XIAOQING ZENG

Water Quality Modeling in Southeastern Lake Management: A Case Study of Lake Lanier, Georgia (Under the direction of TODD C. RASMUSSEN)

Lake biogeochemistry is related to nutrient inputs, water temperature, and hydrologic conditions. Lake Lanier water quality varies spatially and vertically. Stratification is an important concern for within lake and downstream fisheries. A vertical biogeochemical model for Lake Lanier is developed in this dissertation to study the ecosystem behavior, with special reference to the roles of sediment-nutrient interactions and lake biogeochemistry.

Principal components analysis of the water quality data set (from 1996/97) indicates that the spatial variability of suspended sediment concentration, total phosphorus, orthophosphate, total kjeldahl nitrogen, ammonia, total organic carbon, dissolved organic carbon, iron and manganese in the tributaries of Lake Lanier are correlated and generally dominated by non-point source, storm runoff. Therefore a discharge-sediment-nutrient model using the rating curve method was developed to evaluate non-point source (sediment production and nutrient loading) from the watershed into Lake Lanier. Total nutrient loadings (including point source, non-point source, atmospheric deposition, etc.) are estimated using a detailed nutrient budget. Total nutrient loadings serve as inputs for the biogeochemical model.

A one-dimensional vertical thermal model for stratified deep lakes was developed and calibrated in Lake Lanier. In this model, the measured water surface temperature is forced using a sinusoidal function with an annual cycle. The measured thermocline depth variation is utilized to quantitatively determine the position of thermocline that separates epilimnion and hypolimnion. The temperature model avoids the need to perform a heat balance at the air-water interface. Model calibration results using a Monte Carlo simulation method show that the vertical heat dispersion coefficient D_z in Lake Lanier is about 0.35 m²/day during stratification period and the root mean square error of temperature simulation is 0.97 °C. The calibrated vertical heat dispersion coefficient is used as a conservative tracer to estimate vertical mass diffusion, and the simulated vertical temperature profile is used for determining chemical reaction kinetics for the biogeochemical model.

A hydrologic model based on water budget is used to predict dynamic water volumes and water levels of the lake. These results serve as dynamic hydrologic conditions for the biogeochemical model.

A one-dimensional vertical biogeochemical model was developed for stratified lakes. This model includes 15 state variables: phytoplankton biomass, suspended solids, dissolved oxygen, carbonaceous biochemical oxygen demand, sediment oxygen demand, sediment organic matter, organic nitrogen, ammonia nitrogen, nitrate nitrogen, organic phosphorus, orthophosphate, carbon dioxide, bicarbonate, carbonate, and total iron. The model not only predicts vertical distribution of the selected variables, but also explores benthic sediment effects on pelagic water quality. In addition, the model can be used as a diagnostic tool for TMDL (Total Maximum Daily Load) analysis.

INDEX WORDS: Water quality modeling, Sedimentation, Nutrient loading, Lake, Thermal modeling, Stratification, Biogeochemistry, Watershed, Eutrophication, Sediment-water interactions, Cluster analysis, Principal components analysis

WATER QUALITY MODELING IN SOUTHEASTERN LAKE MANAGEMENT: A CASE STUDY OF LAKE LANIER, GEORGIA

by

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DEDICATION

With love and devotion

To my wife, Hui, who accompanies me and always supports me

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There are many individuals whom I should acknowledge and thank for their contribution to my education at Daniel B. Warnell School of Forest Resources, the University of Georgia. First of all, I am greatly indebted to my major professor, Dr. Todd C. Rasmussen, for his guidance and support throughout my study. I really learned a lot from his extremely broad knowledge and kind personality.

