$$

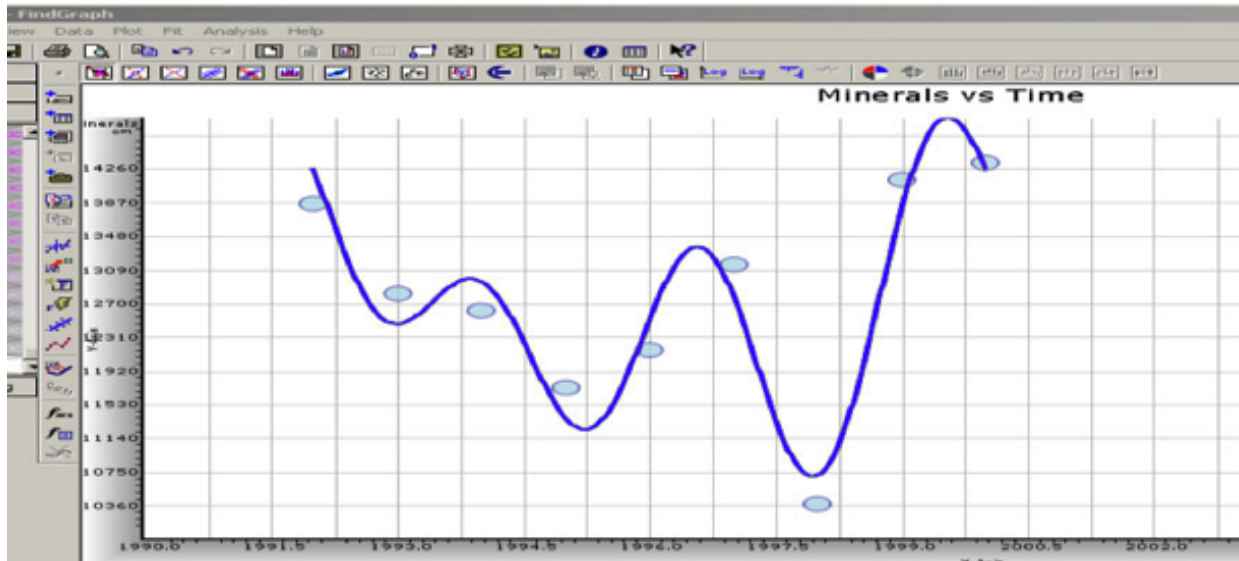


Figure 4.9 Data mining (FindGraph) results.

Figure 4.9 shows the Fourier function with 3 harmonics as found by FindGraph software and in figure 4.10 the actual recorded data for minerals from table 4.5 is plotted against the Fourier time function for comparison.

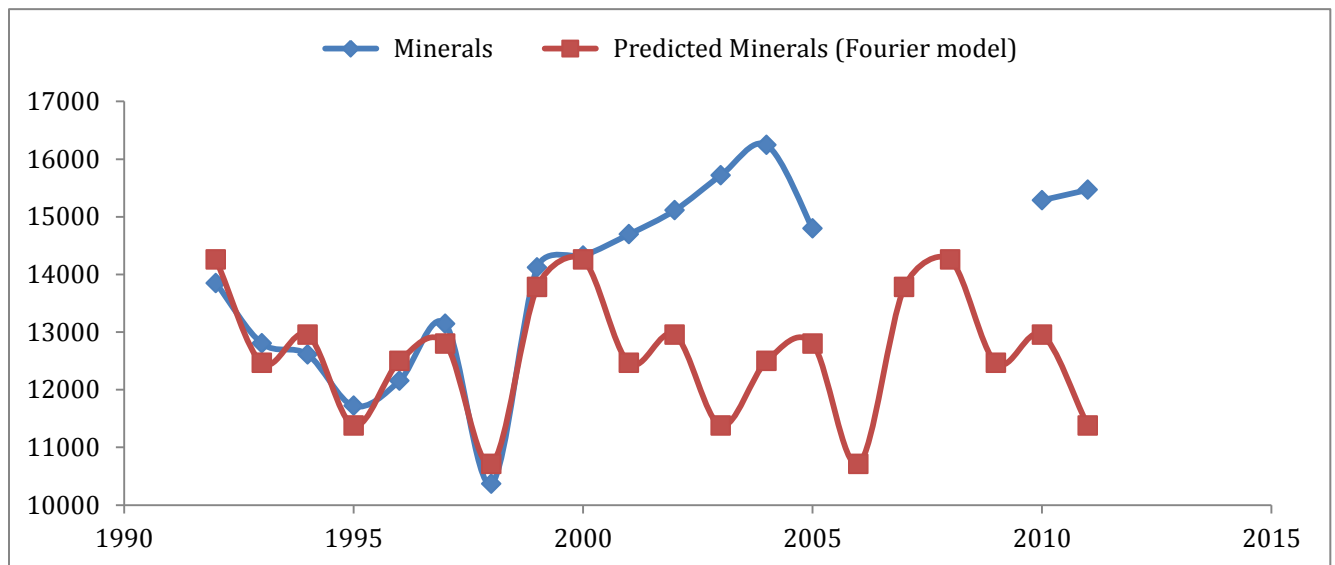


Figure 4.10 Minerals Fourier predictions for station 02

Although the Fourier function provided a good fit for the data between 1992-2001, the function failed to verify and predict the data between 2002-2011. Understanding the way Fourier function works helps to justify the reason for this. In 1807 Joseph Fourier declared that a periodic function can be represented as the sum of a Fourier series (Georgi P., 1976).

$$f(x) = a_0 + \sum_{k=1}^{\infty} (a_k \cos kx + b_k \sin kx)$$

Where

$$a_0 = \frac{1}{2\pi} \int_0^{2\pi} f(x) dx \quad \text{Eq. 4.3}$$

$$a_k = \frac{1}{2\pi} \int_0^{2\pi} f(x) \cos(kx) dx$$

$$b_k = \frac{1}{2\pi} \int_0^{2\pi} f(x) \sin(kx) dx$$

Fourier as a function assumes a cyclic and periodic nature of the signal; meaning that if we split the data into two halves, the left side of a Fourier function will be a mirror image across the y-axis of the right side. Therefore, the Fourier function assumed that the data after 2002 would be a mirror image of the previous years. Despite the failure of the Fourier function, I continued investigating several different nonlinear functions, but the results were the same. All linear and nonlinear (curve fit) functions generated then failed during the verification process, thus indicating that this approach was not applicable for filling in the gaps and the missing ranges for the Lake Champlain data.

B -Extreme and outliers detection

Similar to plants, algae are affected by their surroundings; therefore we cannot underestimate the importance of any monitored variable. However because of the gaps, missing ranges, different monitoring frequency, lack of concurrent data and difficulties to fix all these data problems, it

makes sense to shift the analysis to the yearly timeframe. Yearly data is obtained by averaging monthly data, and the monthly data was obtained by averaging the daily data. The daily data records for the lake water quality parameters were inconsistent, and some months had barely a single data entry, while other months had tens of data records. This problem presents a risk of having the results deviating by one or two extreme values. For example let us assume the following data records for a lake segment.

Data for 1997	Total Phosphorus readings ($\mu\text{g/L}$)						Number of Daily data records
March	10		11		9		3
April	14		15		13		4
May	11				11		2
June	12		14		10		5
July	15		11		8		5
August	12		12		10		6
September	65						1
October	10				14		2

To find total phosphorus typical value for each month, we average the data for that month, for example, on June the monthly average were $= (12+14+10+17+8)/5 = 14.8 \mu\text{g/L}$. In the same way we find the average for the other months.

$$\text{March} = 10 \qquad \text{July} = 12.8$$

$$\text{April} = 12.75 \qquad \text{August} = 13$$

$$\text{May} = 11 \qquad \text{September} = 65$$

$$\text{June} = 12.2 \qquad \text{October} = 12$$

To obtain the yearly data we average the monthly data, the 1997 yearly data $= (10+12.75+11+12.1+12.8+13+65+12)/7 = 18.59$, the question is: was the extreme data record for the month of September a result of human error? Assuming it was an error and dropping it from the analysis will give the following yearly data $= (10+12.75+11+12.1+12.8+13+12)/6 = 11.96$, such a significant difference can be the deciding factor for a lake to meet the federal TMDL criteria or not. If in each year on the same month of September we had similar extreme value, then in this case such a value becomes seasonal high record and is not considered as an anomaly. To judge whether a data record is extreme or not, we must run seasonal tests or visually inspect the overall data distribution. Many methods are available for detecting outliers or extreme values, the simplest of these is to visually screen the data, and typically outliers are spotted at the border of data distribution. For example in figure 4.11 the majority of the daily

data records for the total phosphorus of station 02 are between 25 and 125 $\mu\text{g/L}$ however, in 8/17/2004 there was a data record of TP =235 $\mu\text{g/L}$, such a value is outside the normal data distribution and has not been recorded again for that particular station, therefore it is considered extreme and can be removed from the analysis

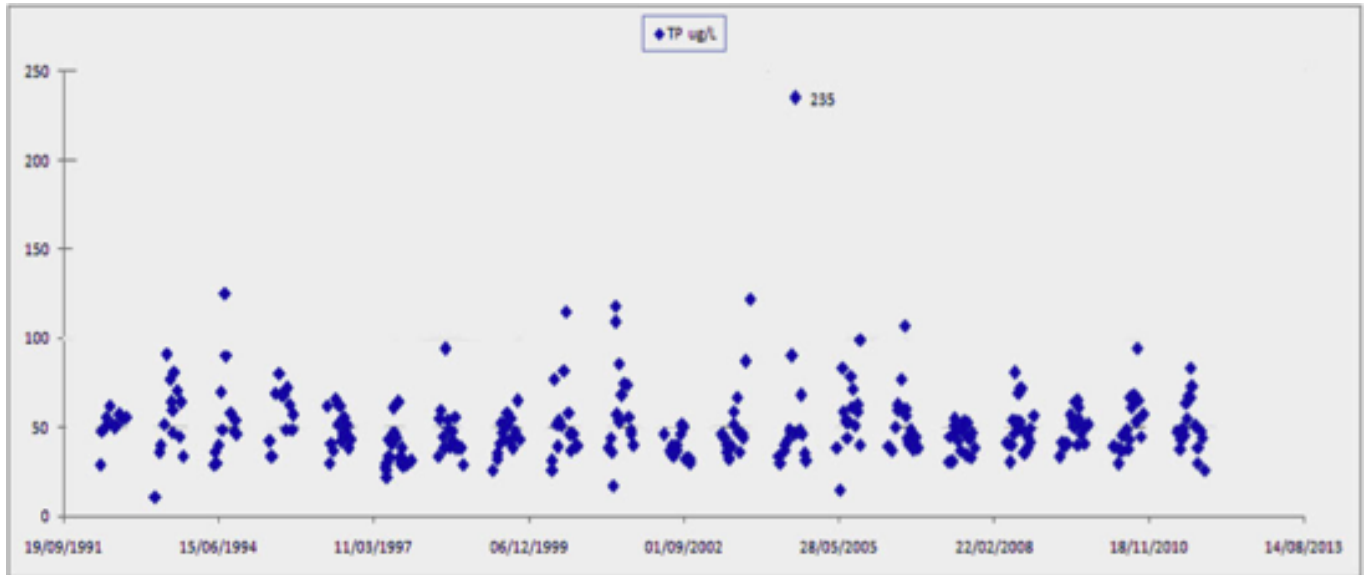


Figure 4.11 Screening outlier daily data of TP for station 02

There are six different criteria set for Lake Champlain segments defined in table 4.2. So while TP =50 $\mu\text{g/L}$ is a typical value in the South segment of the lake, the same value is considered extreme in the main lake segment therefore, it was necessary to investigate extreme values for each monitoring station independently, and for the 12,994 records of daily data between 1992 till 2011, only 125 recordings of outliers were found, those outliers were removed and a record of their value is kept in appendix A. However, it is worth mentioning that due to the huge amount of daily data records, if outliers were not removed their impact would have been reduced during the averaging process to obtain the yearly data.

C -Selecting data range and variables

Water quality monitoring of Lake Champlain at particularly stations (i.e. stations 2, 4, 7, 19, 21, 25, 33, 34, 36, 40, 46, 50) started in 1992, while monitoring for stations 9 and 16 didn't start till later in 2001, and station 51 was added in 2006. Typically, earlier data is used for training while recent data is used for testing. Applying this approach means that data from stations 9, 16 and 51) will not be included in the model creation.

Therefore throughout this study for Lake Champlain, data between 2003- 2011 will be used for model creation, while the data between 1992- 2002 will be used for verification. The R^2 value increases whenever a new predictor is added, so a model with more variables will appear to be a better fit than a model with fewer variables. Thus, it is to our advantage to include as many variables as possible, although the gaps in the Lake Champlain data resulted in dropping few variables. The variables selected for this thesis are listed in table 4.6.

Variable name	Code	Units	Date Range	Lab	Sampling Frequency
Total Phosphorus	TP	µg/L	1992 – 2011	VT & NY	10/year
Chloride	Cl	mg/L	1992 – 2011	VT & NY	10/year
Total Nitrogen	TN	mg/L	1992 – 2011	VT	10/year
Temperature	TempC	deg C	1992 – 2011	VT	10/year
Alkalinity	RegAlk	mg/L	1992 – 2011	VT	3/year
Chlorophyll-a	Chla	µg/L	1992 – 2011	VT & NY	10/year
Secchi Depth	Secchi	m	1992 – 2011	VT & NY	10/year
Time	Date	Years	1992-2011		
Depth	Depth	m	1992-2011		

Table 4.6 Lake Champlain variables monitoring range (modified from lake Champlain phosphorus TMDL, 2002).

In section 2.1.1 Phosphorus Cycle I emphasized on the importance of internal loading in lake modeling analysis, however the lake Champlain data available through the long-term water quality program does not have the internal loading, so I started the analysis of lake Champlain assuming a negligible internal loading, which is a valid assumption for the majorly of the deep monitoring stations.

Water quality parameters causing eutrophication and algae bloom depend on the same factors, including the amount of rain, run off water and human activities, all of which result in a strong correlation between the variables. To simplify the analysis, however, the water quality parameters used for the analysis are assumed to be independent for the purpose of this thesis project.

4.6 Modeling Steps

The objective of this thesis project was to better understand the importance of factors that contribute to the growth of cyanobacteria algal blooms (CABs) in lake Champlain. I used the approach illustrated in figure 4.12, which is explained below.

Firstly, I used historical data from the State of Vermont monitoring stations on lake Champlain (www.watershedmanagement.vt.gov, accessed on Dec 2012), to investigate the links between the levels of the seven selected independent water quality parameters (variables) described in section 5.1, using a correlation matrix. This step determined the relative impact of each variable on the dependent variable chlorophyll a levels (a biomarker for CABs). Secondly, I investigated the compound impact of the water quality parameters on the CABs using modeling techniques, including multiple linear regression (MLR), neural network (NN) and data mining (DM). This step generated a number of chlorophyll a models. Thirdly, I verified each of the chlorophyll models using recent data (as detailed in chapter 5) in order to find the best-fit model.

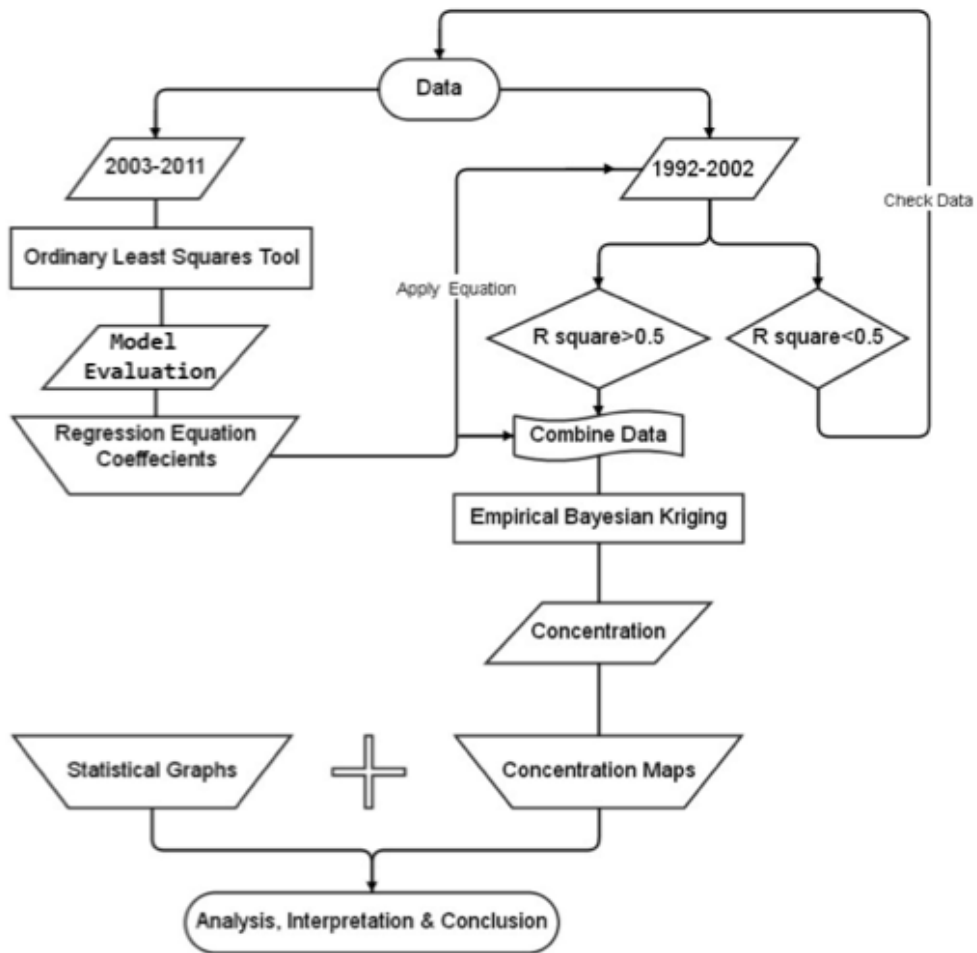


Figure 4.12 Model flowchart verification.

4.6.1 Multiple linear regression

Multiple linear regression (MLR) is a modeling technique which attempts to find the relationship between several explanatory variables and a response variable, by fitting a linear equation to the observed training data set, assuming we want to find the MLR for station 19 of lake Champlain, we then use the yearly data presented in the following table. To avoid potentially biased results, the data is split in two, the first half is used to derive the model while the other half of the data is passed through the model equation and the output is compared with the observed data for verification.

Data set	Station	Year	Depth (m)	TP(µg/L)	Cl (µg/L)	TN (µg/L)	Secchi (m)	Temp C	RegAlk	Chla (µg/L)
		Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Y
Data set 1	19	1993	100	13.89	11495.00	433.75	5.13	14.02	51.57	3.33
	19	1994	100	12.22	11594.44	466.33	5.33	12.68	49.50	4.33
	19	1995	100	8.97	12661.11	452.22	6.41	9.80	52.41	4.16
	19	1996	100	10.84	12461.70	447.08	4.88	8.90	50.38	4.04
	19	1997	100	11.37	11733.89	453.33	4.87	12.00	50.45	4.61
	19	1998	100	11.36	11879.17	396.25	5.20	12.53	50.37	3.86
	19	1999	100	10.64	12310.26	444.05	6.57	21.67	49.03	4.70
	19	2000	100	11.71	12622.00	427.17	6.04	16.78	49.14	3.66
	19	2001	100	10.51	13099.00	430.50	5.46	19.98	49.26	3.43
19	2002	100	7.90	13633.33	403.67	6.50	22.24	48.20	1.52	
Data set 2	19	2003	100	8.57	14706.25	409.33	6.87	21.06	48.23	2.91
	19	2004	100	12.50	14775.28	398.50	6.11	16.53	49.31	3.62
	19	2005	100	12.57	15118.33	409.47	4.84	19.34	51.48	5.34
	19	2006	100	14.48	14686.31	435.12	4.42	19.60	49.83	4.34
	19	2007	100	12.87	13760.00	432.58	4.94	19.18	49.84	3.32
	19	2008	100	13.89	14448.33	436.00	5.40	18.20	49.42	3.34
	19	2009	100	12.75	14293.06	410.14	5.62	18.03	51.32	2.90
	19	2010	100	12.96	13975.71	370.29	4.60	13.00	53.72	3.10
	19	2011	100	16.12	12978.10	387.19	3.48	6.10	51.35	4.62

Table 4.7 Lake Champlain yearly data for 1993-2011.

Solution: The concept of linear regression suggests the existence of a linear relationship between the dependent variable (chlorophyll-a) and the independent variables listed above. In a linear relationship the constant is the slope, so if we use part of the data to find the slope, then we can use the other part of the data to verify the results. First the data in table 4.7 is split in half, the first half will be used to derive the model (slope), and the second half will be used to verify the model. The general format for the multiple linear regression model is

$$Y_i = \beta_0 + \beta_1 z_{i1} + \beta_2 z_{i2} + \dots + \beta_i z_i + \varepsilon \quad \text{for } i = 1, \dots, n$$

The above equation can also be rewritten in a matrix format using the lake variable as follows

$$\begin{bmatrix} Chla_{11} \\ Chla_{21} \\ \vdots \\ Chla_{n1} \end{bmatrix} = \begin{bmatrix} 1 & TP_{11} & TN_{12} & Cl_{13} & Temp_{14} & RegAlk_{15} & Depth_{16} & Secchi_{17} \\ 1 & TP_{21} & TN_{21} & Cl_{23} & Temp_{24} & RegAlk_{25} & Depth_{26} & Secchi_{27} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & TP_{n1} & TN_{n1} & Cl_{n3} & Temp_{n4} & RegAlk_{n5} & Depth_{n6} & Secchi_{n7} \end{bmatrix} = Z\beta + \varepsilon$$

Our target is to use half of the data set to find β and then use it to create the MLR equation, then the model accuracy is evaluated by applying the MLR equation to the second half of the data and comparing the model output with the observed data. The best MLR model is the one where the error =0. Arranging the input and output variables from table 4.7 to match the matrix equation results in:

$$Y_{training} = Chla = \begin{bmatrix} 3.33 \\ 4.33 \\ \vdots \\ 1.52 \end{bmatrix}$$

$$Z_{training} = \begin{bmatrix} 1993 & 100 & 13.89 & 11495.00 & 433.75 & 14.02 & 5.13 & 51.57 \\ 1994 & 100 & 12.22 & 11594.44 & 466.33 & 12.68 & 5.33 & 49.50 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 2002 & 100 & 7.90 & 13633.33 & 403.67 & 22.24 & 6.50 & 48.20 \end{bmatrix}$$

Can be calculated from $\beta=Y/Z$ when error=0, however, this computation is not directly possible since Y and Z are of a different dimensions, so I developed a Matlab code LEF-MLR (see appendix B) to obtain the following answers.

$$\hat{\beta} = Y/Z = (Z^tZ)^{-1}Z^tY = \begin{bmatrix} 0.4095 \\ -8.2418 \\ \vdots \\ 0.2626 \end{bmatrix}$$

$$\hat{Y} = Chla = 0.409 - 8.24 * Year + 0.032 * Depth - 0.0014 * TP + 0.03 * TN - 0.09 * Secchi + 0.445 * Temp + 0.262 * RegAlk$$

For verification of the above model equation, we then used the data from the verification data set 2; and the predicted values of Chla model are then compared to the observed monitoring station values. The model was found to have $R^2= 0.0065$, this is a low value, and this means that our model isn't of a good fit. Thus, the process is repeated again using a different set of input variables, and this continues till a model with a good fit is found. The process of finding the right input data set is a time consuming process, and we may not end up with the right set of variables, because the input variables are highly correlated as seen from the correlation matrix.