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PREFACE

This research project is a subproject of "Community Values and the Long-Term Ecological Integrity of Rapidly Urbanizing Watersheds" which is headed by professor and eminent scholar Dr. M. Bruce Beck. U.S. EPA sponsored the project. Daniel B. Warnell School of Forest Resources, Institute of Ecology (University of Georgia), and School of Policy and College of Architecture (Georgia Institute of Technology) team together to do the research. The whole project seeks to integrate ecological, hydrological, and social/policy sciences in a study of a rapidly urbanizing watershed (Lake Lanier, Georgia), where preservation of long-term ecological integrity is perceived as being at stake. More specifically, the goals are to:

- (i) Develop a concept of environmental decision-making in which science-based models are responsive to identified community values, as they evolve in both the short and long term.
- (ii) Develop and apply a procedure for identifying those scientific unknowns crucial to the "reachability" of the community's desired/feared environmental futures.
- (iii) Improve understanding of basic aspects of lake ecosystem behavior, with special reference to the roles of the microbial foodweb, sediment-nutrient interactions, and geochemistry.

My research is to fulfill part of the third goal under the directions of my major professor -Dr. Todd C. Rasmussen.

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CHAPTER 1

INTRODUCTION

1.1 Motivation

In broad terms there are two reasons for constructing a mathematical model. From a *pragmatic* point of view decisions regarding restoration and protection of the environment must be made. A decision may take one of the two forms: of either an action – figuratively, the enactment of policy in order to push the system in a desired direction; or the collection of future observations – for identification of those parts of the systems that are not well understood, yet crucial to the success of policy initiatives. From a more *philosophical* perspective a mathematical model may be the only means of representing our understanding of the complex behavior of an environmental system. Such a model may be the most appropriate vehicle for interpreting observations of this system's past behavior.

In a more refined sense, there are three objectives of mathematical modeling (Beck et al., 1993):

- Prediction of future behavior under various courses of action, i.e. in the service of informing a decision.
- (ii) Identification of those constituent mechanisms of behavior that are crucial to the generation of a given pattern of future behavior but insufficiently secure in their theoretical or empirical basis, i.e. in designing the collection of further observations.
- (iii) Reconciliation of the observations of past behavior with the set of concepts embodied in the model, i.e. in the modification of theory and in explaining

why a particular input disturbance of the system gave rise to a particular output response.

1.2 Background

A lake or reservoir may serve as both the drinking water supply and the receiving waterbody for wastes generated by communities within its watershed. Protecting the water quality of the lake requires effective management strategies. Central to lake water quality management is the need for a robust model of lake and watershed water quality. The southeastern United States has a warm temperate climate, highly erodible and deeply weathered soils, and growing waste loads. These aspects present a challenging environment for water management. Lake and watershed models must be able to incorporate the region's unique physical, chemical, biological, social, and economic environment.

The primary purpose of water quality modeling in this dissertation is to develop a management model that correctly incorporates the unique physical-biologicalgeochemical processes within southeastern lakes and reservoirs. This study focuses on developing and using physical-biological-geochemical models to better understand the constitutive relationships that govern water quality mechanisms. Few efforts have examined these fundamental relationships in southeastern lakes and reservoirs. The intent in this study is to couple basic scientific principles with known behavior to better specify the mechanisms of southeastern lake water quality in general and Lake Lanier water quality in particular.

Lake water quality models, should, at the minimum, account for the interactions of nutrients with biological productivity, redox-controlled sediment geochemical reactions, and biological mediated sediment - water quality interactions. Specifically, the linkages between thermal stratification, dissolved oxygen concentration, carbonate species, pH, Eh, concentration of total and dissolved phosphorous, nitrogen, iron, and manganese, Chlorophyll a, specific conductance, and sediment should be formulated using kinetic reactions.