4.6.2 Neural network analysis

Unlike other modeling techniques, NN does not generate a model with coefficients but instead produces multilayer neural interconnected processing units that imitate human brain activity, where each neuron in a layer is connected to every neuron in the next layer. Figure 4.13 shows a single neuron in a neural network. The output of the NN model is weights that are saved as an xml file; the file can be then used in forecasting and verification of a different data set.

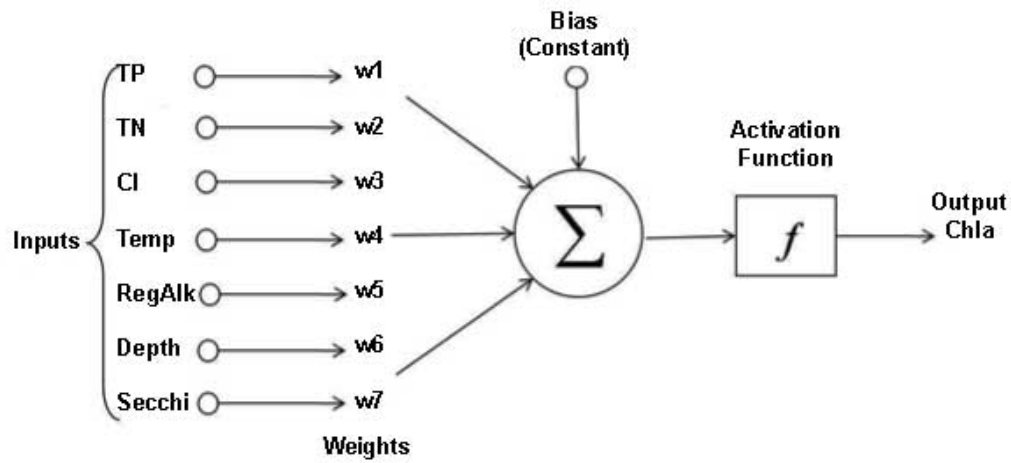


Figure 4.13 Neuron in a neural network (Bishop, 2006)

In NN, the input data goes through the NN model where it is multiplied by the weights (brain) in a forward direction, the information is then processed and the output is compared with the observed value. The resulting error from the comparison is back propagated and becomes an input for the next prediction while the model weight (brain) is adjusted to minimize the error, via several iterations. The data is plotted as a variable importance chart, which shows the impact of the variable to the model, and also as a synaptic weight chart which shows the influence of the neuron (Iyer et al., 2013).

4.6.3 Data mining

Also known as BLACK BOX MODEL, because it is computer written sophisticated algorithms to reveal and extract hidden information from a data set (Maimon and Rokach, 2011, Data Mining and Knowledge Discovery Handbook). Data mining technique is employed in this study to:

- A. Estimate the equations for the independent input parameters that were discontinued from the monitoring program or newly introduced, in an attempt to fill the gaps within the data.
- B. Estimating the nonlinear regression equation of the combined chemical and biological parameters for Chlorophyll-a.

4.6.4 Geostatistical analysis

ArcGIS version 10.1-geostatistical analysis package was used to investigate the impact of lake location on cyanobacterial algal bloom in lake Champlain. Two files were needed for the analysis are derived from:

- 1) Lake Champlain LTM QAPP/Work Plan Document Revision 1.4 provided the geographical locations information for the monitoring stations.
- 2) The ArcGIS map shape file for lake Champlain, was partially available in the United States USGS Water Resources web site (water.usgs.gov; accessed on Dec 2012). However, a big section of the lake polygon was missing. Figure 4.14 shows a summary of the steps used to create the lake polygon file, where firstly, the none relevant information was removed from the USGS file, then USGS map was edited using the US topology map as a background image to manually draw the missing parts for the northern and southern parts of the lake. Finally, the entire lake shape was combined into one polygon for GIS analysis. The longitude and latitude information was added to the lake data file and imported into ArcGIS.

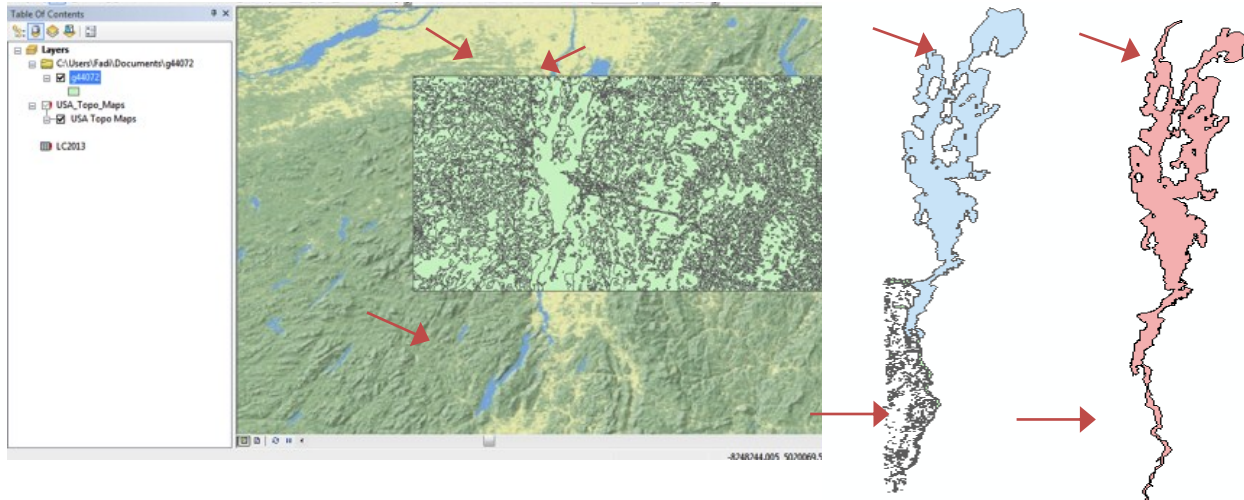


Figure 4.14 Lake Champlain polygon creation.

Spatial analysis utilizes location information in the relationships, so if the data set under investigation changes with location, then spatial analysis will reveal this information when running the OLS regression test. The OLS tool is available through ArcToolbox menu from ArcMap, If the location was found to be important then by using geographically weighted regression (GWR) analysis, we can develop a linear regression model which will have the location as one of its input variables. The OLS test is only valid when we have found the best MLR model. OLS does not have the stepwise selection option which was available in SPSS, so the OLS test does not know which set of input variables will produce the best regression model.

The variance inflation factor (VIF) value from the OLS test can help to determine if a variable is important to the model or not, a VIF value > 7.5 indicates that the input variable is redundant and should be omitted from the model. Although the OLS test does not consider the location as an input, it automatically runs a test to determine the location importance for the linear regression modeling. The Koenker statistic test is the one to determine the locations importance: if the p-value < 0.05 , then the model equation is likely to change with the locations across the study area. In this case we should consider the location as an input variable and use GWR analysis instead.

Since stepwise selection is not available as in IBM SPSS, several iterations are need before reaching significant a model. Alternatively, time can be saved by directly using the input variables set obtained using the stepwise in IBM MLR

CHAPTER 5

LAKE CHAMPLAIN CHLOROPHYLL- A STATISTICAL MODELING RESULTS

5.1 Correlation Matrix Analysis Results

The result of the cross correlation analysis are presented in table 5.1 and figure 5.1 for the first part of the study, which examined the relationship and impact of seven independent water quality parameters (variables; yearly data) on the dependent variable, chlorophyll-a (a biomarker for cyanobacteria algal blooms; CABs) in lake Champlain.

VARIABLE	YEAR	DEPTH	TP	CL	TN	TEMPC	SECCHI	REGALK	CHLa
YEAR	1.000								
DEPTH	-0.026	1.000							
TP	0.096	-0.484	1.000						
CL	-0.243	0.125	-0.147	1.000					
TN	-0.086	-0.229	0.703	-0.398	1.000				
TEMPC	-0.064	-0.107	0.116	-0.085	-0.041	1.000			
SECCHI	-0.274	0.402	-0.894	0.088	-0.562	-0.117	1.000		
REGALK	0.070	-0.130	0.432	0.731	-0.069	0.003	-0.460	1.000	
CHLa	0.057	-0.341	0.803	-0.328	0.734	0.093	-0.757	0.127	1.000

Table 5.1 Pearson's correlation matrix.

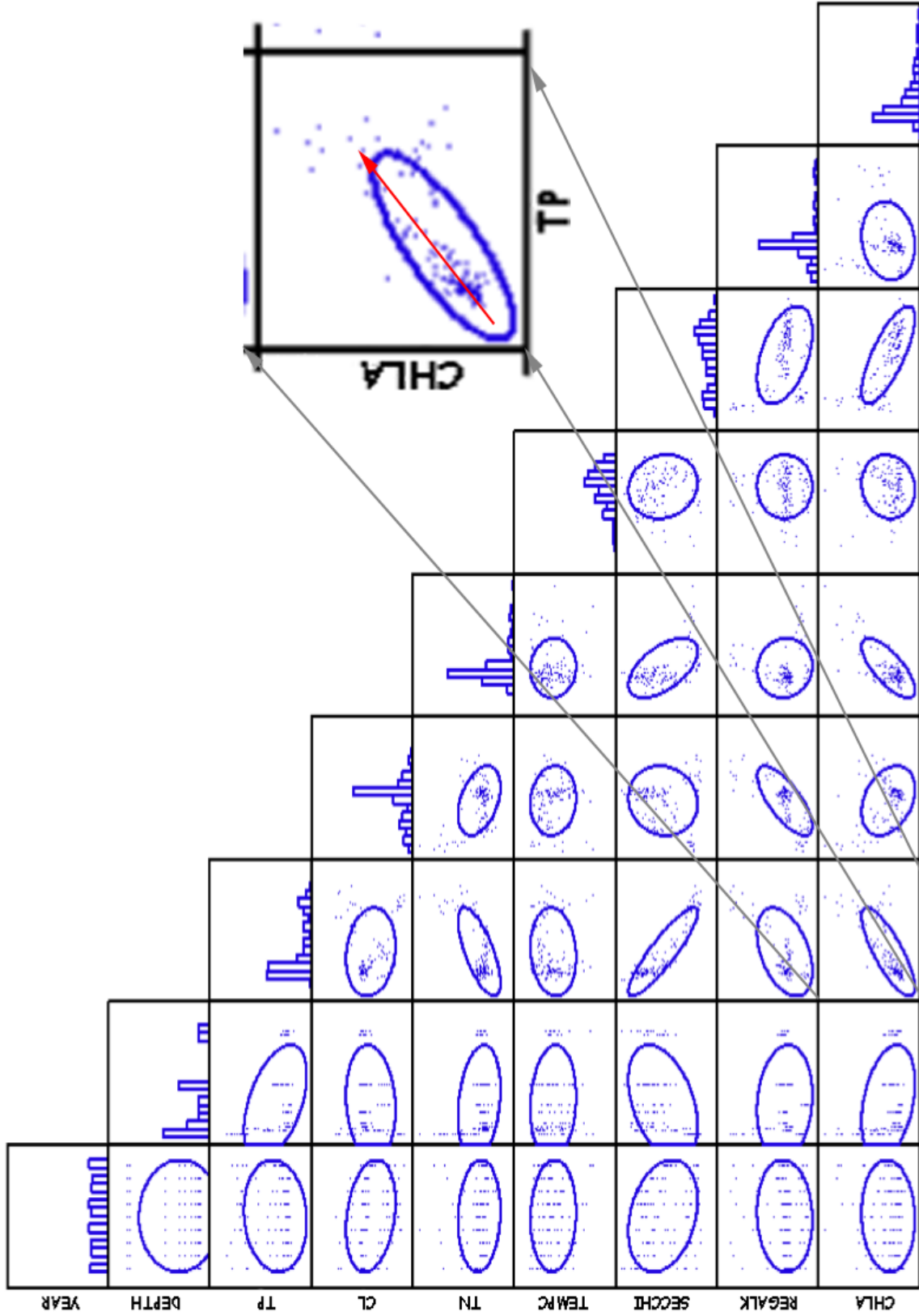


Figure 5.1 Cross correlation scatter plots showing the relationship between the 8 independent water quality variables (lake Champlain yearly data) and the dependent variable chlorophyll-a (at the bottom). Abbreviations: Date, 1992-2011 (YEAR); total phosphorus (Tp); Chloride (CL); total nitrogen (TN); temperature in degrees C (TE MPC); Secchi depth (SECHI); Alkalinity (REGALK); chlorophyll-a (CHLA).

As expected, the cross correlation analysis indicated:

- 1) A significant strong positive linear relationship between the assumed independent variable total phosphorus (TP; $r=0.803$), a nutrient for CABs growth (Correll, 1998), and the dependent variable chlorophyll-a.
- 2) A significant strong positive linear relationship between the assumed independent variable total nitrogen (TN; $r=0.734$), a nutrient for CABs growth (Correll, 1998), and the dependent variable chlorophyll-a.
- 3) A significant strong negative linear relationship between the independent variable secchi depth ($r=-0.757$), a measure of water clarity (Prescott, 2006) which is reduced by the growth of CABs (George et al., 2010), and the dependent variable chlorophyll-a.

Also as expected, the analysis confirmed:

- 4) A significant strong positive linear relationship between two of the independent variables, total phosphorus (TP) and total nitrogen (TN) ($r=0.703$), because they are both nutrients for CABs growth (John A. Downing et al., 1992).
- 5) A significant strong negative linear relationship between the assumed independent variable secchi depth (water clarity) and the assumed independent variable total phosphorus (TP; $r=-0.894$).
- 6) A less significant trend towards a negative linear relationship between the assumed independent variable secchi depth (water clarity) and the assumed independent variable total nitrogen (TN; $r=-0.562$).

These results suggest that our modeling approach should be successful if we assume that the levels of total phosphate (TP) and total nitrogen (TN) are indeed positively linearly related to chlorophyll-a/CAB growth, and that conversely, secchi depth is negatively linearly related to chlorophyll-a/CAB growth.

5.2 Determination of Analysis Data Set

I used MS Excel and Matlab to analyze lake Champlain yearly data over two different time periods:

- 1) Early years yearly dataset: 1992-2002.
- 2) Later years yearly dataset: 2003 to 2011.

The early years and later years datasets were tested as either the training dataset or the verification dataset for my modeling study, and the later years dataset worked better as a training data set. This was because several new important monitoring stations were set up during the later years time period, and the additional data from these stations improved the accuracy of the models. Therefore, the later years yearly dataset was chosen for constructing the chlorophyll-a models, and the early years dataset was used to verify the models.

5.3 Chlorophyll-a Modeling Using Multiple Linear Regression (MLR)

5.3.1 SPSS statistical analysis:

It is statistical software package that was used to analyze the lake Champlain later year dataset as the model training dataset, with the critical value for the models = 95%, the error range = -1.96 to 1.96 (models with errors outside this range were rejected). The assumed independent 7 variables used for modeling were those listed in table 4.1 The dependent variable was chlorophyll -a (a biomarker for cyanobacteria algal blooms; CABs). The Stepwise selection feature in IBM SPSS software was used to determine whether each input variable was significant for the model or not. The results of this modeling analysis are shown in table 5.2 and the chlorophyll-a (Chla) MLR coefficients of the lake Champlain MLR models are presented in table 5.3.

5.3.2 ANOVA analysis of the variance of the MLR models

ANOVA provides a method to judge between the different models. Table 5.4 shows the results of the ANOVA and variance analysis, which indicated that although all six MLR models found were significant ($p = 0.00$), the last two models (models #5 and #6) had the smallest error mean square, meaning that of the all models, these provided the more accurate predictions.

5.3.3 Multiple linear regression (MLR) results

MLR model number #6 (table 5.2, yellow highlighted cells) was found to be the most accurate chlorophyll-a model, because it had the smallest ANOVA error mean square, highest Pearson product-moment correlation coefficient ($R = 0.925$), indicating the strength of the linear relationship between the variables; the highest coefficient of determination (R^2 value = 0.857), indicating the goodness of fit of the linear model; the highest adjusted R^2 value = 0.854, is also indicating goodness of fit of the linear model (but it avoided the biased errors that sometimes result from calculating R^2); and the lowest standard error = 1.80, indicating how good the estimation from the linear regression model is, as the error in the sample mean with respect to true mean was low.

MLR model #6 results were that 4 of the 7 tested (assumed) independent water quality variables were significant predictors of chlorophyll-a levels over the Later years time period (2003-2011), and thus of CABs growth. Two variables were positively correlated with chlorophyll-a levels (total phosphate (TP) and total nitrogen (TN)), and a third variable was negatively correlated with chlorophyll-a levels (secchi depth; secchi; water clarity). These results supported the results of the correlation analysis (section 5.1), in agreement with the scientific literature (Brown et al., 2012).

MLR model #6 results revealed that Chloride (Cl) was a fourth new significant predictor of chlorophyll-a (Chla), which was negatively correlated with Chla. This result was not obtained with the correlation analysis (section 5.1) and is in agreement with the scientific literature (Shillito et al., 1992).

MLR models #2 to #6 indicated that total phosphorus (TP) was the most significant predictor of chlorophyll-a levels and therefore CABs growth, which is supported by most of the scientific literature (Correll, 1998).

Time (date: over the range 2003-2011) was not found to be a predictor for any of the MLR models, suggesting that the above four variables (TP, TN, Secchi, Cl) were significant predictors of chlorophyll-a levels (and CABs growth) over the entire time period of 9 years, and potentially generally useful predictors which should be tested with historically earlier and later data.

Therefore, MLR model #6 was chosen for further studies (verification and validation) and its equation is shown below:

$$\text{Chla} = 4.13 + 0.07 * \text{TP} - 14.9 * 10^{-5} * \text{Cl} + 0.01 * \text{TN} - 0.70 * \text{Secchi} \quad \text{Eq. 5.1}$$

MLR model #	R	R ²	Adjusted R ²	Std. Error of the Estimate	Predictors
1	0.452	0.204	0.194	3.3741	Constant, Depth
2	0.839	0.704	0.694	2.0740	Constant, Depth, TP
3	0.838	0.702	0.690	2.0704	Constant, TP
4	0.874	0.763	0.761	1.9435	Constant, TP, Cl
5	0.910	0.828	0.825	1.8620	Constant, TP, Cl, TN
6	0.925	0.857	0.854	1.8040	Constant, TP, Cl, TN, Secchi

Table 5.2 Lake Champlain MLR modeling results for (2003-2011). Abbreviations used: monitoring depth (Depth); total phosphorus (TP); chloride (Cl); total nitrogen (TN), secchi depth (Secchi).

MLR model #		Unstandardized Coefficients		t	Sig.	95.0% Confidence Interval for B	
		B	Std. Error			Lower Bound	Upper Bound
1	(Constant)	7.185092	0.427	16.808	0.000	6.339	8.031
	Depth	-0.039765	0.010	-4.183	0.000	-0.059	-0.021
2	(Constant)	0.782799	0.518	1.510	0.134	-0.244	1.809
	Depth	0.007074	0.007	1.056	0.293	-0.006	0.020
	TP	0.205891	0.014	14.324	0.000	0.177	0.234
3	(Constant)	1.185673	0.351	3.373	0.001	0.490	1.881
	TP	0.198475	0.013	15.815	0.000	0.174	0.223
4	(Constant)	4.448068	0.830	5.360	0.000	2.805	6.091
	TP	0.187970	0.012	15.654	0.000	0.164	0.212
	Cl	-0.000233	0.000	-4.283	0.000	0.000	0.000
5	(Constant)	0.341967	1.427	0.240	0.811	-2.482	3.166
	TP	0.145900	0.017	8.725	0.000	0.0113	0.179
	Cl	-0.000145	0.000	-2.508	0.013	0.000	0.000
	TN	0.009236	0.003	3.466	0.001	0.004	0.015
6	(Constant)	4.131727	1.874	2.205	0.029	0.421	7.842
	TP	0.070080	0.030	2.331	0.021	0.011	0.130
	Cl	-0.000149	0.000	-2.652	0.009	0.000	0.000
	TN	0.010803	0.003	4.101	0.000	0.006	0.016
	Secchi	-0.701711	0.234	-2.994	0.003	-1.166	-0.238

Table 5.3 Chlorophyll-a (Chla) MLR coefficients of the six lake Champlain MLR models.

The best model, MLR model #6, had four independent significant variables (all close to zero). The t- test was used to check the significance of each of the regression coefficients of the models. It was clearly noted that adding a significant variable to a regression model makes the model more effective, for example model #6 was more significant than model #5 because it had more significant variables. The confidence interval (CI) for the coefficients was the smallest for model #6, indicating that this was the best model, since the error limit boundary for accepting or rejecting a model was small for all the variables.

MLR model #		Sum of Squares	df	Error Mean Square	Sig	F	
1	Regression	199.220	1	199.220	0.000	17.499	Constant, Depth
	Residual	1411.707	124	11.385			
	Total	1610.926	125				
2	Regression	1081.807	2	540.904	0.000	125.739	Constant, Depth, TP
	Residual	529.119	123	4.302			
	Total	1610.926	125				
3	Regression	1077.006	1	1077.006	0.000	250.128	Constant, TP
	Residual	533.921	124	4.306			
	Total	1610.926	125				
4	Regression	1146.290	2	573.145	0.000	151.725	Constant, TP, Cl
	Residual	464.636	123	3.778			
	Total	1610.926	125				
5	Regression	1187.946	3	395.982	0.000	114.213	Constant, TP, Cl, TN
	Residual	422.980	122	3.467			
	Total	1610.926	125				
6	Regression	1217.124	4	304.281	0.000	93.494	Constant, TP, Cl, TN, Secchi
	Residual	393.802	121	3.255			
	Total	1610.926	125				

Table 5.4 ANOVA analysis of the six lake Champlain MLR models

5.3.4 Discussion of MLR model # 6

A. Elimination of data with non-random high errors

As explained in section 4.5.C the lake Champlain yearly water quality monitoring data for the period early years (1992-2002) was used for verification of MLR model #6. The verification data set produced an $R^2 = 0.812$, which is lower than the $R^2 = 0.857$ obtained from the MLR training dataset. Examination of the standard error distribution histogram in figure 5.2 revealed that the model errors had a uniform distribution with few errors outside of the standard distribution range. Plotting the model #6 predicted Chla values against the model's observed values (figure 5.3 and figure 5.4), revealed that most of the model #6 prediction errors were obtained from lake Champlain monitoring stations 02, 04, 50 and 51, and these errors were not

random, as shown in (figure 5.4). Omitting the data from stations 02, 04, 50 and 51 from the verification data set, improved the R^2 to 0.829, which suggested further investigation of this data.

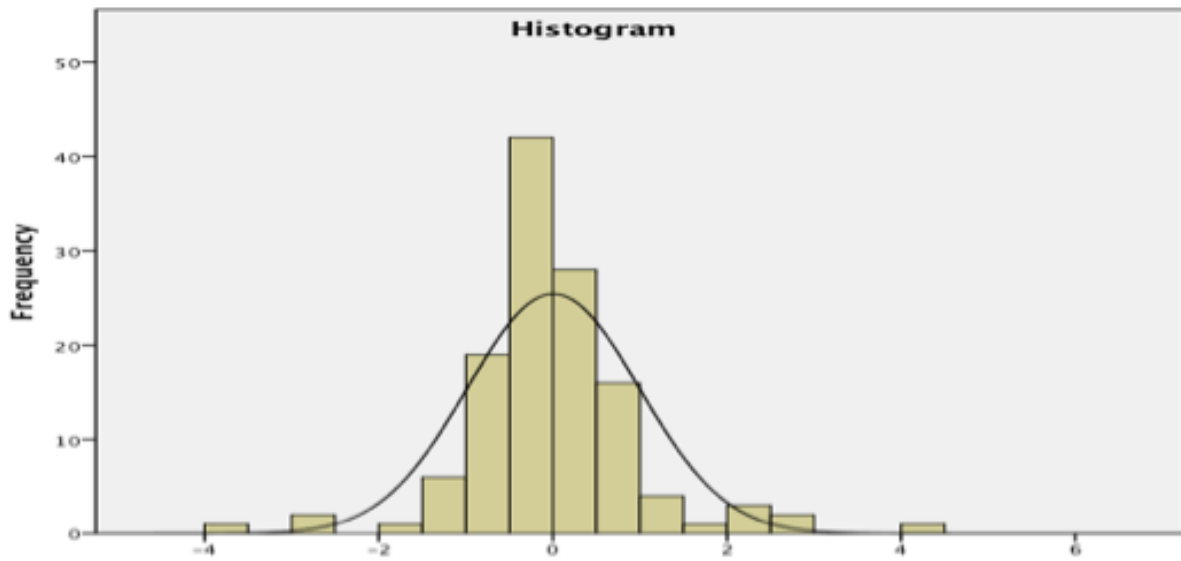


Figure 5.2 MLR model #6 standard error distribution

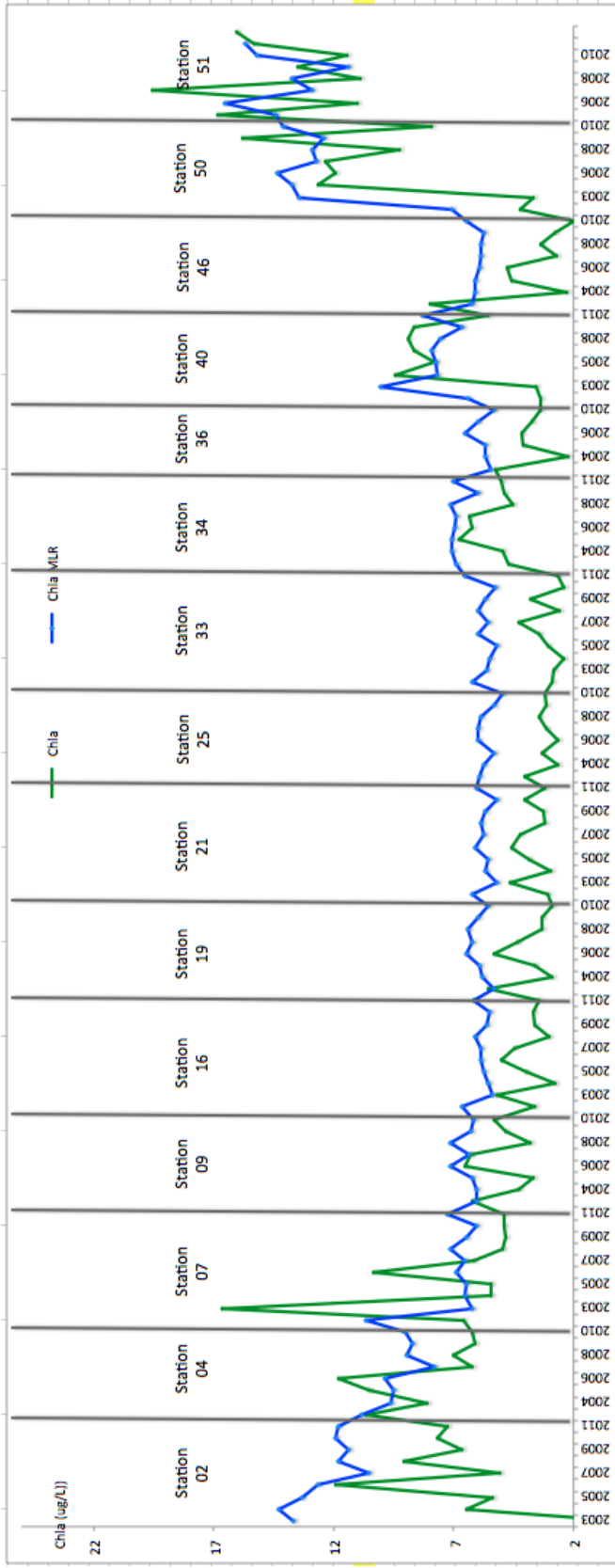


Figure 5.3 Lake Champlain chlorophyll-a levels by years (2003-2011) with MLR. $R^2=0.857$, showing the actual monitoring station data (Chla; green line), compared to the MLR model #6 predicted chlorophyll-a values (Chla MLR; blue line). The data from stations 02, 04, 50 and 51 had large errors that were non-random

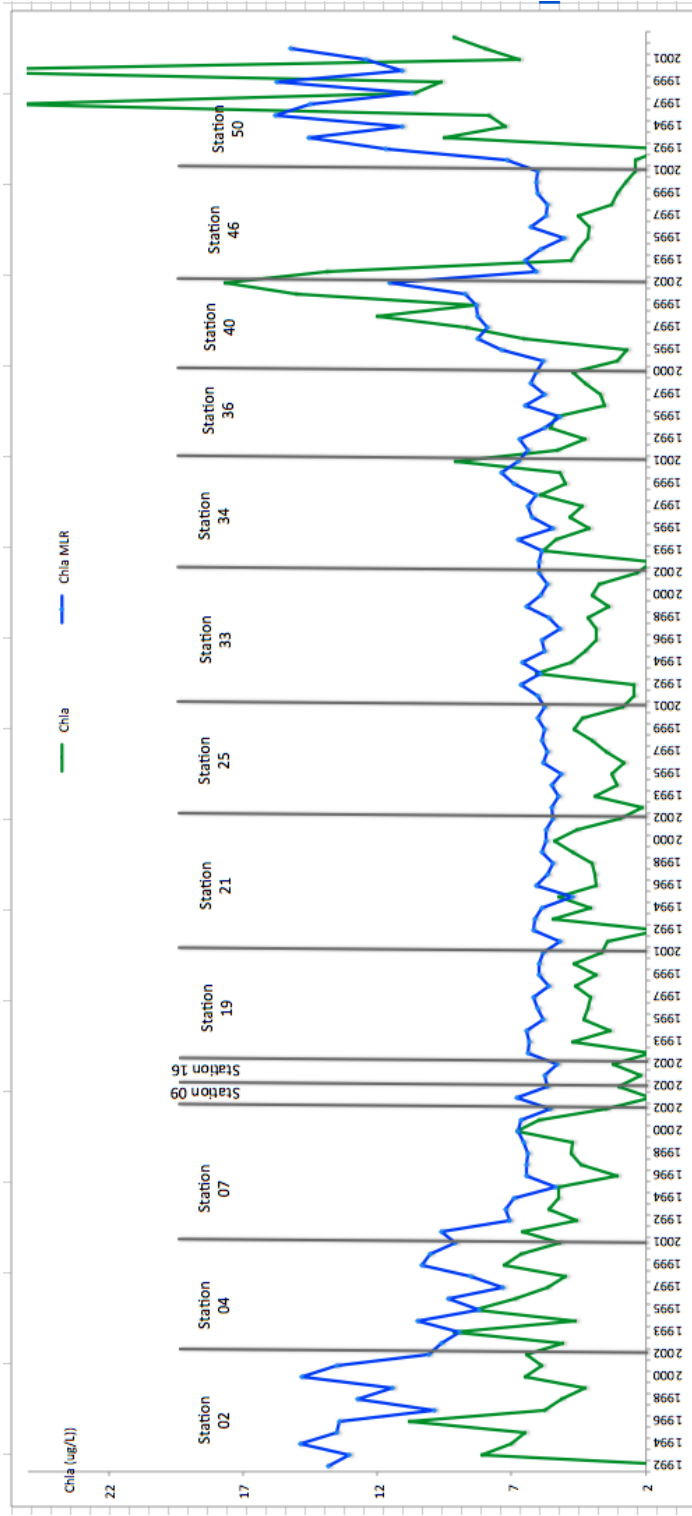


Figure 5.4 Lake Champlain chlorophyll-a levels by years (1992-2002) with MLR. $R^2=0.812$, showing the actual monitoring station data (Chla; green line), compared to the MLR model #6 predicted chlorophyll-a values (Chla MLR; blue line). The prediction for stations 02, 04, 50 and 51 also had large errors, which were non-random

B. Bootstrapping

According to IBM SPSS software documentation, bootstrapping is a process that can improve modeling results by making them more accurate, by revealing more information about the properties of estimators for “unknown” populations and ill-behaved parameters.

Bootstrapping was used on the lake Champlain early years yearly data and generated the eight models shown in table 5.5.

Model#	R	R ²	Adjusted R ²	Std. Error of Estimate	Sig	Predictors
1	0.303	0.090	0.070	3.589	0.315	Constant, Year
2	0.601	0.360	0.216	3.375	0	Constant, Year, Depth
3	0.905	0.820	0.764	2.081	0	Constant, Year, Depth, TP
4	0.921	0.849	0.812	1.927	0	Constant, Year, Depth, TP, Cl
5	0.926	0.859	0.828	1.873	0	Constant, Year, Depth, TP, Cl, TN
6	0.927	0.86	0.826	1.879	0	Constant, Year, Depth, TP, Cl, TN, TempC
7	0.934	0.873	0.848	1.802	0	Constant, Year, Depth, TP, Cl, TN, TempC, Secchi
8	0.934	0.874	0.849	1.805	0	Constant, Year, Depth, TP, Cl, TN, TempC, Secchi, RegAlk

Table 5.5 Lake Champlain early years data, bootstrapping model results

Bootstrapping option is only available in IBM SPSS when stepwise modeling option is disabled; therefore, the predictors in table 5.5 appear in an increasing order. Also It can be seen that bootstrapping did not significantly improve R², slight increase is due to the increase number of variables in the model, more important the resulting models haven't produced better predictions for stations 02, 04, 50 and 51.

It appears that MLR models are not accurate at high water quality variable (nutrient) levels, further modeling analysis for stations 02 and 04 model using 2002-2011 yearly data, resulted in following MLR model equation with R²= 0.488:

$$\text{Chla} = 16.346 - 4.65 * 10^{-3} * \text{Cl} \quad \text{Eq. 5.2}$$

R²= 0.488 is relatively low, however an interesting finding is that the water quality parameter Chloride (independent variable) which was negatively correlated with chlorophyll-a, was the only variable found to affect the chlorophyll-a model for the Southern section of lake Champlain. This suggested the presence of high levels of Chloride in the Southern sections. Further investigation confirmed this finding and revealed high chloride concentrations at Station

04 that were coming from the river mouth and from road runoff were affecting the accuracy of model #6.

Supplementary MLR model analysis was conducted using data for stations 50 and 51 (2002-2011 yearly data), and the following model equation was found with $R^2 = 0.329$

$$\text{Chla} = -2.973 + 0.024 * \text{TN} \quad \text{Eq. 5.3}$$

R^2 is relatively low, but another interesting finding is that the only variable influenced chlorophyll-a in the model was the total Nitrogen (TN) which positively correlated with chlorophyll-a concentrations, thus indicating high levels of nitrogen in the northern sections of lake Champlain.

This high lake water chloride concentrations in the south and the high lake water nitrogen concentrations in the north are a major factors for the reduced accuracy of MLR model #6 and possibly a main reason behind the errors in MLR model.

5.4 Lake Champlain Chlorophyll-a Modeling Using Multiple Nonlinear Regression (MNR)

Analysis of the lake Champlain early years yearly data was not possible using this method because each of the lake monitoring stations has a different chlorophyll-a data distribution, so no common function could be defined to proceed with the analysis (see appendix C).

5.5 Lake Champlain Chlorophyll-a Modeling Using Neural Networks (NN)

Several studies suggested using neural networks (NN) to provide effective chlorophyll-a prediction (Karul, et al., 1999). The IBM SPSS multilayer perceptron (MLP) NN tool was used to explore NN models using the lake Champlain monitoring station data. As described in methods section 4.6.2, the dataset was split and used as follows:

1) Approx. 70% of the later years (2003-2011) yearly data was used to create the NN models, while the remaining 30% of the data was used to simultaneously verify each model as it was

created. After reviewing the literature, I found that most references suggest that for large amounts of data, the data should be split 50% for training the models and 50% for verification of the models. The literature also suggested that for handling smaller amounts of data, splitting it 70% for training models and 30% for verification models was best (Oded et al., 2010)

2) The results of the NN model analysis of the lake Champlain water quality monitoring data are shown in Figures 5.5 and 5.6. Coefficient of determination for NN model #8 is $R^2 = 0.851$.

3) Early years (1992-2002) yearly data was used to verify NN model #8.

NN importance chart (figure 5.5, top panel) is a measure of how much the network's model-predicted value changes for different values of the independent variable; and this value is divided by the largest value present them as a percentage. The results of the analysis showed that the independent variable total phosphorus (TP) had the greatest effect on how the network classifies chlorophyll-a models, followed by the variables secchi depth (Secchi; relative importance (ri =40%), chloride (Cl; ri=20%) and total nitrogen (TN; ri=20%). Interestingly, the NN analysis suggested that RegAlk was also important (ri=30%). The remaining variables tested were considered relatively unimportant (ri <20%). These results agree with the earlier MLR modeling study (section 5.3) and also agree with the correlation analysis (section 5.1). They also do agree with the published literature (Karul et al., 1999).

A plot of the observed Chla data verses NN model predicted Chla values are shown in figure 5.5 (bottom panel). It can be seen that the error in prediction using NN model #8 is low for low to moderate Chla levels (<10 $\mu\text{g/L}$) and the prediction becomes less accurate at higher Chla levels (>10 $\mu\text{g/L}$). This is in good agreement with the MLR modeling study results (MLR model #6, section 5.3)

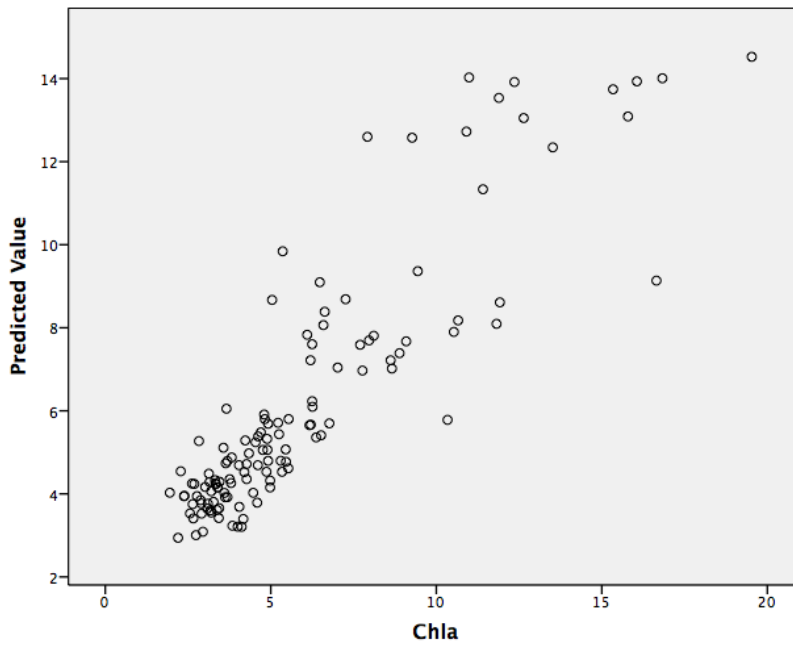
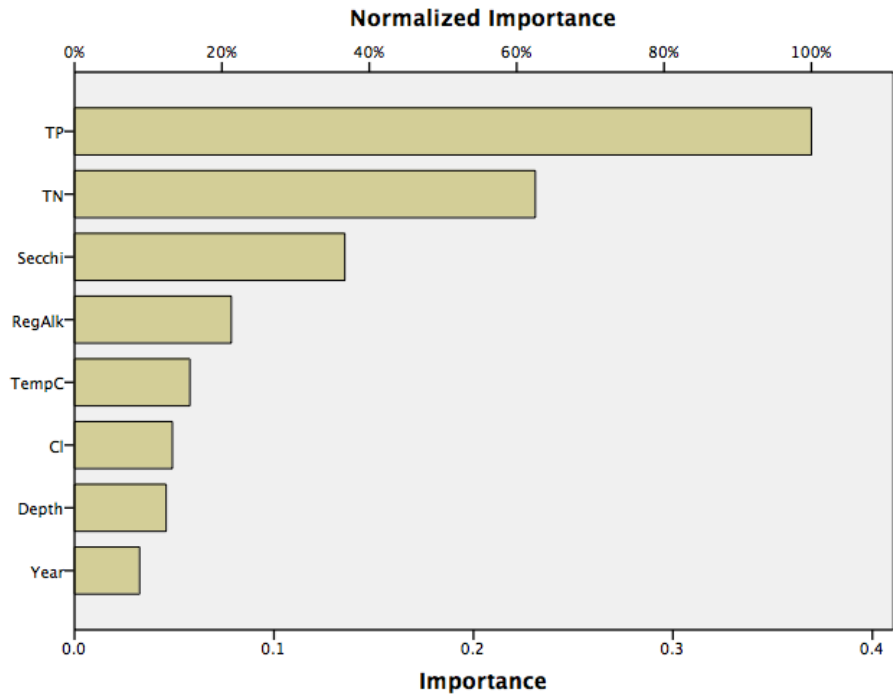


Figure 5.5 NN analysis water quality variables importance chart (top panel) and Chla observed values vs. NN model #8 predicted values for Chla in $\mu\text{g/L}$ (bottom panel).

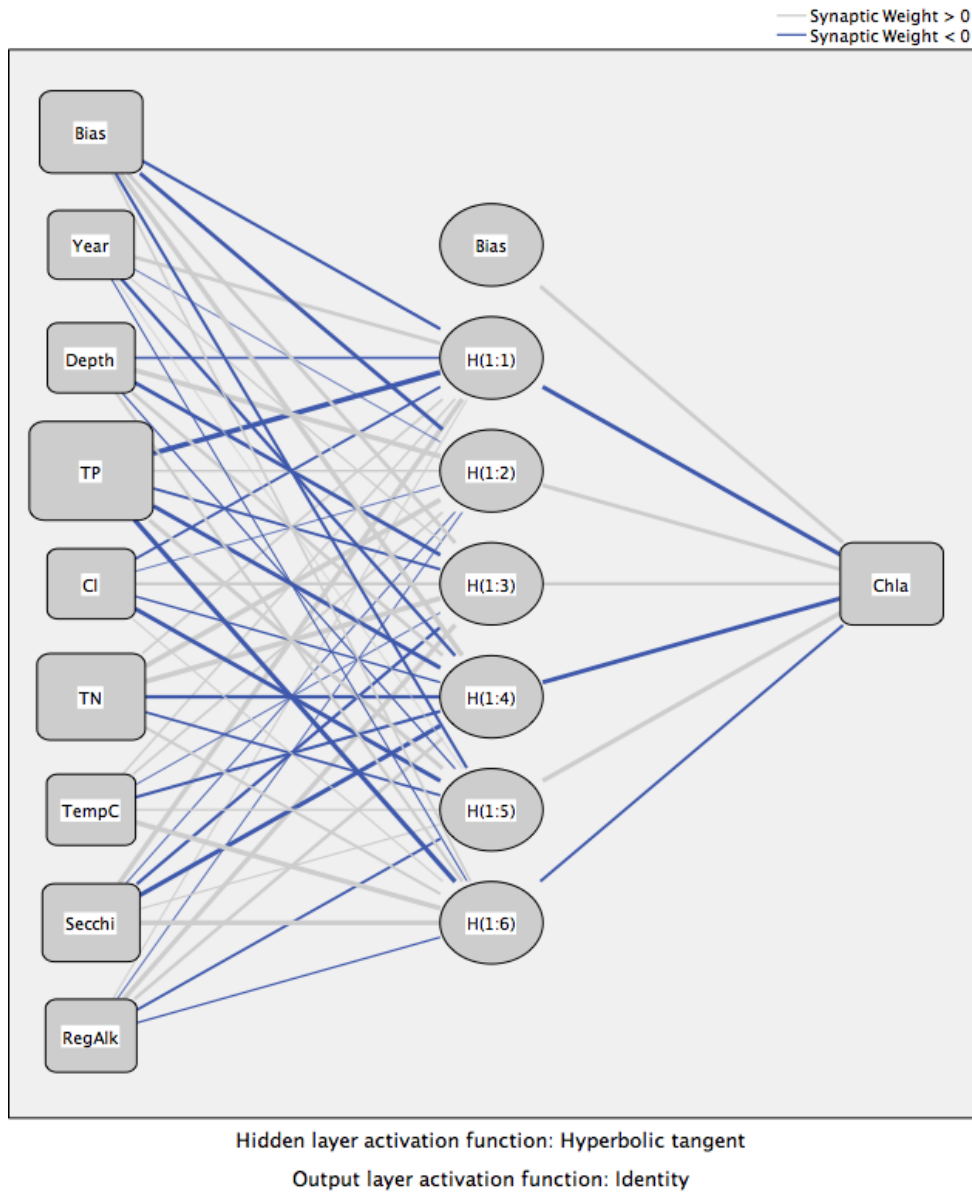


Figure 5.6 NN synaptic weight chart for lake Champlain later years data (2003-2011) model #8

Figure 5.6 displays the results of the NN synaptic weight chart which shows the feed forward NN chlorophyll-a model architecture as connections flowing forward from the input layer to the output layer without any feedback loops.