1.3 Research Objectives

The objectives of this dissertation are to:

- (1) Identify water quality issues using existing data. Data sources include: i) Holder (monthly, 1966/67); ii) EPA's National Eutrophication Survey (1973); iii) EPA's Clean Lake Study (1991, monthly); iv) Upper Chattahoochee River Basin Group's Study (monthly and biweekly, 1996/97); v) Supplementary sampling data in August 1999 and December 1999. Identification of water quality issues is useful for the selection of model state variables.
- (2) Quantify temporal (including daily, seasonal, annual and long-term variations) and spatial changes (including horizontal and vertical variations) in lake water quality. Idenditification of water quality characteristics is very important for model development.
- (3) Develop a daily non-point source model to estimate the pollutant loading of a lake watershed and use it with detail nutrient budget (including non-point source, point source, atmospheric deposition, etc.) to generate inputs for our water quality model.
- (4) Develop and calibrate a vertical temperature model to determine hypolimnetic heat dispersion coefficient and to simulate vertical temperature profile in Lake Lanier. The calibrated hypolimnetic heat dispersion coefficient is used for estimation of vertical mass diffusion and the simulated temperature results are used for determining chemical reaction kinetics for our water quality model.

- (5) Develop and calibrate a hydrologic model to predict water volume and water level for the lake. The predicted results serve as dynamic hydrologic conditions for our water quality model.
- (6) Develop and calibrate a physical-geochemical-biological model suitable for southeastern lakes and reservoirs, which focuses on vertical distribution of water biogeochemistry. Lake Lanier water quality has obvious vertical variation, and stratification is an important concern for within lake and downstream fisheries. A simplified CSTR (Continuously Stirred Tank Reactor) model is not suitable to study the ecosystem behaviour of the stratified deep lake.
- (7) Study the effects of benthic sediment on lake water quality. For a stratified deep lake, this can be done by using a reliable vertical biogeochemical model.
- (8) Provide mitigation alternatives for lake management based on above research results.

1.4 Methodology

1.4.1 General technical approach

The general technical approach used in this dissertation (shown in Figure 1-1) can be summarized as follows:

Data collection \rightarrow information extraction \rightarrow system understanding (knowledge) \rightarrow exploration of unknowns, conclusions and management suggestions (wisdom).

Data collection is the basis to understand an ecosystem. Data include historical data and current data. While there are many observations in Lake Lanier, we need to extract information from these different kinds of data, such as daily, seasonal, annual and longterm variations, spatial variations, lake stratification and mixing, sediment-nutrient relationships from tributary inflows, and water quality issues, etc. Once the water quality characteristics have been identified, we use our knowledge about the ecosystem (e.g. physical, biological, and geochemical theory) to develop a mathematical model that can be used to simulate the ecosystem for a range of management purposes. Suggestions of management alternatives are provided based on the modeling results.

1.4.2 Model calibration and evaluation

Model calibration and evaluation are important steps for model development. Field observations for a single period of time are used for what is called "model calibration", which is the process of adjusting the model parameters to best describe observed water quality for a particular data set. The calibrated model is then used to predict water quality using additional data. The process of comparing model prediction to multiple data sets is called model evaluation. The overall reliability of the model to predict future conditions increases in proportion to the amount of historical data that the model is able to describe successfully (note: the data sets must come from a range of conditions, otherwise the model reliability will be limited).

1.4.3 Modeling systems and usage

Modeling systems include hydrologic modeling, nutrient load modeling, spatial distribution modeling, vertical thermal modeling, vertical biogeochemical modeling, and sediment-water interaction modeling. Model components and usage are shown in Table 1-1.

1.4.4 Model connections and modeling strategy

Figure 1-2 indicates the model connections. The model running steps are as follows:

- Use a hydrologic model to generate lake water volumes and evels. The results serve as dynamic hydrologic conditions for the biogeochemical model.
- (ii) Apply nutrient load model to generate nutrient inputs for the biogeochemical model.

- (iii) Use a temperature model to generate dynamic vertical distributions of temperature. The simulated temperatures are used for determining chemical reaction kinetics for the biogeochemical model
- (iv) Implement the vertical biogeochemical model to study the lake ecosystem behavior and benthic sediment effects on lake water quality.