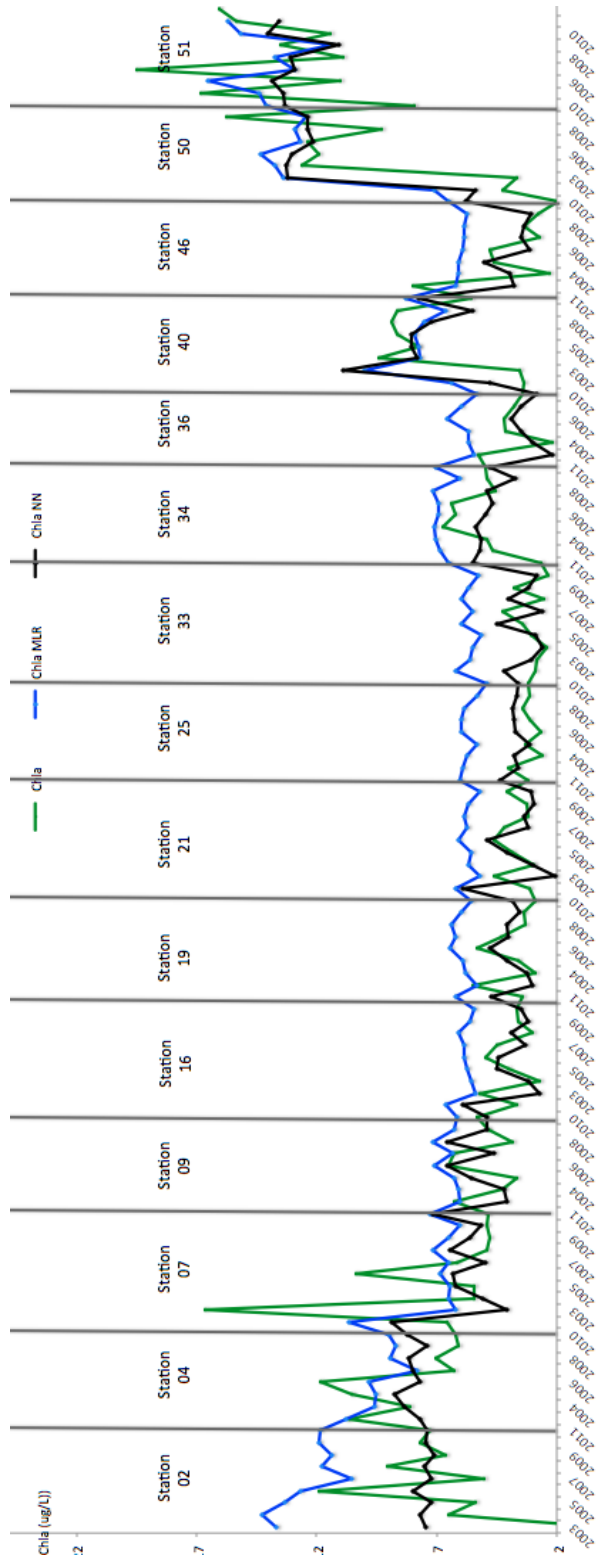


Figure 5.7 Lake Champlain chlorophyll-a levels by years (2003-2011), NN model $R^2=0.851$
 Observed lake Champlain monitoring data (Chla, green line), compared to predictions generated using two chlorophyll a models (MLR model #6 (blue line) and NN model #8 (black line), using the same datasets

5.5.1 NN model #8 verification

To verify NN model #8 ($R^2=0.851$), which was created using the lake Champlain monitoring station later years variable data (2003-2011)(see section 5.5), the model was tested with variable data from lake Champlain early years (1992-2002). NN model #8 results were compared with: 1) the actual observed results (Chla); and, 2) MLR model #6 results (section 5.3) as shown in figure 5.8

Although the NN model #8 verification for the years between 1992-2002 resulted in ($R^2=0.795$) which is lower than verification of the MLR model #6 ($R^2= 0.812$) for the same period, however it produced a better fit since the average absolute error between the NN model #8 curve and the observed Chla data curve is less than 1.33, while for MLR model #6 the average absolute error between the MLR model #6 curve and the observed Chla data curve was 2.19, this can also be noticed on prediction results of figure 5.8

It should be noted that running the same data set using NN model #8 will result in a different NN model and result for each run, and this is due to the fact that NN is a learning algorithm that works by minimizing the error successively from the previous equation. Improving the NN results is an iterative and time-consuming process. Previous studies suggested manipulating the number of layers and the ratio between the training and prediction data. I have already implemented many of the recommended techniques to improve the prediction of the NN model, but since NN does not produce any modeling equation, I decided to present only the best model (model #8) that I found from the NN analysis.

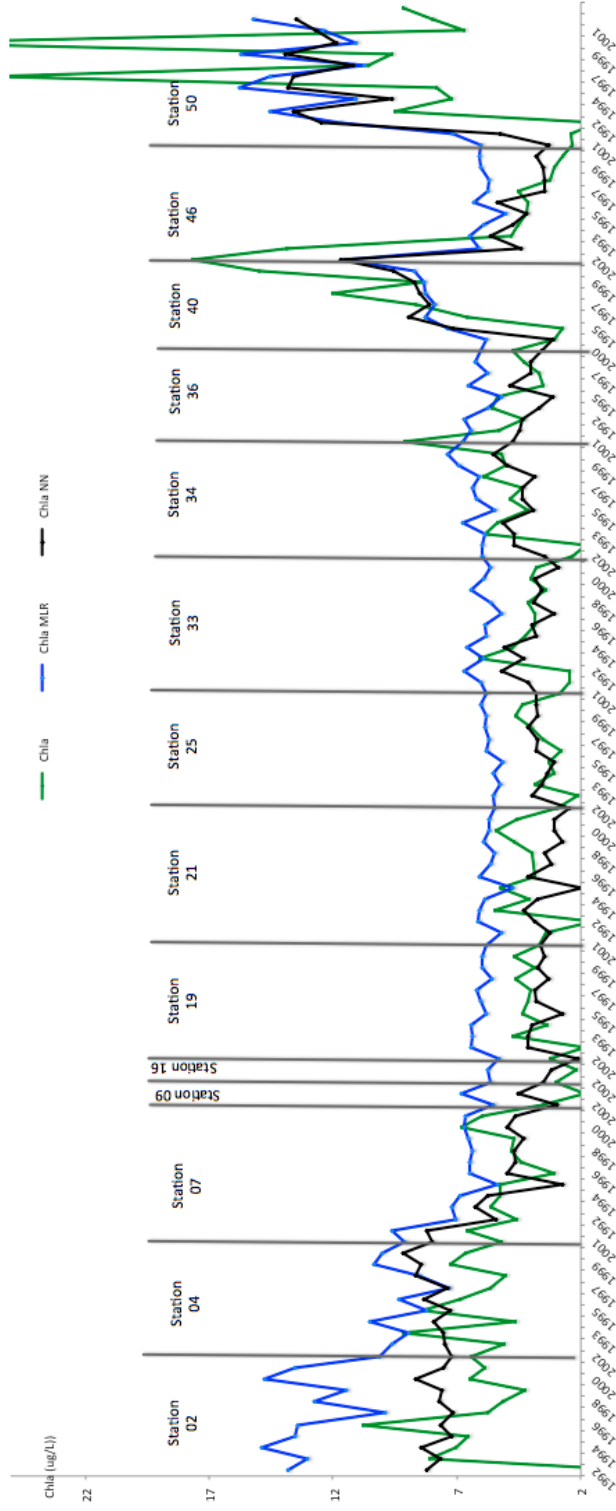


Figure 5.8 Lake Champlain chlorophyll-a levels by years (1992-2002), NN model $R^2 = 0.795$
 Observed lake Champlain monitoring data (Chla, green line), compared to predictions generated using two chlorophyll
 a models (MLR model #6 (blue line) and NN model #8 (black line), using the same datasets

5.6 Lake Champlain Chlorophyll-a Modeling Using Data Mining (DM)

EUREQA DM software was used to analyze the lake Champlain total yearly dataset for all years (early years + late years: 1992-2011) and produced several models. The complete analysis is presented in appendix D. The best model found was arbitrarily named DM model #1 (figure 5.9) with a high goodness of fit ($R^2=0.815$), and is detailed in table 5.6.

5.6.1 DM modeling and water quality variables

Table 5.6 (left panel) shows the equation for DM model #1 which was produced after the Eureka DM software screened the lake Champlain total yearly dataset (1992-2011), which included all the seven water quality variables listed in Table 4.1. It was found that the following variables were the most significant and relevant variables for modeling and that these were related in a complex manner: total phosphorus (TP), secchi depth (water clarity), and total nitrogen (TN). This is in agreement with MLR model #6 results (section 5.3) and NN model #8 results (section 5.5).

DM model equation was nonlinear and the scatters plot for DM model #1 (table 5.6 indicates a uniform and small error distribution, which indicates the high accuracy of this model).

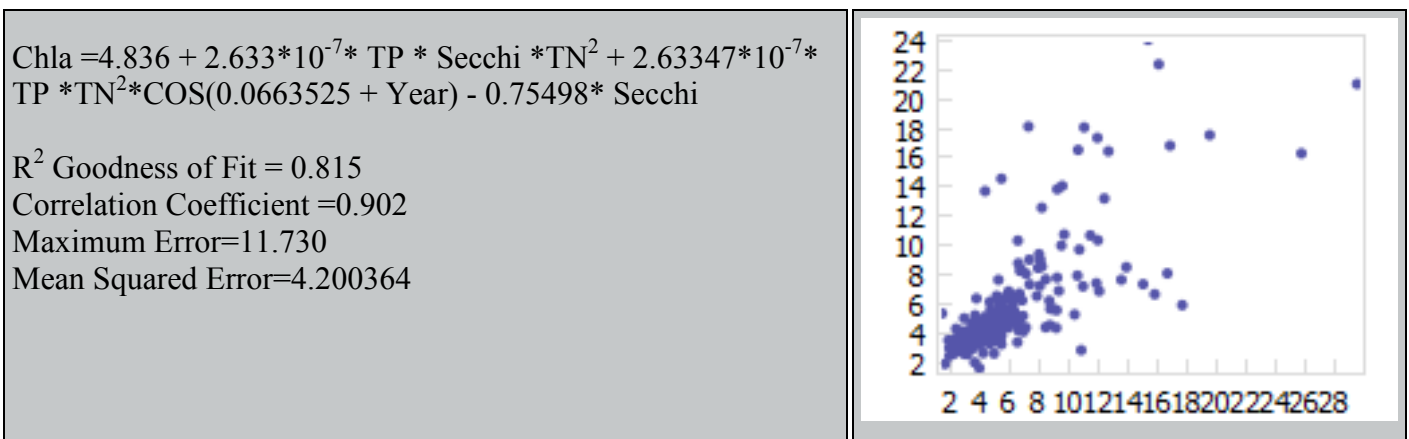


Table 5.6 Results of lake Champlain DM model #1 for (1992-2011)

5.6.2 Lake Champlain DM model #1 verification and comparison with MLR model #6 and NN model #8

The DM modeling equations should be among the best to provide an accurate prediction of lake Champlain chlorophyll-a levels, because the verification process immediately starts after each model is created. To confirm this, all three lake Champlain chlorophyll-a models (MLR model #6, NN model #8, and DM model #1) were compared with each other and with the observed data (see figure 5.9). For this study, the following variables and input datasets were used for the models detailed below.

- 1) Chlorophyll a MLR model #6 ($R^2 = 0.857$) was generated using lake Champlain later years (2003-2011) yearly dataset, which consisted of 50% of the total data, with 7 input variables, while the verification of Chlorophyll a MLR model #6 for the early year (1992-2002) resulted in ($R^2 = 0.812$)
- 2) Chlorophyll a NN model #8 ($R^2 = 0.851$) was generated using lake Champlain later years (2003-2011) yearly dataset. This model was created using 70% of the data, while 30% of the data was used to verify the model, with 7 input variables, while the verification of Chlorophyll a NN model #8 for the early year (1992-2002) resulted in ($R^2 = 0.795$)
- 3) Chlorophyll a DM model #1 ($R^2 = 0.815$) was generated using the lake Champlain total years early data set, which consisted of 50% randomly chosen values from the dataset (years 1992-2011) and the other 50% of this dataset was used to verify the model results, with 7 input variables, however the verification of Chlorophyll a DM model #1 for the early year (1992-2002) resulted in ($R^2 = 0.786$)

The results of this comparison indicated that NN model #8 predictions were more accurate than both MLR model #6 and DM model #1 predictions, by 48% and 12.8%, respectively, this results was obtained by comparing the errors resulted from the each model prediction with the actual observed data between the years of 1992-2002, furthermore all the three models are plotted against each other and against the observed Chlorophyll a data for the entire study period between 1992-2011 in figure 5.9

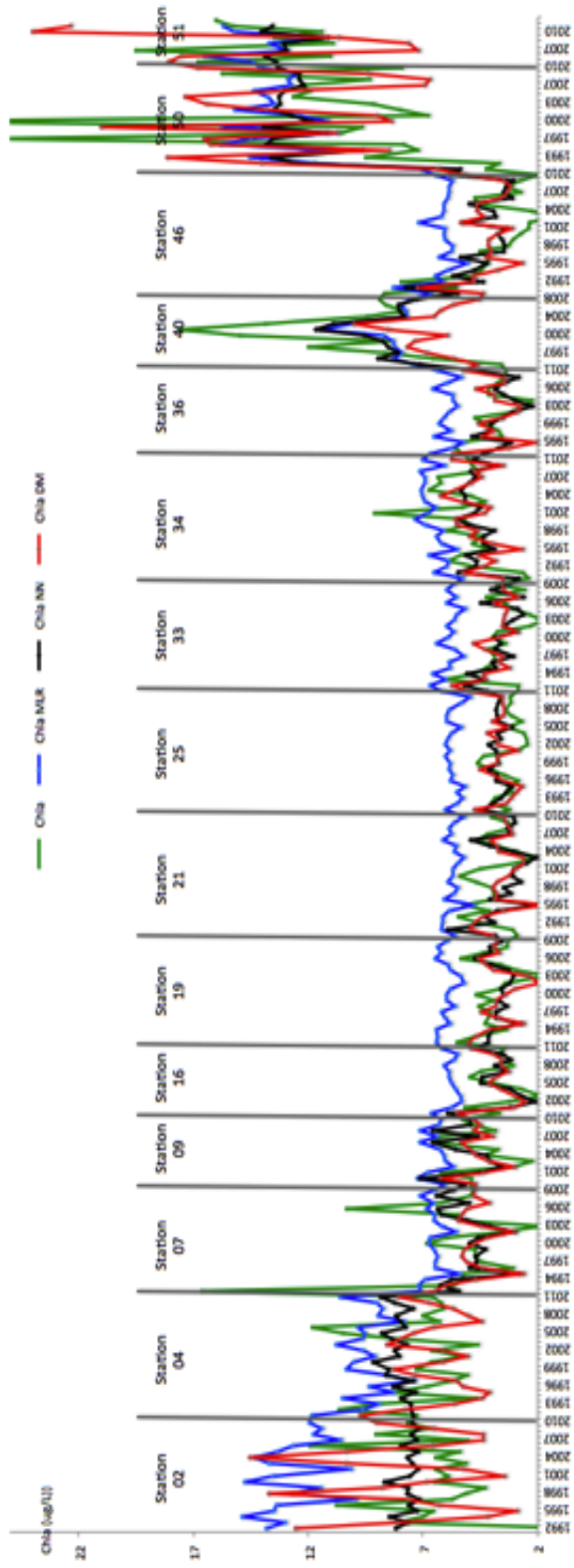


Figure 5.9 Observed lake Champlain monitoring data 1992-2010 (Chl, green line) compared to predictions generated using three chlorophyll-a models (MLR model #6 (blue line), NN model #8 (black line) and DM model #1 (red line), using the datasets, variables, and outlier conditions described in the text.

5.6.3 Comparison of chlorophyll-a DM, NN, MLR models with actual observations

At the beginning of writing this thesis, the lake Champlain data was only available till 2011, and recently in 2014 the data for the years of 2012 and 2013 were added, provided the ability to test and verify the different models that I developed for this lake using the 2012-2013 data (see figure 5.10).

We notice from figures 5.10, 5.11 and 5.12 that NN model #8 predicted results for chlorophyll-a levels were closer to the observed data than those of the other models tested, including MLR model #6 and DM model #1 using recent data for years 2012-2013. Mean absolute errors for MLR, NN and DM models were respectively 0.075, 0.053 and 0.068.

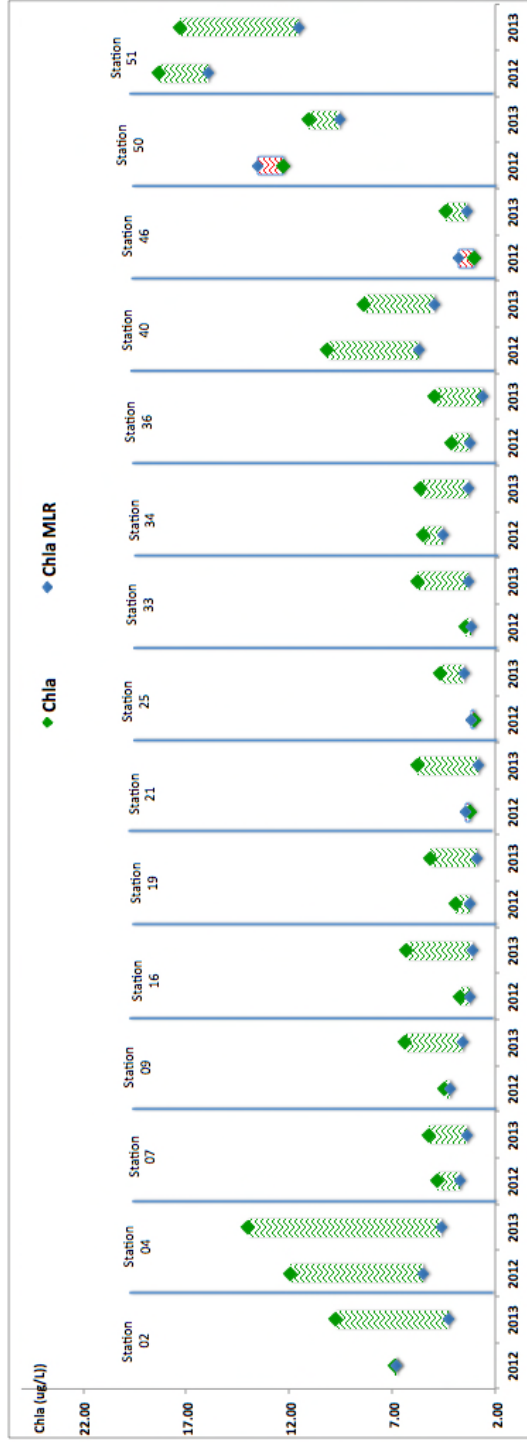


Figure 5.10 Observed lake Champlain monitoring data (2012 and 2013) compared to predictions from MLR model

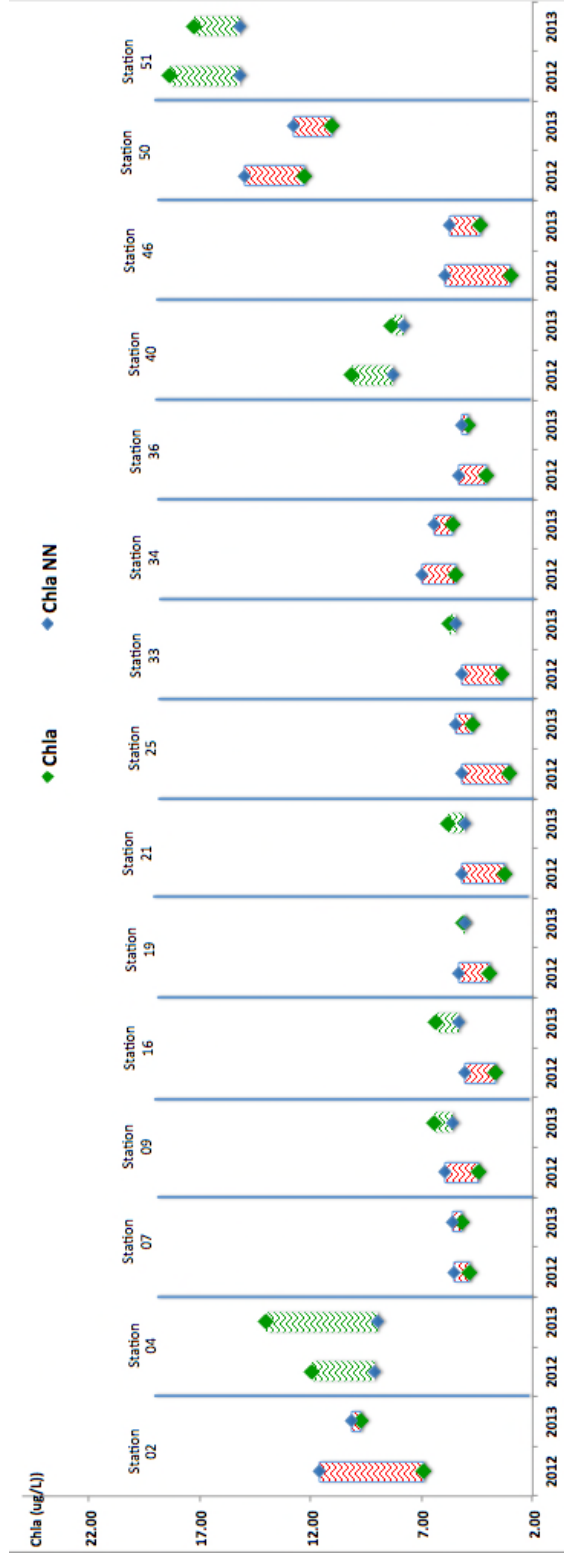


Figure 5.11 Observed lake Champlain monitoring data (2012 and 2013) compared to predictions from NN model

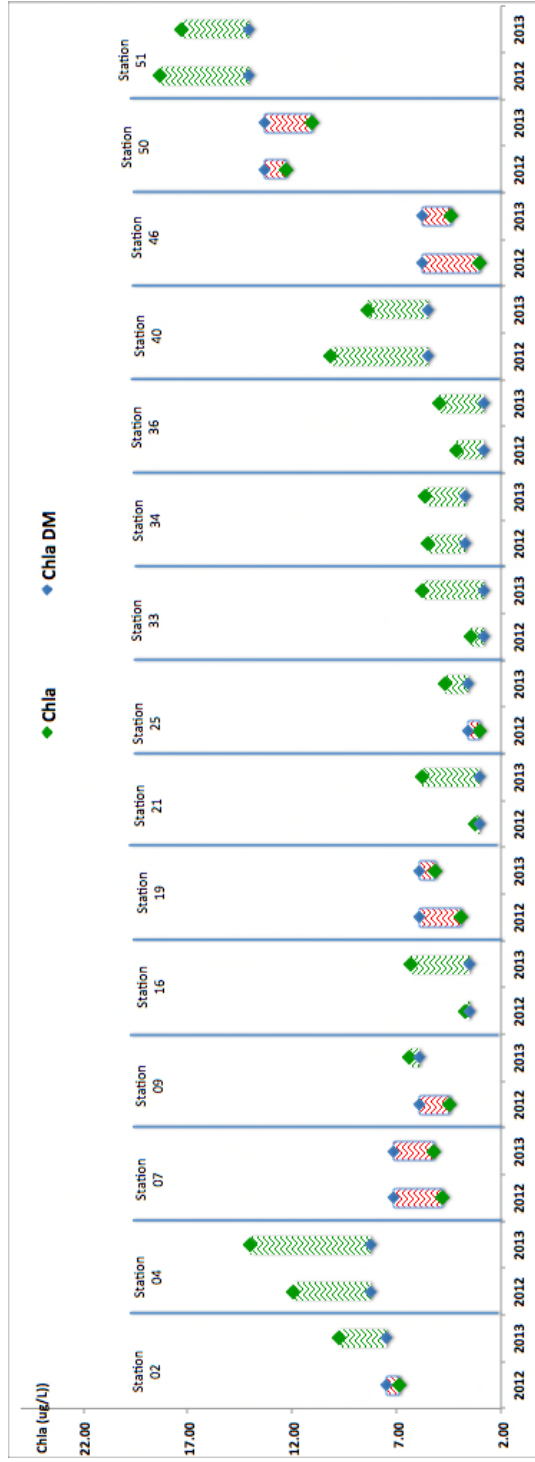


Figure 5.12 Observed lake Champlain monitoring data (2012 and 2013) compared to predictions from DM model

5.7 Discussion of The Results

5.7.1 Low to moderate water nutrient conditions

For most of lake Champlain, where low to moderate levels of nutrients (e.g. $<10 \mu\text{g/L}$) were recorded at the majority of water quality monitoring stations, a linear relationship was observed between the levels of water quality parameters and chlorophyll-a (a biomarker for cyanobacteria algal blooms; CABs). In some cases this relationship was positive linear (e.g for water nutrients such as total phosphorus (TP) and total nitrogen (TN) which are needed for CABs growth. In other cases a negative linear relationship was found (e.g. for secchi depth, a measure of water clarity, which is reduced by the growth of CABs). All of the modeling approaches tested (MLR, NN, DM) were able to give models with good fit R^2 values for these lake conditions.

5.7.2 High water nutrient conditions

In areas of lake Champlain with high levels of water nutrients ($10 > \mu\text{g/L}$), which are found at the southern water quality monitoring stations 02 and 04 (located at the mouth of a river that empties nutrients into the lake); and also at stations 50 and 51 (located near agricultural fertilizer runoff into the lake), a nonlinear relationship was observed between water quality parameters and chlorophyll-a. In high water nutrient conditions, the best approach to accurately predicting chlorophyll-a and thus CABs growth in lake Champlain was by using NN model does not provide a modeling equation, data mining was used to find the nonlinear model to accurately predict chlorophyll a levels, and therefore cyanobacteria algal blooms in lake Champlain.

Model	Variables	R^2	Notes
MLR model #6	TP, Cl, TN, Secchi	0.857	Close prediction for most of lake Champlain, but poor predictions for water high level nutrient data obtained at stations 02,04 50 51 and 25
NN model #8	Year, Depth, TP, TN, Cl, Secchi, Temp	0.851	Provided better R^2 and more accurate results but no equation only xml file
DM model #1	Years, TP, TN, Secchi	0.815	Nonlinear model with high accuracy

Table 5.7 Summary of chlorophyll-a models described in this thesis.

5.7.3 Causes of the model errors

Investigation of the models errors revealed that:

The errors in MLR model were due to:

- a. High correlation between the lake input variables (Diebold et al., 2007).
- b. Chla general distribution is nonlinear, which was proven in appendix C, and it was observed from the data mining that Chla model in general is not linear, so it is likely that linear regression was not able to fully address the nonlinear part of the lake data.
- c. The model most significant errors were for the northern as southern parts of the lake and were due to the extreme concentrations of Chloride (Cl) in the southern part of the lake, and extreme concentrations of nitrogen (TN) in the northern part of the lake.

NN model provided better accuracy than the MLR; the main cause of errors in the model was due to the extreme concentrations of Chloride (Cl) in the southern part of the lake, and extreme concentrations of nitrogen (TN) in the northern part of the lake.

DM model was more responsive to extreme changes as it used complicated algorithms to derive the DM model, and similar to NN model the DM model main cause of errors were due to the extreme concentrations of Chloride (Cl) in the southern part of the lake, and extreme concentrations of nitrogen (TN) in the northern part of the lake.

Further investigation of the data generated by the lake Champlain water quality monitoring stations that were causing problems in model prediction accuracy revealed that, the southern monitoring stations 02 and 04 are located in shallow water at the mouth of the Poultney river that contributes large amount of nutrients into the lake. Furthermore, farms and agricultural lands that likely contribute fertilizer into the lake surround the northern monitoring stations 50 and 51. The results obtained in this thesis project have been confirmed by other studies in the literature, which showed that the MLR model approach is not accurate at high water nutrient concentrations (Li et al., 2013).

Results of model comparison indicated that NN model #8 predictions were more accurate than both MLR model #6 and DM model #1 predictions, by 48% and 12.8%, respectively.

CHAPTER 6
LAKE CHAMPLAIN
CHLOROPHYLL-A GIS SPATIAL ANALYSIS
RESULTS

In the previous chapter using statistical analysis we revealed several chlorophyll-a models for lake Champlain. The best model comprised a set of 3 different equations found through data mining. One model was for the southern part of the lake, another for the northern and a final set for the main lake body. Such distribution suggests that location might be a factor in modeling algae in lake Champlain. In this chapter I'll present geostatistical analysis to investigate the location importance to the algae bloom in Lake Champlain and show the spread of the different variables contributing to the algae model across the lake.

6.1 GIS Based Modeling Results

In the previous chapter, the variables contributing to chlorophyll-a models for lake Champlain were identified through statistical analysis, and it was noted that the different models found were less accurate at the northern and southern parts of the lake, further investigation revealed that northern parts of the lake suffers from excess levels of nitrogen, while southern parts of the lake suffers from excess levels of chloride, such phenomena suggests that the location might be a factor in modeling algae in Lake Champlain, so in this section geostatistical analysis is used to investigate the location impact on algae bloom for lake Champlain, furthermore the geostatistical analysis will be used to mathematically interpolate the levels of variables throughout the volume of the lake.

6.2 Determination of the Statistical Model Variables

The purpose of this test is to determine the location importance to the MLR chlorophyll-a model. ArcGIS is advanced geostatistical analysis software, however it lacks the stepwise selection option available in IBM SPSS, therefore in the MLR variables test, all of the variables for lake Champlain water quality parameters were used. The data for later years 2003-2011 was used to generate the model equation, while the early years data 1992-2002 was used to verify the model results. The processing extent and snap raster of the analysis were set to the lake Champlain boundary. Figure 6.1 shows the GIS ordinary least square (OLS) setup interface.

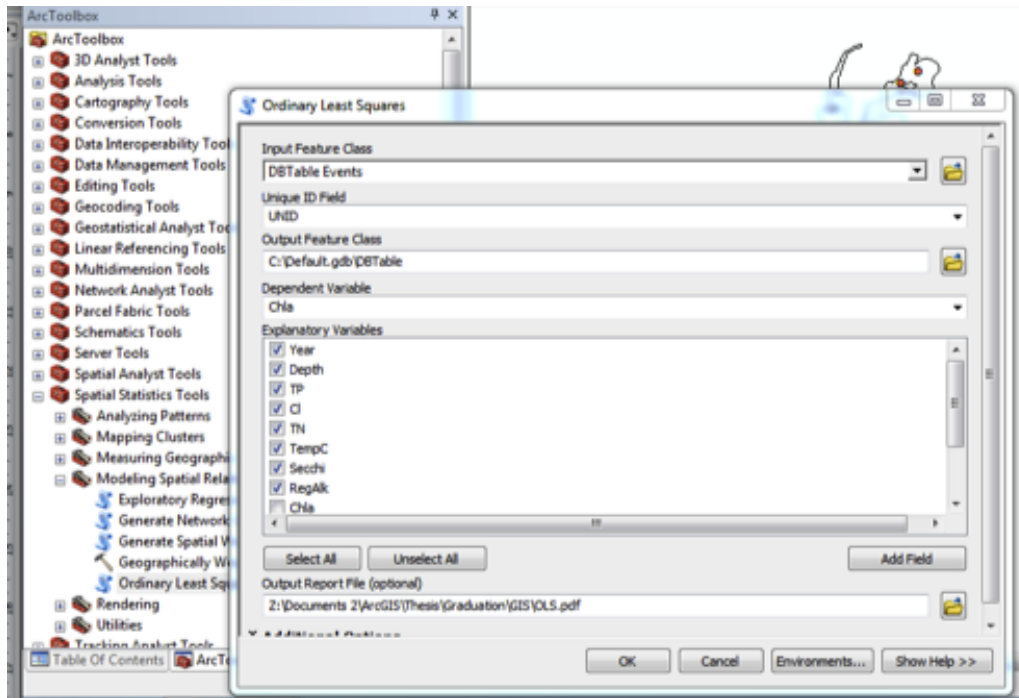


Figure 6.1 GIS -ordinary least squares interface.

6.3 Model Results and Model Configuration

6.3.1 Statistical model with all input variables

Variable	Coefficient	StdError	t-Statistic	Probability	Robust SE	Robust t	Robust Pr	VIF [c]
Intercept	221.672	172.710	1.283	0.201	159.858	1.386	0.168	-----
YEAR	-0.107	0.085	-1.255	0.211	0.079	-1.352	0.178	1.881
DEPTH	0.003	0.006	0.604	0.546	0.003	1.142	0.255	1.495
TP	0.086	0.043	2.020	0.045*	0.044	1.934	0.055	15.509
CL	-97×10^{-6}	141×10^{-6}	-0.688	0.492	152×10^{-6}	-0.640	0.522	8.182
TN	0.008	0.003	2.474	0.014*	0.003	2.122	0.035*	4.134
TEMPC	95×10^{-5}	0.032	0.029	0.976	0.030	0.031	0.974	1.117
SECCHI	-0.868	0.261	-3.316	0.001*	0.263	-3.295	0.001*	6.699
REGALK	-0.032	0.040	-0.793	0.429	0.053	-0.604	0.546	10.078

Joint F-Statistic	47.162	Dependent Variable:	Chla
Joint Wald Statistic	297.831	Number of Observations:	126
Koenker (BP) Statistic	27.664	Multiple R-Squared	0.763
Jarque-Bera Statistic	108.340	Adjusted R-Squared	0.747

Table 6.1 GIS-based model #1 (OLS) results.

From table 6.1, we notice that the Koenker test value is >0.05 . This means that the geographical location of the water quality parameters (variables) may not have a significant impact on the GIS based model. However, the MLR model obtained in this step was not the optimal solution, since there were several variables with $VIF >7.5$, indicating that some variables might be redundant (dismissible).

6.3.2 Statistical model with selected variables

Previously, we found through use of correlation analysis, that lake Champlain variables were strongly correlated, thus removing the variables with $VIF >7.5$ may not be the best approach (e.g. total phosphorus (TP) and total nitrogen (TN), particularly at high levels). Therefore several iterations are required to find the best set of input of variables that produce the optimal MLR model, or we can use the set of input variables obtained from the MLR model stepwise selection since we already know they produced the optimal MLR model. GIS based model (OLS) run results are presented in the following table.

Variable	Coefficient	Std Error	t-Statistic	Probability	Robust SE	Robust t	Robust Pr	VIF [c]
Intercept	4.131	1.874	2.204	0.029*	2.297	1.798	0.074	-----
TP	0.070	0.030	2.331	0.0213	0.034	2.004	0.047*	6.591
CL	- 0.00015	0.000056	- 2.651	0.009*	0.00007	-2.123	0.035*	1.290
TN	0.010	0.002	4.101	0.00008*	0.003	3.460	0.0007**	2.733
SECCHI	- 0.701	0.2343	-2.994	0.003*	0.232	-3.024	0.003*	5.369
Joint F-Statistic		93.493		Dependent Variable:			CHLa	
Joint Wald Statistic		241.618		Number of Observations:			126	
Koenker (BP) Statistic		25.555		Multiple R-Squared			0.857	
Jarque-Bera Statistic		73.763		Adjusted R-Squared			0.854	

Table 6.2 GIS- based model# 2 (OLS) results

The set of input variables used for this run resulted in all of the variables having their $VIF <7.5$, thus confirming that we chose the right set of variables which were significant for this model. The Koenker test value was >0.05 , indicating the insignificance of the geographical location impact on the algae model. Furthermore, the JarqueBera statistic of > 0.05 indicates the

residuals (errors) are normally distributed and the model is well distributed and not biased. The other outputs from the OLS test, (e.g. the robust probabilities, Robust_SE, Robust_t, Joint Wald Statistic and Joint F-Statistic), all became insignificant, as we only considered their value when the Koenker Statistic was < 0.05. The equation from OLS model with the selected input variables is:

$$\text{Chla} = 4.13 + 0.07 * \text{TP} - 14.9 * 10^{-5} * \text{Cl} + 0.01 * \text{TN} - 0.70 * \text{Secchi} + \varepsilon \quad \text{Eq. 6.1}$$

With $R^2 = 0.857$

Recall equation 5.1 using IBM SPSS MLR stepwise selection.

$$\text{Chla} = 4.13 + 0.07 * \text{TP} - 14.9 * 10^{-5} * \text{Cl} + 0.01 * \text{TN} - 0.70 * \text{Secchi} + \varepsilon \quad \text{Eq. 5.1}$$

The two equations are identical; this result was expected because when the location has no impact on the chlorophyll-a model, then ArcGIS produces similar results to those obtained by statistical analysis tools like IBM SPSS, or Systat 13. This finding suggests that high/low levels of chlorophyll-a and thus cyanobacteria algal blooms (CABs) could occur anywhere throughout lake Champlain, depending on the seasons and natural and man-made environmental conditions (e.g. presence of farm fertilizer runoff into the lake in some years but not in others and prevailing wind/currents in the lake that distribute the phosphorus and nitrogen throughout the lake).

6.4 Spatial Trend Analysis

Spatial analysis is also required to show the spread, distribution and extent of the variables affecting the chlorophyll-a model for cyanobacterial algal bloom growth. ArcGIS uses the interpolation technique Empirical Bayesian Kriging to create a continuous surface, a method well suited to handle extreme and minor changes within data records. Using Kriging, the surrounding measured values are weighted to derive a predicted value for an unmeasured location. Weights are based on: the distance between the measured points, the prediction locations and the overall spatial arrangement among the measured points. The Empirical Bayesian Kriging (EBK) tool is available in ArcGIS to automate calculation of the interpolated surface for the various water quality input parameters, generating maps that represent the distribution of the variable over the entire lake volume and surface.

In the EBK interface input menu, the water quality parameters (phosphorus, nitrogen, chloride, secchi depth, alkalinity and chlorophyll-a) that we wish to interpolate and have their values projected on a map throughout the lake are added one by one. The EBK surface output is stored in the Z value field from EBK interface menu. In the environment settings, the processing extent and the snap raster are set to be the lake Champlain boundary and in the layer properties the clip options are set to lake Champlain layer, the last step is necessary to limit the analysis to the lake boundary.

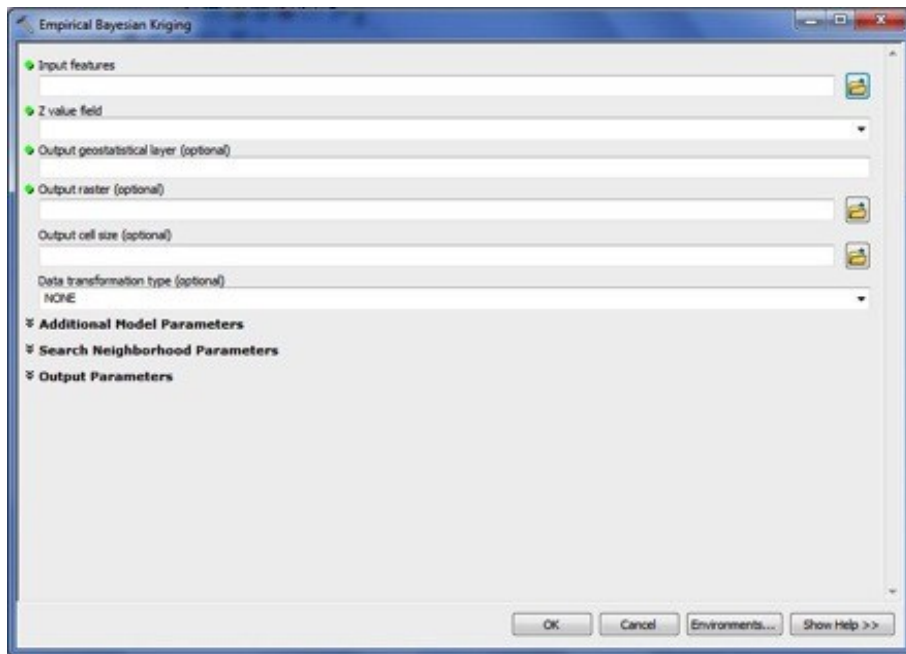


Figure 6.2 GIS Kriging inputs.

Figure 6.3 shows a summary of the total phosphorus (TP) levels obtained from the water quality monitoring stations in lake Champlain from years 1992 to 2011, illustrated in an interpolated (EBK) map. This figure shows the normal seasonal and yearly variations in the lake phosphorus levels, which are generally lower in the center of the lake (blue colour) and higher in the Northern and Southern sections of the lake (red colour), likely due to farm fertilizer runoff (in the North) and the rivers (in the South). The addition of a water quality monitoring station 51 in 2005 confirmed the high phosphorus levels previously observed at monitoring station 50 in the Northern section of the lake (red colour).

Figure 6.4 and 6.5 for the EBK map which clearly highlights the problem causing the deviated results in the models predictions, as we can see extreme concentrations of chloride (Cl) in the southern part of the lake, thus confirming the analysis in section 5.3 and the MLR model equation 5.2, similarly we can see extreme concentrations of total nitrogen (TN) in the northern part of the lake, thus confirming the analysis in section 5.3 and the MLR model equation 5.3. This is rendering the two sections (the northern and southern) parts of the lake as different extreme environment.

Figure 6.6 shows the results for secchi depth monitoring in lake Champlain between 1992-2011, the EBK maps for the secchi depth confirm the correlation analysis in section 5.1 and MLR model #6 and equation 5.1 as well as the data mining modeling equation 5.4, as we notice that secchi depth which is a measure of the water clarity is reduced by increasing levels of cyanobacterial algal bloom (CABs) growth

Figure 6.7 shows a different trend for alkalinity monitoring in lake Champlain between 1992-2011. Alkalinity is the ability of a solution to neutralize acids. Alkalinity levels are subject to minor changes through the years thus it seems that the CABs growth in lake Champlain is not being affected by alkalinity, and this is supported by the analysis in chapter 5 as none of the modeling equations contain the alkalinity as a predictor.

Phosphorus Concentration in Lake Champlain from 1992-2011

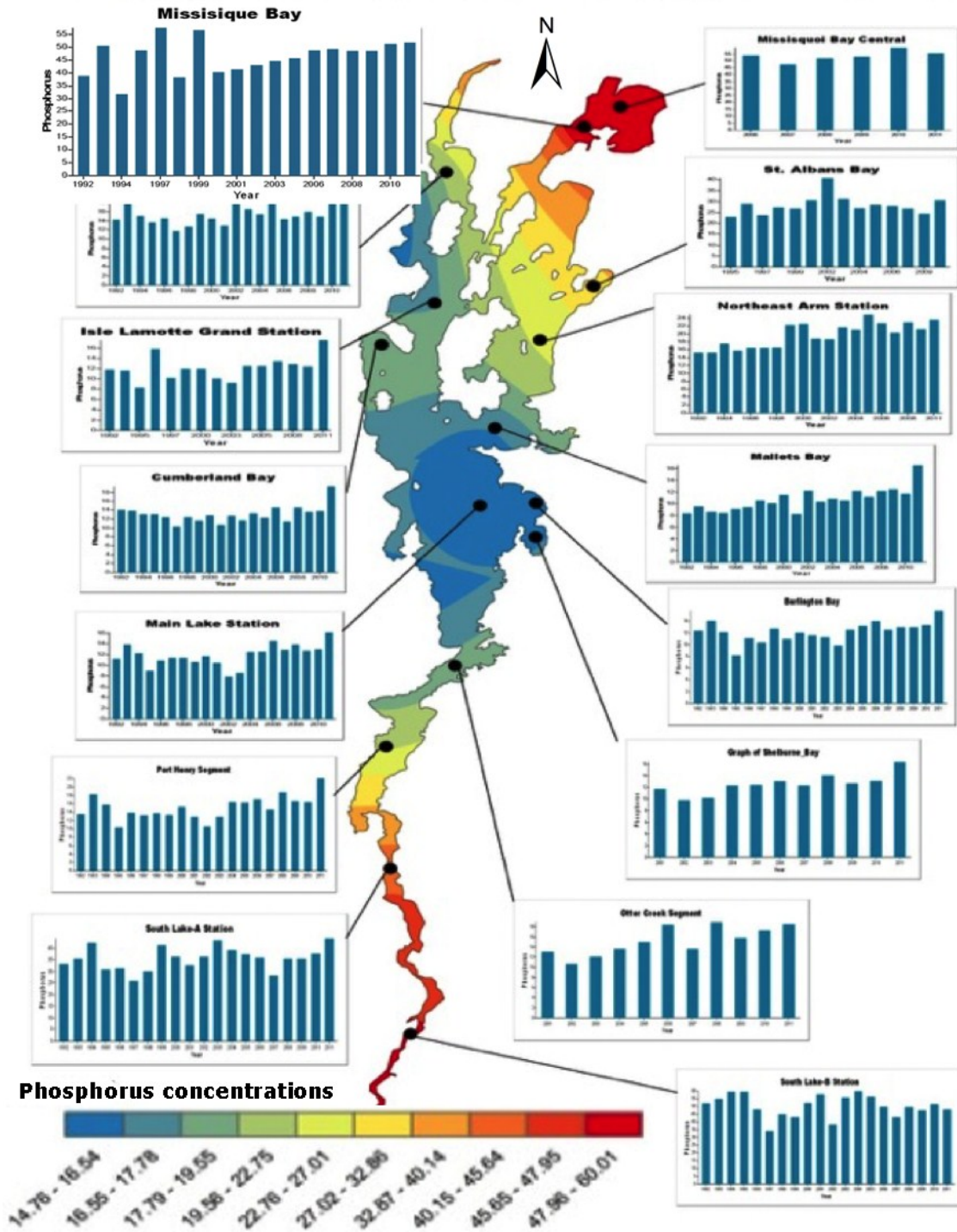


Figure 6.3 GIS map showing a summary of lake Champlain total phosphorus (TP) levels monitored at various stations throughout the lake from 1992-2011.