1.5 Summary of Original Contributions

- (i) Principal components analysis and cluster analysis are used to characterize the spatial variability of the watershed and reservoir water quality. These analyses have a common theme, "how can we simplify monitoring and assessment of a lake system and still accurately represent the system?" This has important ramifications for both water quality monitoring and water quality modeling.
- (ii) The Rating-Curve method is used to estimate short- and long-term watershed nutrient loadings, and the rating-curve bias correction factors for different variables in Lake Lanier watershed. The estimated nutrient loadings can be used for parameter calibration for GIS-based models, and the rating-curve bias correction factors can be used for annual loading correction when annual inflows and annual mean concentrations are used to estimate annual loadings.
- (iii) A simplified thermal model for stratified deep lakes is proposed based on thermal transport physics and observations. The model avoids the estimation of a heat budget at the atmosphere-water interface.
- (iv) A new biogeochemical model is developed which couples benthic sediment with pelagic water quality, and simulates pH based on carbonate chemistry.

Models	Model Components	Model Usage
	- Inflow	- Provide hydrologic
	- Outflow	conditions needed for
Hydrologic	- Rainfall	water quality modeling
model	- Evaporation	
	- Water level, surface area, and water	
	volume variation with time	
	- Watershed based	- Estimate the total
	- Instream water quality	nutrient loading directly
	- Runoff of water and dissolved	into the lake
Nutrient load	materials (or nutrients) on and through	- Determine the loading
model	the land surface	transfer coefficient from
	- Erosion of sediment and associated	the whole watershed to
	constituents from the land surface	the lake
Temperature	- Surface temperature	- Relate to biological
vertical profile	- Thermocline depth	and geochemical proces
model	- Heat dispersion coefficient	- Mixing and isolation
	- Characterization of physical-	- Predict short-term
Lake water quality	biological-geological chemistry	water quality, especially
vertical	- Vertical distribution	during algal growing
distribution model	- Model calibration	season
		- Study of hypolimnion
		water quality features
		- Study of sediment
		effects on water quality
	- Nutrient settling	- Predict seasonal and
Sediment-water	- Nutrient release	long-term water quality
interaction model	- Nutrient burying	- Provide information of
	- Nutrient utilization	sediment effect on wate
		quality

 Table 1-1
 Model Systems and Model Usage



Figure 1-1 General Study Procedures



Figure 1-2 Model Connections

CHAPTER 2

REVIEW OF WATERSHED AND LAKE WATER QUALITY MODELS

Lake water quality models require model inputs. Watershed water quality models can serve as the purpose of generating inputs for lake water quality models. In this chapter, we first introduce the various water quality models, and then discuss their relative strengths and weaknesses. Review of some commonly used and well-documented watershed models indicates that existing watershed models are not suitable for our lake water quality modeling objectives on a daily basis. Similarly, review of widely used lake models can not meet our modeling objectives to explore benthic sediment effects.

2.1 Review of Watershed Models

2.1.1 General Review

Until the late 1960s in the United States, *end of pipe* emissions of chemicals into the environment were believed to be the primary cause of water quality problems. Non-point source (NPS) pollution was almost an unrecognized phenomenon. Since the passage of the Water Pollution Act Amendments in 1972 (with its two later versions of 1977 and 1987, collectively referred to as the Clean Water Act), hundreds of billions of dollars have been spent on pollution cleanup. However, water quality of many rivers, lakes, and estuaries still were not sufficiently improved. During the 1970s and early 1980s, a number of influential research and management programs gradually led to the recognition that NPS from landscape features driven by hydrologic processes was a significant and often a major source of pollutant loads. These programs include the Pollution from Land