Total Nitrogen Concentration in Lake Champlain from 1992-2011

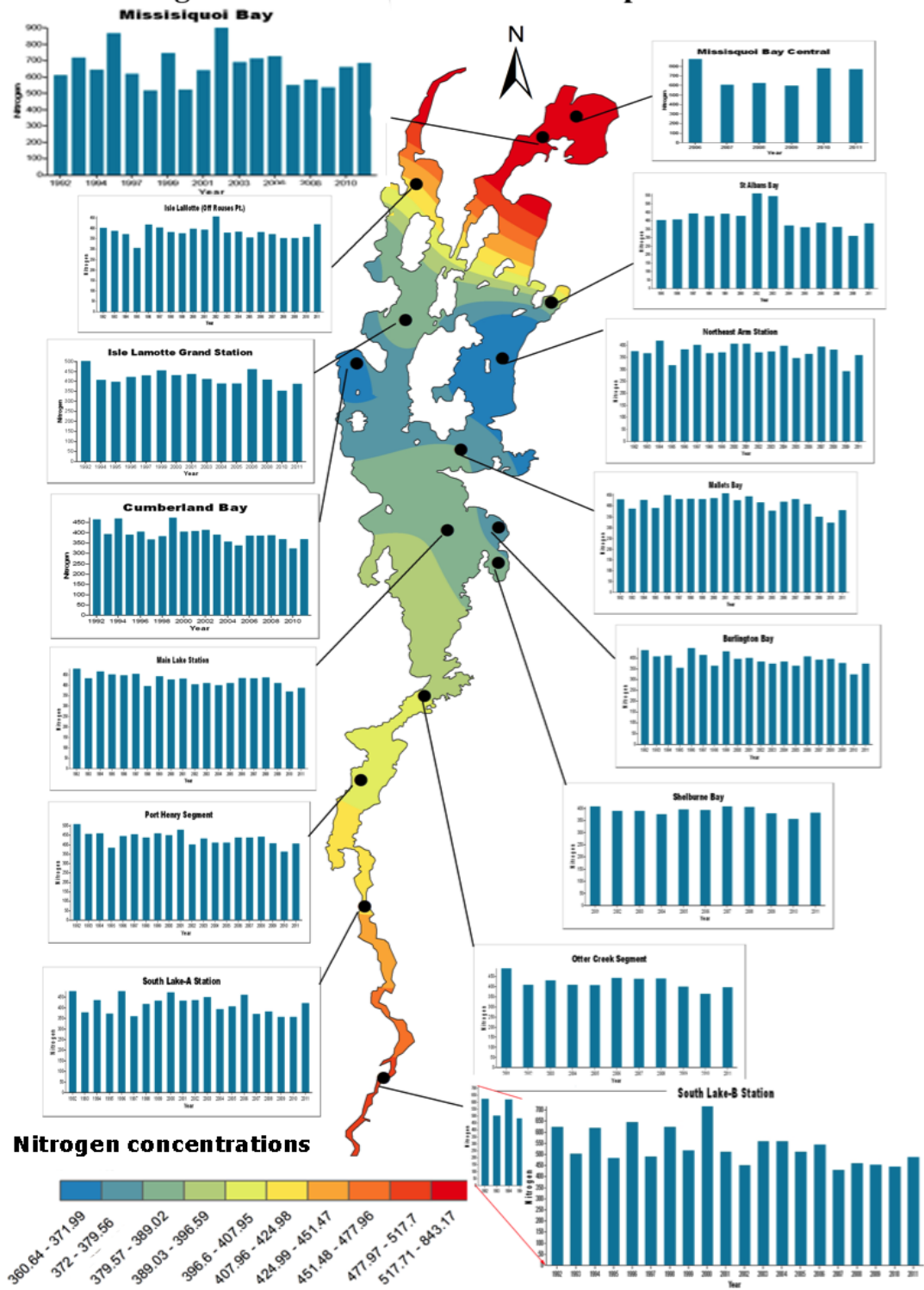


Figure 6.4 GIS map showing a summary of lake Champlain total nitrogen (TN) levels monitored at various stations throughout the lake from 1992-2011.

Chlorine Concentration in Lake Champlain from 1992-2011

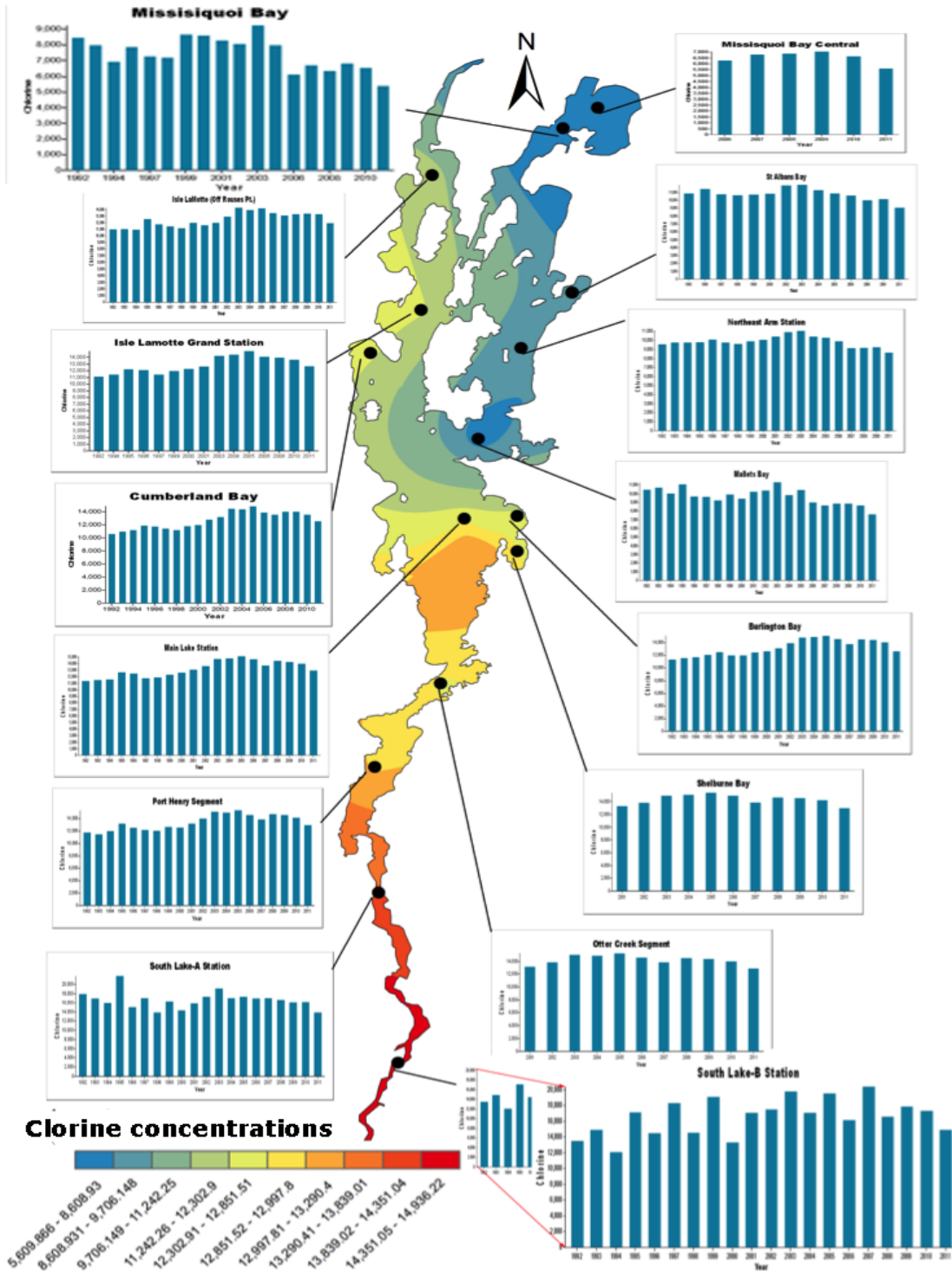


Figure 6.5 GIS map showing a summary of lake Champlain chloride (Cl) levels monitored at various stations throughout the lake from 1992-2011.

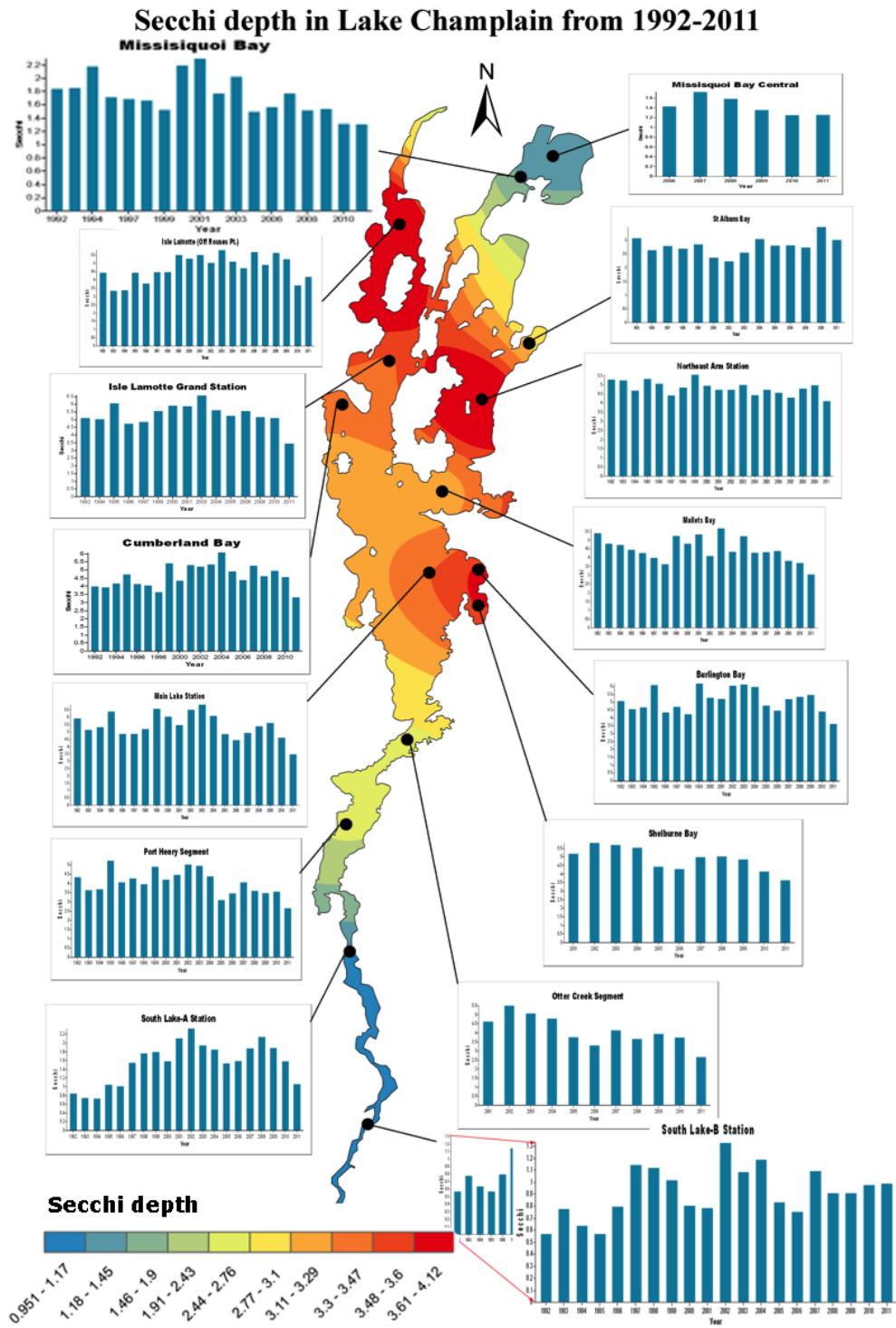


Figure 6.6 GIS map showing a summary of lake Champlain secchi depths (a measure of water clarity) monitored at various stations throughout the lake from 1992-2011.

Alkalinity levels in Lake Champlain from 1992-2011

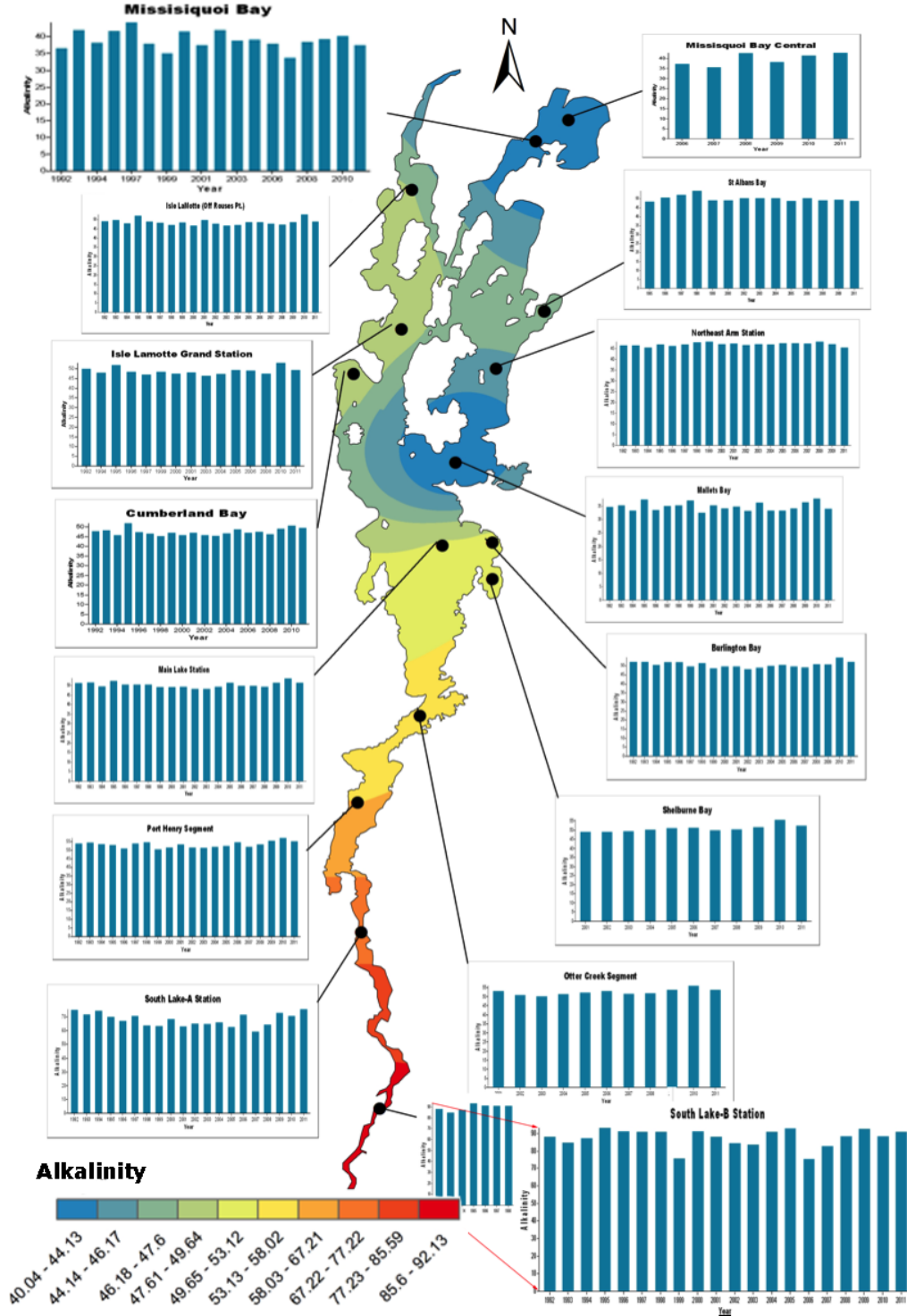


Figure 6.7 GIS map showing a summary of lake Champlain alkalinity levels (an inverse measure of water acidity) monitored at various stations throughout the lake from 1992-2011.

6.5 GIS Based Statistical Model Validation and GIS Results for TP and Chla

In section 6.4 the interpolated EBK maps of lake Champlain water quality monitoring data were used to show the trend for the variables appearing in the cyanobacterial algal bloom (CABs) model, and the EBK maps came to confirm the results of the different models, furthermore for better visualization for the results presented for the MLR in figure 6.8 we can use the EBK maps to present the cyanobacterial algal bloom spread side by side by the main factors contributing in the MRL cyanobacteria model thus helping to better understand and verify the model.

Figure 6.8 presents a pair of maps for the observed chlorophyll-a (Chla) side by side by the Total Phosphorus (TP) which was found to be the most dominant factor affecting cyanobacterial algal bloom (CAB) according to the multiple linear regression, neural network and data mining models, where we can clearly see the similarity between the TP and Chla spread of concentrations throughout the years of lake Champlain, thus verifying the results obtained by the multiple linear regression, neural network and data mining models

Figure 6.9 and 6.10 respectively present a pair of maps showing the prediction results from the GIS (OLS) model #2 output verses the observed recorded values. We can see that the chlorophyll-a GIS (OLS) model #2 results, were accurate and consistent in the main lake body and the accuracy tends to drop in the northern and southern parts of the lake for the reason discussed earlier in this chapters.

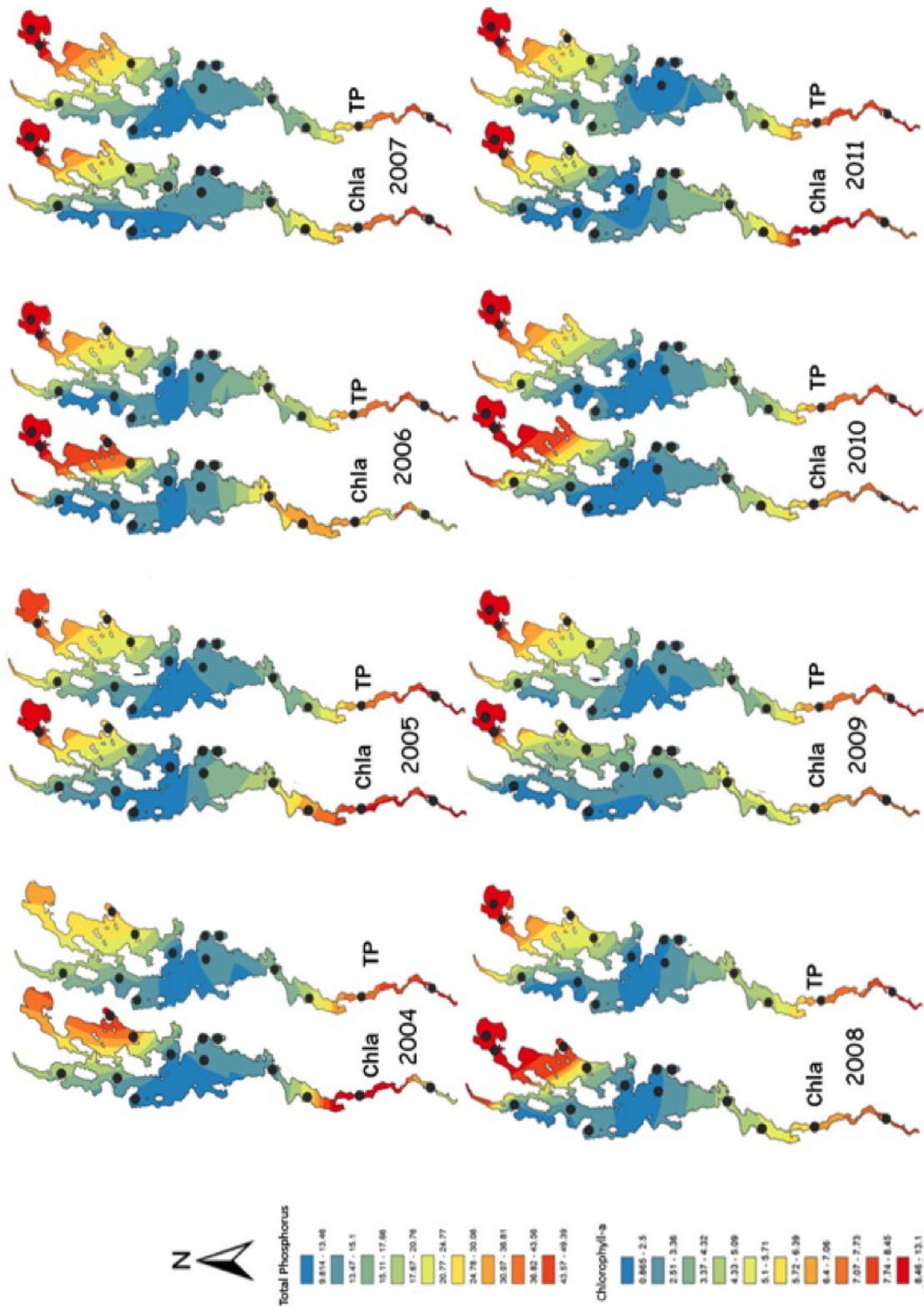


Figure 6.8 GIS maps comparing lake Champlain chlorophyll-a observed levels with total phosphorus (TP) observed levels between 2004-2011.

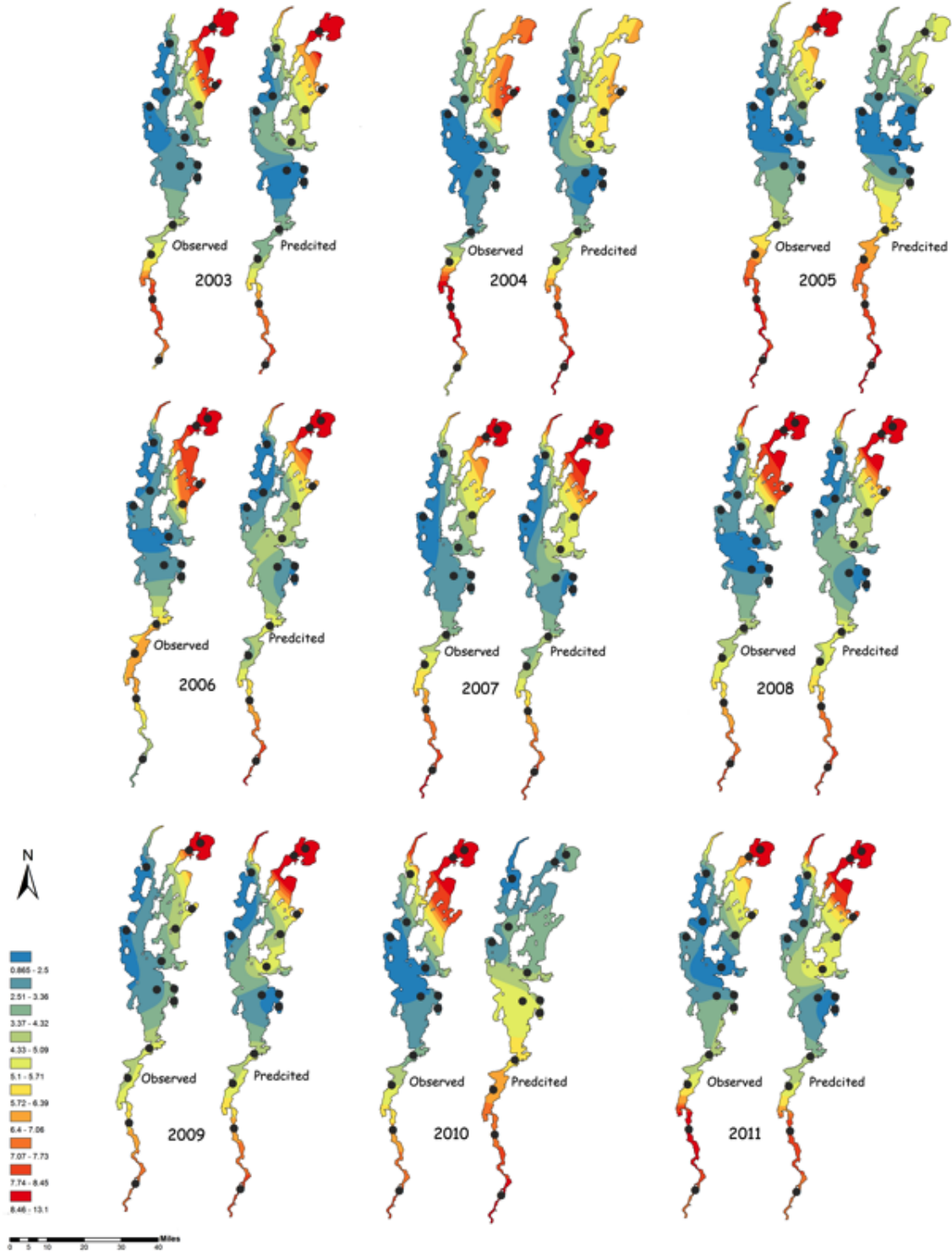


Figure 6.9 Lake Champlain water quality monitoring station observed chlorophyll-a levels (Chla a biomarker for CABs) compared to the GIS model #2 predicted levels.

Chlorophyll-a concentration in Lake Champlain from 1992-2011

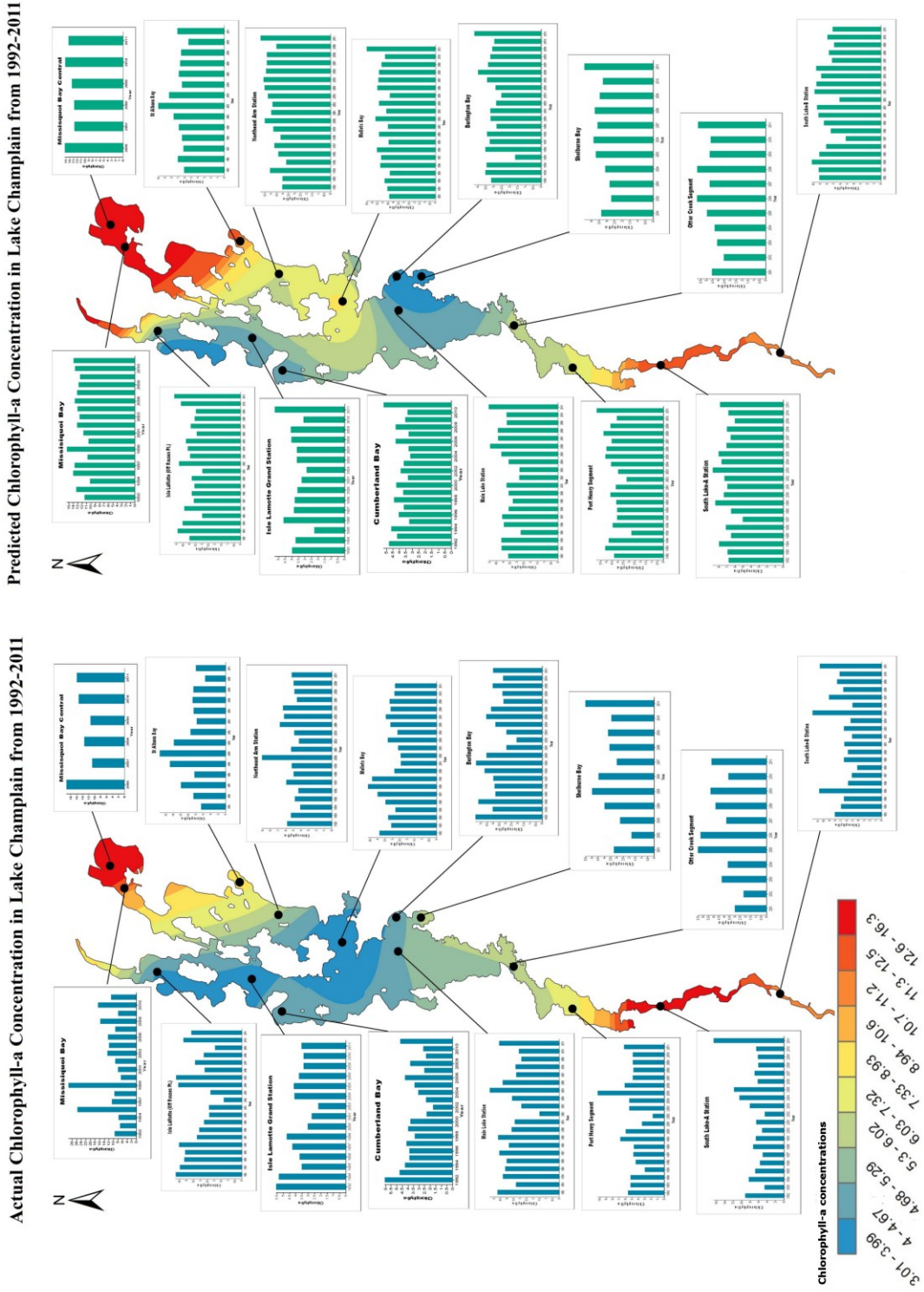


Figure 6.10 Lake Champlain monitoring station observed chlorophyll-a levels vs. the MLR model #6 predicted levels.

CHAPTER 7

CONCLUSION AND CONTRIBUTION

7.1 Conclusion

This study provided information, data and an overview of research on modeling of the factors affecting cyanobacterial algal bloom as well as my subjective opinions related to the factors affecting the water quality in lake Champlain.

A statistical analysis and simulation models including: (a) multiple linear regressions (MLR); (b) artificial neural network (ANN) based on back propagation algorithms; (c) data mining (DM) were developed using multiple water quality parameters such as the total phosphorus, total nitrogen, temperature, water monitoring depth, water clarity as an input while using the chlorophyll-a levels which is a biomarker for algal growth as an output to these models. A GIS modeling structure of lake eutrophication was developed to support the statistical analysis. The results of the statistical analysis indicate that neural network model had the most accurate predictions followed by data mining, then the multiple linear regression and that's due to the fact that Chla growth is nonlinear. The developed chlorophyll-a models showed various degrees of accuracy in predicting chlorophyll-a levels, the results of the MLR in particular are less accurate due to the high correlation between the input variables, and the nonlinear characteristics of Chlorophyll-a at high levels of lake variables, while in NN and data mining the errors were not random, they came from stations 02, 04, 50 and 51. The analysis indicates that excessive levels of Chloride at the southern section of lake Champlain and excessive levels of Nitrogen at the northern section of the lake were the two factors affecting the NN and data mining chlorophyll-a model accuracy.

The water quality parameter (variable) found to be most significantly correlated with chlorophyll-a levels was total phosphorus (TP). The phosphorus cycle in lake Champlain shows that there are many natural and human sources of phosphorus in the lake, including the mouth of a river bringing phosphorus-rich sediment into the southern section of the lake, and farms with fertilizer runoff located at the northern part of the lake. This suggests that the natural environment as well as human activity contribute perhaps equally to lake eutrophication and algae blooms. The natural and man made high levels of phosphorus and other nutrients such as nitrogen promoting algal growth and controlling these levels are the key issue related to minimizing the probability of algal blooms.

The geostatistical analysis indicated that hi/low levels of chlorophyll-a and thus cyanobacterial algal blooms (CABs) could occur anywhere throughout lake Champlain, and it is independent of the location.

The investigation of the different lake Champlain timeframes, suggests that: smaller timeframes such as daily and weekly, doesn't not support developing a significant model; and since the significant models came from the yearly timeframes, then it means that the developed model can't be used as an early alert for increasing levels of algae or eutrophication but rather as a tool to help developed proper lake management programs.

7.2 Contributions of the Research

As the regulations are being developed and enforced to protect and improve water quality in lakes, rivers and reservoirs, understanding algal blooms (using the biomarker chlorophyll-a) is becoming more and more important. In the present thesis study, several analytical techniques were used to uncover the water quality parameters that are correlated with algal bloom. Several models for chlorophyll-a were developed, and for these different models, the degree to which each environmental variable contributed to chlorophyll-a levels varied. Taken together, the set of different chlorophyll-a models that were developed using different approaches (e.g. multiple linear regression (MLR), neural network (NN), and data mining (DM), all indicated a strong linear relationship between the dissolved total phosphorus (TP) levels and chlorophyll-a levels in the lake water, most likely because phosphorus is an important nutrient for algal growth. This relationship was found to be linear at low to medium concentrations of TP. However, at high concentrations of total phosphorus ($>10 \mu\text{g/L}$), the relationship became nonlinear.

The contributions of the present thesis can be summarized as follows:

1) Analysis of lake Champlain data indicates that using the mean values of the data (yearly) have had refined to a relatively high degree of statistical precision and to create the models. The later years dataset worked better as a training data set. This was because several new important monitoring stations were set up during the later years time period.

2) Although MLR model had the highest R^2 value, however the model produced the least accurate predictions. The deviation in the model accuracy was due to 1) high correlation between the environmental variables. 2) extreme levels of nitrogen in north and chloride in the south. 3) Chlorophyll-a has nonlinear characteristics at high levels of lake variables. 4) and in section 4.5.C I ignored the impact of internal loading which in this case should be considered as those are shallow stations with lots of sediment interaction. The best predictions came through NN model, however NN model did not provide a model equation to help future researchers investigation, the alternative came through data mining, which provided a significant accurate model with an equation that can be used to further investigate the lake on future studies.

3) Model verifications indicated less accurate results for the northern and southern parts of the lake, further investigation supported by Empirical Bayesian Kriging (EBK) maps highlighted the cause of the problem to be due to the extreme concentrations of chloride (Cl) in the southern part of the lake, and extreme concentrations of total nitrogen (TN) in the northern part of the lake.

4) Modeling studies in this thesis for chlorophyll-a indicate that: the total dissolved phosphorus has the strongest impact on algae production and the main cause to water quality degradation due to its persistence in lake water at high levels.

5) Earlier studies for lake Champlain haven't produced a good prediction equation (Smeltzer et al., 2009); this study is one of the first to produce several modeling equations with high prediction accuracy to address the algal problem in lake Champlain. The developed chlorophyll-a models showed various degrees of accuracy in predicting chlorophyll-a levels therefore, it is ill advised to assume that one model can account for all the variations in the chlorophyll-a equation. Furthermore, we cannot generalize the use of any of these models for other lakes because each lake will respond differently to its environment.

In general, this study helped to identify the water quality factors that most significantly affect chlorophyll-a levels (correlated with cyanobacterial algal bloom growth) in lake Champlain. Although the models developed for the case study may not apply for a different lake, the factors affecting the algal blooms may be similar for all lakes.

7.3 Future Studies

This section highlights the scope of future work, which may be conducted on the basis of the work presented in this thesis.

1. Lake recovery from eutrophication depends in part on the quantity of phosphorus that has accumulated over time in the lake bottom sediment and in the quantity of dissolved phosphorus in the water volume in contact with the sediment. Reduction of external phosphorus loading may not necessarily produce swift improvement, since sediment release can compensate for this reduction, consequently, both internal and external loading data reduction should be considered in preparing a proper lake management program.
2. It was not possible to utilize multiple nonlinear regression due to the inconsistency of the monitored data, however with the aid of new technology such as GIS analysis we were able to expose the hidden information patterns and the problems in the north and south parts of the lake. The scientific works published on GIS lake eutrophication models are still very limited. Further and deeper scientific research should be conducted in this area in the future.
3. The comprehensive statistical analysis exposed that the northern and southern parts of the lake have complicated and uncertain patterns, and were ill defined using multiple linear regression, therefore for future studies fuzzy and/or stochastic modeling methods can be used to further address uncertainties.
4. ArcGIS in comparison to other professional statistical analysis software like IBM SPSS or data mining has limited capabilities and has less accuracy. Future studies should try to import models developed outside GIS and import and implement those models into the GIS for enhanced and improved predictions.
5. The goal of any monitoring plan is to be able to take action before the problem becomes uncontrollable. Huge efforts were made in collecting lake Champlain water quality monitoring data, however, the daily data for lake Champlain did not help much in

producing any of the chlorophyll-a models. lake Champlain data would also have been much more valuable if it was collected concurrently.

6. During the modeling process, I assumed that all the lake variables are independent however, this is not the case in fact most of the variables are correlated with the climate conditions, so climate impact on lake water quality is a subject for further investigation.

7. The developed models can be further used to find an effective methodology for lake Champlain management, and suggest programs/regulations, which can help improve the lake water quality.

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APPENDICES

Appendix A: Lake Champlain Outliers

Station	Date	TP µg/L	Cl µg/L	TN µg/L	TempC deg C	RegAlk µg/L	Secchi	Cl
02 - Sout Lake B	17/08/2004	235						
02 - Sout Lake B	17/06/1998			1190				
02 - Sout Lake B	22/08/2011			1720				
02 - Sout Lake B	12/06/2007							34.1
02 - Sout Lake B	28/09/2011							36.5
04 - Sout Lake A	27/10/1993		31800					
04 - Sout Lake A	11/08/1992			810				
04 - Sout Lake A	03/07/1998							44.35
04 - Sout Lake A	12/08/2005							47.5
04 - Sout Lake A	28/07/2011							52.6
04 - Sout Lake A	11/08/2011							39.6
07 - Port enry Segment	14/07/1993	41						
07 - Port enry Segment	28/08/2006							25.9
07 - Port enry Segment	23/06/2005							22.4
09 - Otter Creek Segment	28/05/1996	31						
09 - Otter Creek Segment	07/06/2006	38.4						
09 - Otter Creek Segment	05/08/2008	56.9						
09 - Otter Creek Segment	07/08/2008	42.5						
09 - Otter Creek Segment	14/08/2008	42.8						
09 - Otter Creek Segment	24/05/2010	66.4						
09 - Otter Creek Segment	28/07/2011		10000					
09 - Otter Creek Segment	12/09/2001			620				
09 - Otter Creek Segment	21/07/2005			570				
09 - Otter Creek Segment	01/05/2006			590				
16 - Selburne Bay	07/07/2011	30.1						
16 - Selburne Bay	12/07/2005			550				
16 - Selburne Bay	03/10/2005			620				
16 - Selburne Bay	18/08/2010			170				
16 - Selburne Bay	23/08/2011			160				
16 - Selburne Bay	19/08/2011			180				
16 - Selburne Bay	07/07/2011							15.3
19 - Main Lake	16/06/1993	26						
19 - Main Lake	11/07/1995		15800					
19 - Main Lake	10/10/1995		8100					
19 - Main Lake	22/07/1992			650				
19 - Main Lake	03/09/1994			240				
19 - Main Lake	02/05/1995			690				
19 - Main Lake	16/08/1995			670				
19 - Main Lake	08/07/2009			690				
19 - Main Lake	18/08/2010			170				
19 - Main Lake	06/07/1998							15.25
21 - Burlington Bay	20/05/1992	25						
21 - Burlington Bay	20/05/1993	30						
21 - Burlington Bay	18/08/1993	30						
21 - Burlington Bay	24/06/1998	33						
21 - Burlington Bay	09/07/2007	32.8						
21 - Burlington Bay	07/06/2011	38						
21 - Burlington Bay	10/10/1995		8800					
21 - Burlington Bay	08/06/1998		19500					
21 - Burlington Bay	25/07/2011		10000					
21 - Burlington Bay	05/06/2006			680				
21 - Burlington Bay	30/06/1999			650				
21 - Burlington Bay	01/06/2000							16.36
21 - Burlington Bay	07/06/2011							15.4
21 - Burlington Bay	28/09/1999							14.06
21 - Burlington Bay	13/07/2009							14.1
25 - Malletts Bay	22/07/1997	25						
25 - Malletts Bay	03/06/2011	30.9						
25 - Malletts Bay	12/06/2008	22.1						
25 - Malletts Bay	09/05/2011	24.3						
25 - Malletts Bay	01/09/2011	21.2						
25 - Malletts Bay	18/08/1997		6300					
25 - Malletts Bay	16/08/1995		13100					
25 - Malletts Bay	02/07/1997		12600					

25 - Malletts Bay	27/07/2011		4900					
25 - Malletts Bay	10/08/1992			700				
25 - Malletts Bay	29/07/1994			650				
25 - Malletts Bay	09/09/1996			690				
25 - Malletts Bay	19/08/2010			110				
25 - Malletts Bay	23/08/2011			130				
25 - Malletts Bay	07/07/1998							26.2
33 - Cumberland Bay	14/08/1995	34						
33 - Cumberland Bay	06/06/2011	37.9						
33 - Cumberland Bay	06/06/2011	29.3						
33 - Cumberland Bay	22/07/2011	29.8						
33 - Cumberland Bay	31/08/2011	29						
33 - Cumberland Bay	21/10/1999			1030				
33 - Cumberland Bay	30/06/2006			160				
33 - Cumberland Bay	18/08/2010			150				
33 - Cumberland Bay	06/06/2011							9.47
34 - Northeast Arm	18/08/1997		12600					
34 - Northeast Arm	24/07/1997			830				
34 - Northeast Arm	27/07/1994			640				
34 - Northeast Arm	11/07/2008			760				
34 - Northeast Arm	02/05/2000							20.49
34 - Northeast Arm	07/07/1998							17.6
36 - Isle LaMotte (off Grand Isle)	18/10/1996	75						
36 - Isle LaMotte (off Grand Isle)	16/06/1999	50						
36 - Isle LaMotte (off Grand Isle)	10/10/1995		9500					
36 - Isle LaMotte (off Grand Isle)	06/06/2001		6200					
36 - Isle LaMotte (off Grand Isle)	21/07/1992			910				
36 - Isle LaMotte (off Grand Isle)	13/07/1998			660				
36 - Isle LaMotte (off Grand Isle)	13/07/1998			690				
36 - Isle LaMotte (off Grand Isle)	14/04/2006			660				
36 - Isle LaMotte (off Grand Isle)	09/06/2005							21.8
36 - Isle LaMotte (off Grand Isle)	09/08/2007							19.9
40 - St. Albans Bay	13/08/2003			990				
40 - St. Albans Bay	30/08/1999							77.57
40 - St. Albans Bay	22/08/2000							53.82
40 - St. Albans Bay	10/08/2000					1		52.73
46 - Isle LaMotte (off Rouses Pt)	08/05/2001		5000					
46 - Isle LaMotte (off Rouses Pt)	31/08/2011		9800					
46 - Isle LaMotte (off Rouses Pt)	03/10/2000		9300					
46 - Isle LaMotte (off Rouses Pt)	25/08/2000		8900					
46 - Isle LaMotte (off Rouses Pt)	23/07/1997			800				
46 - Isle LaMotte (off Rouses Pt)	17/06/2002			760				
46 - Isle LaMotte (off Rouses Pt)	01/07/2002			710				
46 - Isle LaMotte (off Rouses Pt)	31/08/2011			880				
46 - Isle LaMotte (off Rouses Pt)	08/09/2004							32.2
46 - Isle LaMotte (off Rouses Pt)	21/06/2005							25.5
50 - Missisquoi Bay	25/06/2002			1710				
50 - Missisquoi Bay	01/07/2002			1610				
50 - Missisquoi Bay	26/07/1999							112.72
50 - Missisquoi Bay	06/08/1999							116.36
50 - Missisquoi Bay	20/08/1999							98.18
50 - Missisquoi Bay	20/09/1996							79.02
50 - Missisquoi Bay	04/10/1996							80
50 - Missisquoi Bay	12/08/2008							72.6
51 - Missisquoi Bay Central	04/10/2010	150						
51 - Missisquoi Bay Central	23/05/2006			1720				
51 - Missisquoi Bay Central	04/10/2010			1540				
51 - Missisquoi Bay Central	06/10/2006							112
51 - Missisquoi Bay Central	08/09/2006							57.6

Appendix B: Multiple Linear Regression MLR-LEF

Matlab code for the example in section 4.6.1 multiple linear regressions MLR

```
%=====
%                               MLR Matlab code for the example in Chapter 4
% A line started with the % is only for comments, and will not be executed
%=====
% The first two commands lines were to clear the memory and the screen
clear
clc
% The Data from table 4.7 lake Champlain station 19 is used for the analysis
%-----|
%   Step 1: data division   |
%-----|
% The first step is to divide the data into two halves
% The first half of the data is between 2003-2011 and is used to create the regression model (
% The second half of the data between 1993-2002 and is used for model verification
%-----|
%   Step 2: data input     |
%-----|
% We enter the first half of the data into the Matlab, according to MLR equation
%        $Y = bZ + e$ 
% Where :
%       Y is the chlorophyll-a (Chla) and is the dependent variable
%       Z is the water quality parameters and the independent variables
%       e is the error
% The complete data vector is Y
Y=[3.33
4.33
4.16
4.04
4.61
3.86
4.70
3.66
3.43
1.52
2.91
3.62
5.34
4.34
3.32
3.34
2.90
3.10
4.62]
```

```

% The training data vector for the dependent variable
Y_train= [3.33
4.33
4.16
4.04
4.61
3.86
4.70
3.66
3.43
1.52]
% The verification data vector for the dependent variable
Y_verify= [2.91
3.62
5.34
4.34
3.32
3.34
2.90
3.10
4.62]
The complete independent Z matrix
z = [1993  100 13.89  11495.00  433.75 14.02  5.13  51.57 ;
1994  100 12.22  11594.44  466.33 12.68  5.33  49.50 ;
1995  100 8.97  12661.11  452.22 9.80  6.41  52.41 ;
1996  100 10.84  12461.70  447.08 8.90  4.88  50.38 ;
1997  100 11.37  11733.89  453.33 12.00  4.87  50.45 ;
1998  100 11.36  11879.17  396.25 12.53  5.20  50.37 ;
1999  100 10.64  12310.26  444.05 21.67  6.57  49.03 ;
2000  100 11.71  12622.00  427.17 16.78  6.04  49.14 ;
2001  100 10.51  13099.00  430.50 19.98  5.46  49.26 ;
2002  100 7.90  13633.33  403.67 22.24  6.50  48.20 ;
2003  100 8.57  14706.25  409.33 21.06  6.87  48.23 ;
2004  100 12.50  14775.28  398.50 16.53  6.11  49.31 ;
2005  100 12.57  15118.33  409.47 19.34  4.84  51.48 ;
2006  100 14.48  14686.31  435.12 19.60  4.42  49.83 ;
2007  100 12.87  13760.00  432.58 19.18  4.94  49.84 ;
2008  100 13.89  14448.33  436.00 18.20  5.40  49.42 ;
2009  100 12.75  14293.06  410.14 18.03  5.62  51.32 ;
2010  100 12.96  13975.71  370.29 13.00  4.60  53.72 ;
2011  100 16.12  12978.10  387.19 6.10  3.48  51.35 ]
% Following is the section of Z matrix that will be used for training and model creation
z_train = [1993  100 13.89  11495.00  433.75 14.02  5.13  51.57;
1994  100 12.22  11594.44  466.33 12.68  5.33  49.50 ;
1995  100 8.97  12661.11  452.22 9.80  6.41  52.41 ;
1996  100 10.84  12461.70  447.08 8.90  4.88  50.38 ;