Use Reference Group (PLURP) of the International Joint Commission (IJC) established in 1972 for determining the levels and causes of pollution in the Great Lakes, the U.S. EPA Chesapeake Bay Program started in 1976, the U.S. EPA National Urban Runoff Project (NURP) from 1978 to 1983, and the federally sponsored Rural Clean Water Program (RCWP) beginning in 1980 (Novotny and Olem, 1994). Since the late 1970s, the study of NPS pollution has been an integral part of environmental science and engineering. The first treatise on NPS pollution (Novotny and Chesters, 1981) summarized the early studies and systematically examined the scientific basis and engineering techniques for NPS management and control. Recently this milestone text has been augmented to nearly double its original size by incorporating large amounts of new information accumulated over the past decade (Novotny and Olem, 1994). Since 1984, the U.S. EPA, as mandated by the Clean Water Act, has prepared a National Water Quality Inventory Report to Congress every two years to document the water quality status and impairments in rivers, lakes, and estuaries. The first report (U.S. EPA, 1984) pointed out that virtually every state identified some sort of NPS pollution problem. Agricultural was listed as the most pervasive source, followed by urban runoff, and mining and construction. Silviculture was considered as a substantial but localized problem.

A watershed model provides quantitative information and support for decisionmaking on watershed planning and management. A well-constructed watershed model incorporates both hydrology and water quality. Hydrologic models simulate the dynamic behavior of significant flow and storage processes, generating water balance information (e.g. quantity and associated hydraulic characteristics, sources and pathways, residence time.). Using the simulated water balance information, water quality models simulate pollutant loadings, physical transport, chemical and biological transformation processes within the surface, subsurface, and receiving water systems. Since the creation of the Stanford Watershed Model in the mid-1960s (Crawford and Linsley, 1966), many hydrologic models have been developed around the world. Historically, most of the early hydrologic models were designed for estimating water quantities in engineering applications such as flood forecasting, reservoir design, and water supply. Later, water quality components were developed and incorporated into water balance models. The rapid proliferation of watershed models and numerous application studies have attributed to many theoretical and technological advances.

2.1.2 Review of Existing Watershed Models

Many watershed models are readily available. The review in this chapter is intended to summarize models that are commonly used and well documented. The watershed models summarized here can be categorized as either urban or non-urban. Models intended for use in urban areas include STORM, SWMM, and DR3M-QUAL. Models intended for use in non-urban areas include CREAMS/GLEAMS, EPIC, SWRRB, PRZM, AGNPS, HSPF, WEPP, and SWAT. While several of these watershed models have been applied in both settings, they are categorized here based on their initial development. The following review focuses on modeling characteristics in hydrology, sediment production, and nutrient loading for different existing watershed models.

1) DR3M

The Distributed Routing, Rainfall, Runoff Model (DR3M) was developed by the U.S. Geological Survey (USGS) to simulate urban runoff at points within the watershed. The hydrographs generated by DR3M are used by a companion model, DR3M-QUAL, to simulate runoff water quality (Alley and Smith 1982b).

Hydrology

DR3M (Alley and Smith 1982a) segregates runoff into four types of segments: overland, channel, reservoir, and nodal. Each segment computes runoff differently. Runoff from overland segments is computed using the kinematic wave approximation. Infiltration is approximated using Green-Ampt methodology to compute rainfall excess. Two types of overland segments are considered, pervious and impervious. A portion of the rainfall may be stored in impervious areas but does not infiltrate. The time step and distance used in the kinematic wave approximation are set by the user. Routing in the channel segments is also done using kinematic wave. The user must specify the channel shape and size. Flow into a pipe may be simulated by specifying a circular channel shape. Reservoir routing can be simulated by linear storage or modified pulse routing. Nodal segments are those where three or more segments meet. Flow out of the nodal segment is computed as the sum of the segments entering the nodal segment. Nodal segments may also be used to input a hydrograph or remove runoff.

Sediment and other pollutants

The production of sediment is computed in DR3M-QUAL (Alley and Smith 1982b) as a function of time between storms, build up/wash off, for the impervious areas. Sediment from the pervious areas is computed using a regression relationship developed from the Universal Soil Loss Equation (USLE). Other constituents may be simulated as a fraction of the sediment. Soluble contaminants are not modeled. Pollutants in the channels are assumed not to mix, and the transport is simulated using Lagrangian methods. It is assumed reservoirs are plug flow and do not mix. Settling is allowed in reservoirs following Stokes' Law.