```

```

1997 100 11.37 11733.89 453.33 12.00 4.87 50.45 ;
1998 100 11.36 11879.17 396.25 12.53 5.20 50.37 ;
1999 100 10.64 12310.26 444.05 21.67 6.57 49.03 ;
2000 100 11.71 12622.00 427.17 16.78 6.04 49.14 ;
2001 100 10.51 13099.00 430.50 19.98 5.46 49.26 ;
2002 100 7.90 13633.33 403.67 22.24 6.50 48.20 ]
% The section of Z matrix which will be used for model verification
z_verify = [2003 100 8.57 14706.25 409.33 21.06 6.87 48.23 ;
2004 100 12.50 14775.28 398.50 16.53 6.11 49.31 ;
2005 100 12.57 15118.33 409.47 19.34 4.84 51.48 ;
2006 100 14.48 14686.31 435.12 19.60 4.42 49.83 ;
2007 100 12.87 13760.00 432.58 19.18 4.94 49.84 ;
2008 100 13.89 14448.33 436.00 18.20 5.40 49.42 ;
2009 100 12.75 14293.06 410.14 18.03 5.62 51.32 ;
2010 100 12.96 13975.71 370.29 13.00 4.60 53.72 ;
2011 100 16.12 12978.10 387.19 6.10 3.48 51.35 ]
%-----|
% Step 3: calculation of Beta |
%-----|
% The best linear model is found when the error=0, thus the linear regression model becomes
%  $Y = bZ + e$ 
% Using the training values we can find the coefficient matrix B, where Beta =  $b=Y/Z$ 
% Since we will use the training data set we will rewrite the above equation
%  $b\_hat = Y\_train/z\_train$ 
% We can't directly obtain the value of b_hat since z_train and Y_train
% are of different dimensions.
% To get around this problem we know that a matrix can be decomposed into
% two orthogonal matrices, therefore we can decompose the Z matrix into Q and R
% z_train matrix into Q and R
% Q is orthogonal matrix with n by p dimensions
% R is triangular p by p matrix
% Thus  $b\_hat = z\_train/Y\_train = R \backslash (Q' * Y\_train)$ 
% The last equation is the same as the least square equation
% Using the info on the Z matrix, we can define n and p
n=10; % the number of observations.
p=8; % the number of independent variables.
% The Matlab command to decompose z matrix into two orthogonal matrices is
[Q,R] = qr(z_train,0);
% Now to can calculate  $b\_hat = Y\_train/z\_train = R \backslash (Q' * Y\_train)$ 
b_hat = R \ (Q' * Y_train);
%-----|
% Step 3: Prediction |
%-----|
% Beta matrix can be used in the linear regression equation
%  $Y = bZ + e$ 
% To predict the values for the verification data set so

```

```

%% % Yhat = z_verify * b_hat = z_train*(R\ (Q'*Y_train));
Y_hat= z_verify*b_hat;
% where Yhat is n by 1 vector of fitted (or predicted) values of Y.
%-----|
%   Step 4: Verification   |
%-----|
% The predicted Yhat is compared to Y_verify using the error and
% the R Pearson correlation coefficient and R^2 the coefficient of determination
e = Y_verify -Y_hat;
% The mean squared error is defined as
mse = e'*e./(n-p);
% Square the residuals and total them to obtain the residual sum of squares:%
SSresid = sum (e.^2);
% Compute R Pearson correlation coefficient
r=corr(Y_verify , Y_hat);
% Compute R^2 coefficient of determination
rsq =r^2;
%-----|
%   Step 5 : Output       |
%-----|
% The results are plotted analysis
Plot(Y_verify ,'r-', 'LineWidth', 2);
% Label the curve for function f in red
Text(7.5, 5.4, 'Y Observed Chla', 'Color', 'r', 'LineWidth', 2);
Hold all
Plot(Y_hat,'b-', 'LineWidth', 2);
Text(7.5, 5.2, 'Yhat Predcited Chla', 'Color', 'b', 'LineWidth', 2);
xlabel('x=Years 2003 to 2011','FontSize',12);
ylabel('Chla concentration µg/L', 'FontSize',12);

```

Appendix C: Multiple Nonlinear Regressions

The concept in developing a nonlinear regression model is based on understanding the distribution shape of the data under investigation. First we search for a known nonlinear function that shares a similar shape for the data distribution in question, then by MNR model is obtained by adjusting the coefficients of the known nonlinear function to fit in the data distribution.

Figure C.1 is a screen shot for the IBM SPSS multiple nonlinear regression setup menu, illustrating where a known nonlinear a function is required to commence with MNR modeling.

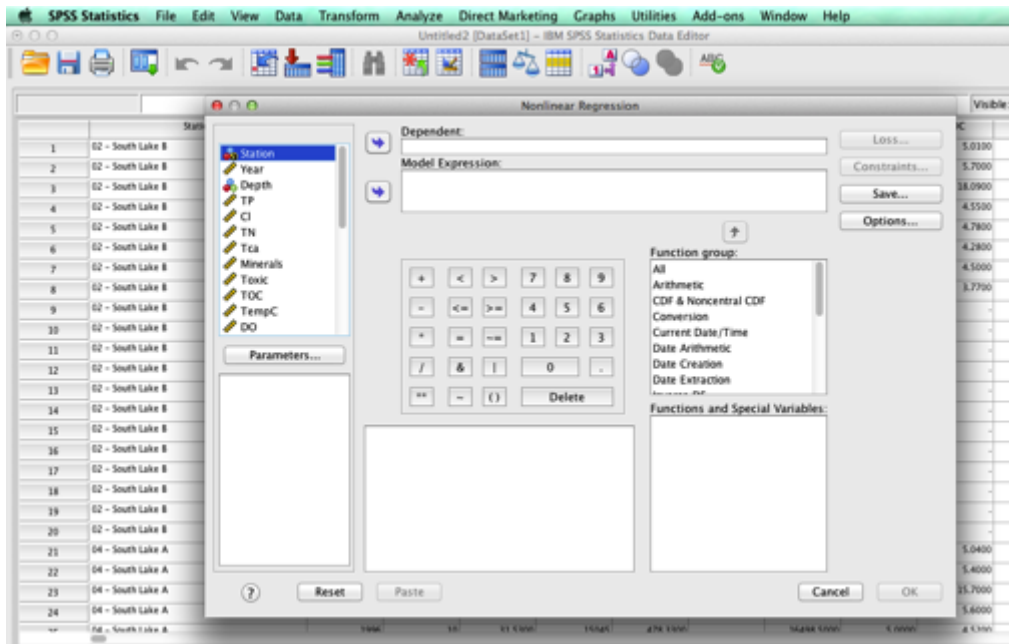


Figure C.1 IBM SPSS, MNR setup menu

The first task is to start with the MNR modeling to find a nonlinear function that shares similar shape to chlorophyll-a observed data distribution for Lake Champlain, for this step the chlorophyll-a observed data distribution records for the 15 monitoring stations of lake Champlain are presented in table C.1 is plotted as a graph on figure C.2

From figure C.2 we notice that almost each station has its unique oscillating shape and that there isn't a common or specific function that can be used to describe the distribution of all the stations; consequently, we can't proceed with the multiple nonlinear analysis

Year	Chla 02	Chla 04	Chla 07	Chla 09	Chla 16	Chla 19	Chla 21	Chla 25	Chla 34	Chla 33	Chla 34	Chla 36	Chla 40	Chla 46	Chla 50	Chla 51
1992	8.11	9.15	5.63			4.74	5.48	3.88	5.84	6.08	5.84	5.57		4.8	9.5	
1993	7.04	4.62	5.25			3.33	4.07	3.08	5.37	4.76	5.37			4.5	7.2	
1994	6.52	8.37	5.27			4.33	5.25	3.3	4.11	4.26	4.11	5.36		4.17	7.85	
1995	10.79	6.85	3.05			4.16	3.86	2.8	4.86	3.87	4.86	3.54	6.57	4.12		
1996	5.77	5.67	4.44			4.04	3.91	3.49	4.38	3.86	4.38	3.71	8.69	4.54	25.77	
1997	5.16	5.01	4.78			4.61	3.99	4.02	5.95	4.14	5.95	4.28	12.01	3.26	10.58	
1998	4.25	7.28	4.72			3.86	4.72	4.66	5.01	3.38	5.01	4.74	8.38	3.09	9.63	
1999	6.51	6.63	6.83			4.7	5.43	4.38	5.22	4	5.22	3.05	15	2.74	29.56	
2000	5.85	5.22	5.98			3.66	4.56	2.87	9.12	3.77	9.12	2.73	17.66	2.37	6.72	
2001	6.45	6.61	3.49	3.02	3.25	3.43	2.95	2.43	5.31	2.33	5.31			2.39	8.01	
2002	5.09	4.57	1.82	2.19	1.83	1.52	2.11	2.46	4.28	1.76	4.28	2.2	13.86	1.32	9.16	
2003	6.48	8.11	5.46	4.27	2.74	2.91	2.95	2.62	4.92	2.39	4.92	4.12	9.44	2.28	12.64	
2004	5.36	10.53	5.45	3.69	4	3.62	3.84	3.33	6.77	3.08	6.77	4.17	7.77	4.61		
2005	11.92	11.82	10.34	6.52	4.98	5.34	4.59	2.66	6.21	3.43	6.21	3.76	8.62	4.76	11.89	
2006	5.04	6.25	6.17	6.26	4.47	4.34	4.2	3.15	6.37	4.27	6.37		8.89	2.69	12.36	19.53
2007	9.09	7.02	4.92	3.82	3.02	3.32	3.18	3.45	4.54	2.56	4.54	3.4		3.39	9.27	10.91
2008	6.63	6.1	4.8	4.82	3.6	3.34	3.27	3.13	4.89	3.8	4.89		8.66	2.77	15.79	13.52
2009	7.7	6.2	4.9	5.3	3.69	2.9	4.05	3.2	4.98	2.38	4.98	3.38	5.54	1.95	7.92	11.41
2010	7.26	6.59	4.87	3.64	3.44	3.1	3.2	2.88		2.64		3.57		4.23	16.83	15.34
2011	10.66	16.65	6.25	5.22	5.53	4.62	4.04	2.83	5.25	4.7	5.25		7.97	3.66	10.99	16.06

Table C.1 Chla yearly data records for lake Champlain

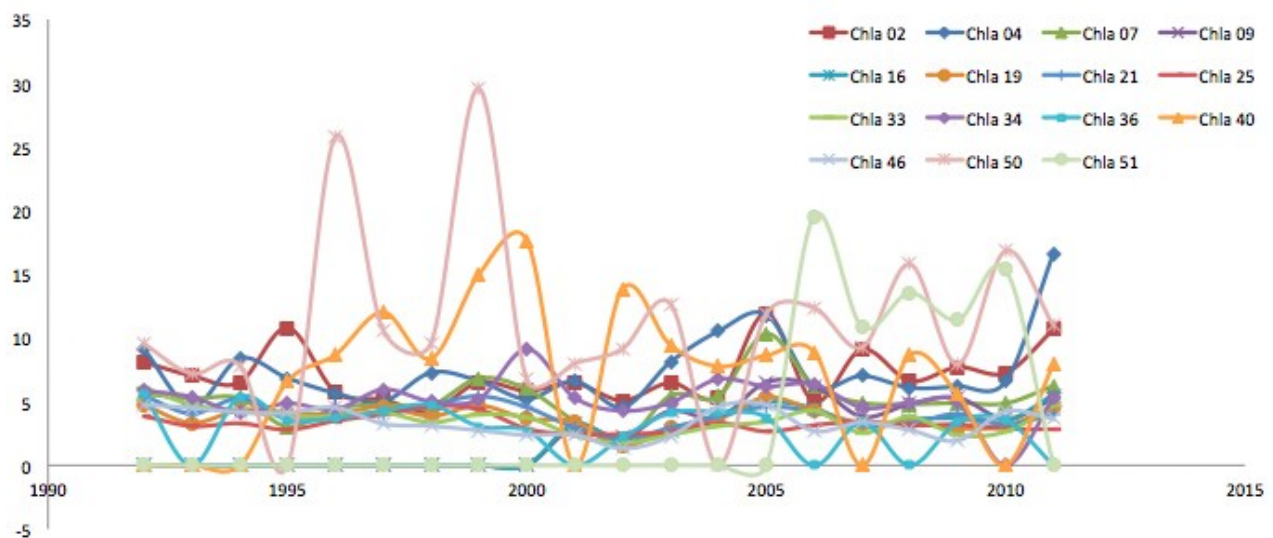
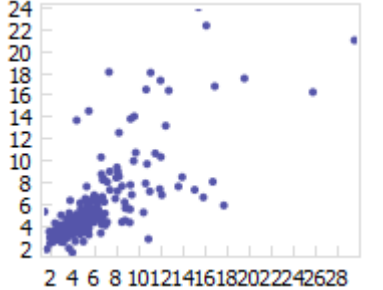
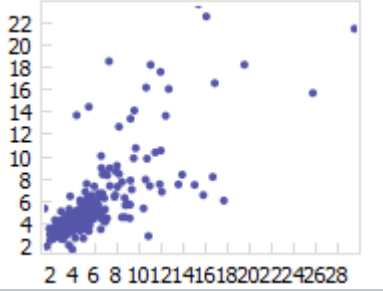
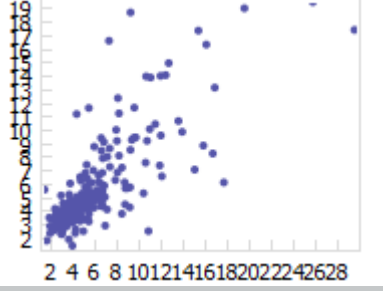
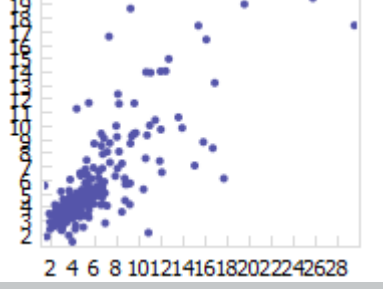


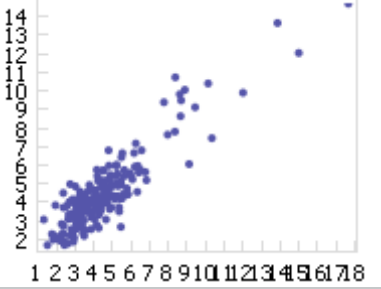
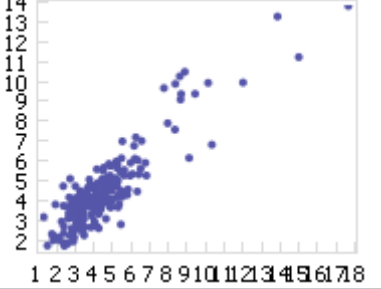
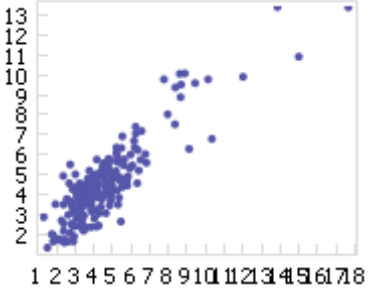
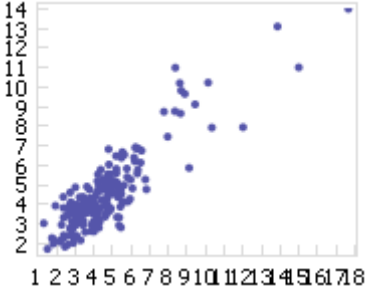
Figure C.2 Lake Champlain Chla yearly data

Appendix D:

D.1 Data Mining Results for Entire Lake Data

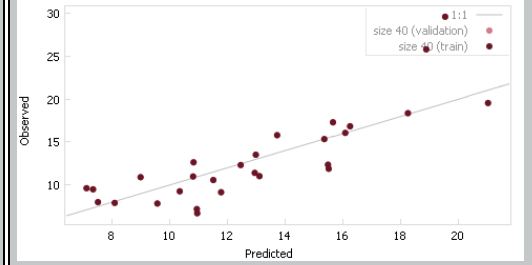
$\text{Chla} = 4.83662 + 2.63347e-7 \cdot \text{TP} \cdot \text{Secchi} \cdot \text{TN}^2 + 2.63347e-7 \cdot \text{TP} \cdot \text{TN}^2 \cdot \cos(0.0663525 + \text{Year}) - 0.75498 \cdot \text{Secchi}$	
$\text{Chla} = 4.8539 + 2.63347e-7 \cdot \text{TP} \cdot \text{Secchi} \cdot \text{TN}^2 + 2.63347e-7 \cdot \text{TP} \cdot \text{TN}^2 \cdot \cos(\text{Year}) - 0.75498 \cdot \text{Secchi}$	
$\text{Chla} = 4.78993 + 2.63347e-7 \cdot \text{TP} \cdot \text{Secchi} \cdot \text{TN}^2 + 2.55028 \cdot \cos(\text{Year}) / (0.0752586 + \text{Secchi}) - 0.753823 \cdot \text{Secchi}$	
$\text{Chla} = 4.7918 + 2.4918 \cdot \cos(\text{Year}) / \text{Secchi} + 2.63347e-7 \cdot \text{TP} \cdot \text{Secchi} \cdot \text{TN}^2 - 0.753823 \cdot \text{Secchi}$	

D.2 Data Mining Results for Main Lake Data (Without Stations 02,04,50 and 51)

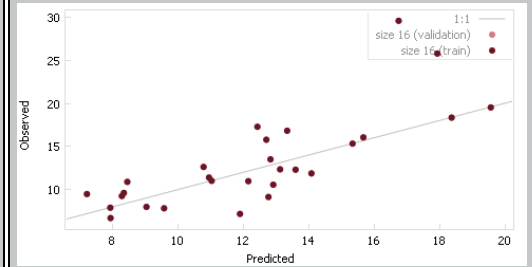
$\text{Chla} = 1.660 + (\text{TP} \cdot \text{RegAlk} + 228.652 \cdot \cos(-0.870 \cdot \text{Year}) + 219.920 \cdot \cos(2085.364 \cdot \cos(-0.8577 \cdot \text{Year}))) / (44.149 \cdot \text{Secchi} + \text{TempC} \cdot \text{Secchi})$	
$\text{Chla} = 1.758 + (0.015 \cdot \text{TP} \cdot \text{RegAlk} + 3.602 \cdot \cos(-0.870 \cdot \text{Year}) + 3.725 \cdot \cos(2085.391 \cdot \cos(-0.857 \cdot \text{Year}))) / \text{Secchi}$	
$\text{Chla} = 1.849 + (0.014 \cdot \text{TP} \cdot \text{RegAlk} + 3.973 \cdot \cos(2085.427 \cdot \cos(-0.857 \cdot \text{Year}))) / (\text{Secchi} + \cos(-0.889 \cdot \text{Year}))$	
$\text{Chla} = 1.730 + (\text{TP} \cdot \text{RegAlk} + 236.708 \cdot \cos(-0.851 \cdot \text{Year}) + 175.643 \cdot \cos(1.363 \cdot \text{Year})) / (46.559 \cdot \text{Secchi} + \text{TempC} \cdot \text{Secchi})$	

D.3 Data Mining Results for North Lake Data Stations 50 and 51

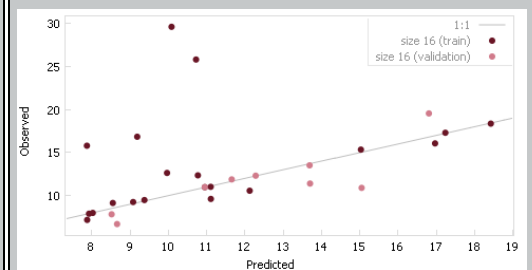
$$\text{Chla} = 38.493 \cdot 10^{-5} \cdot \text{TP} \cdot \text{TN} + 3.122 \cdot \sin(\text{Year} - \text{Cl} - \cos(\text{RegAlk}))$$



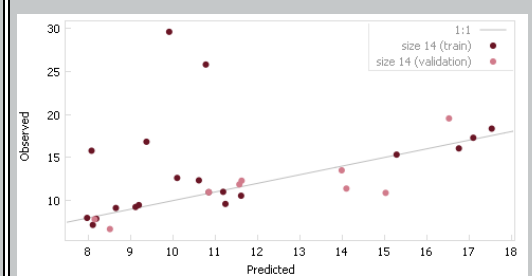
$$\text{Chla} = 37.157 \cdot 10^{-5} \cdot \text{TP} \cdot \text{TN} + 2.178 \cdot \sin(5.974 + \text{Year} - \text{Cl})$$



$$\text{Chla} = 5.940 \cdot \text{Depth} + 0.0422 \cdot \text{TP} \cdot \sin(7.1271 \cdot \text{Year}) - 13.99$$

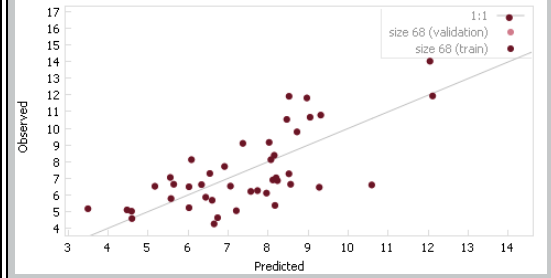


$$\text{Chla} = 5.908 \cdot \text{Depth} + 1.834 \cdot \sin(7.123 \cdot \text{Year}) - 13.829$$

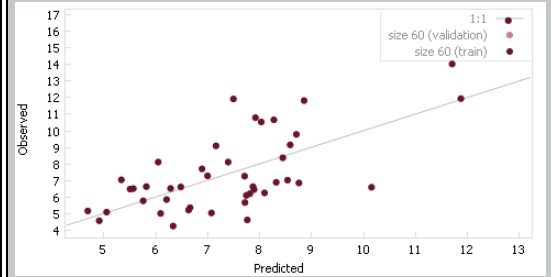


D.4 Data Mining Results for South Lake Data Stations 02 and 04

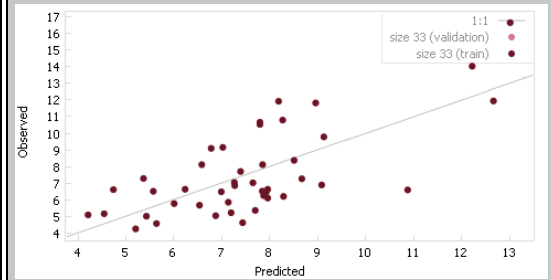
$$\text{Chla} = 0.076 \cdot \text{TP} + 0.032 \cdot \text{Year} \cdot \text{Depth} + 1.480 \cdot \exp(\cos(\text{Year})^2) - 3.711 \cdot \text{Secchi} - 65.1131 \cdot \text{Depth}$$



$$\text{Chla} = 4.691 + 0.027 \cdot \text{Year} \cdot \text{Depth} + \exp(\cos(\text{Year})^2) - 3.586 \cdot \text{Secchi} - 53.827 \cdot \text{Depth}$$



$$\text{Chla} = 49281.115 + 0.136 \cdot \text{TempC} + 0.098 \cdot \text{TP} + 0.031 \cdot \text{Year} \cdot \text{Depth} + 0.012 \cdot \text{Year}^2 - 2.392 \cdot \text{Secchi} - 49.199 \cdot \text{Year} - 61.672 \cdot \text{Depth}$$



$$\text{Chla} = 0.125 \cdot \text{TempC} + 0.087 \cdot \text{TP} + 0.030 \cdot \text{Year} \cdot \text{Depth} - 0.485 - 3.350 \cdot \text{Secchi} - 60.663 \cdot \text{Depth}$$