Model use

DR3M-QUAL is not presently available in PC form. DR3M is PC compatible, and the source code for the quality portion of the model is accessible. DR3M has received extensive use and review by USGS. DR3M-QUAL has been used in-house by USGS to a lesser extent.

2) SWMM

The Storm Water Management Model (SWMM) was developed in 1969-71 for the Environmental Protection Agency (EPA) by Metcalf and Eddy, Inc., in conjunction with University of Florida and Water Resources Engineers, Inc. SWMM has been updated several time over the years with version 4.30 being released in May 1994 (Center for Exposure Assessment Modeling (CEAM) 1994). SWMM is one of the most widely used urban water quality models (Wurbs 1995).

Hydrology

Runoff and routing in SWMM are more hydraulic than hydrologic (Viessman et al. 1977). Runoff from small sub-catchments (single parking lots, city lots, etc.) is first routed overland to gutters or storm drains using Manning's equation and continuity. Infiltration is computed using Horton's equation or Green-Ampt methodology. Depression storage fills before overland flow begins. Evapotranspiration is neglected. Once the overland flow enters a gutter or drain, the flow is combined with upstream flow and routed to the final outflow. The Extran Block in SWMM solves the complete dynamic flow routing equations (St. Venant's equation) to accurately simulate backwater, looped connections, surcharging, and pressure flow (CEAM 1994). SWMM may easily be calibrated using measured hydrographs at any point in the flow system.

Sediment and other pollutants

Several methods are available to simulate water quality. Estimation of sediment production from pervious areas is accomplished using USLE. In impervious areas, build-up/wash-off methods, rating curves, or constant concentration can be used. SWMM also simulates deposition and scour in sewers. First-order decay of constituents may be simulated (CEAM 1994).

Model use

SWMM has been widely used for urban sewage planning and has been continually updated and is supported by EPA's CEAM. A commercial PC version, XP-SWMM, is available with better data input interfaces.

3) STORM

The Hydrologic Engineering Center (HEC) developed the Storage, Treatment, Overflow Runoff Model (STORM) for use in urban areas in the early 1970's. The output from STORM is divided into statistics on runoff quality and quantity and pollutographs for individual events. The main use of STORM has been for sizing control structures (HEC 1977).

Hydrology

STORM (HEC 1977) uses three methods to compute surface runoff, the curve number method, a runoff coefficient method, or a combination method where curve numbers are used on pervious areas and coefficients are used on impervious areas. Evaporation and rainfall are user inputs. STORM computes soil moisture conditions from evaporation data to select the proper curve number. Dry weather flows are provided by the user to simulate combined sewers. Flow is routed using a unit hydrograph method. Storage, treatment, and overflow are computed hourly during rainfall events, but not during dry periods.

Sediment and other pollutants

Sediment production from pervious areas is computed using the USLE. Sediment production from other areas is based on daily build-up/wash-off relationships. Nitrogen, phosphorus, biochemical oxygen demand (BOD), and coliforms may also be simulated, but they are only represented by loading functions and do not degrade or cycle (HEC 1977).

Model use

STORM was applied in several runoff studies in the late 1970's and early 1980's (Donigian and Huber 1990). Abbott (1978) compared STORM to other continuous and event models as well as observational data and achieved good results.

4) CREAMS/GLEAMS

The Chemical, Runoff, and Erosion from Agricultural Management Systems (CREAMS) model was the first in a series of models developed by the U.S. Department of Agriculture. The original model focused on surface water quality, but groundwater quality was added to form the Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) model (Knisel 1993). GLEAMS has replaced CREAMS for the most part, but CREAMS is the recognized predecessor for several other models. CREAMS is a field-scale model used to look at edge of field loading sediment, nutrients, and pesticides with various management practices. With the additions in GLEAMS, leaching below the root zone may also be examined (Knisel 1993). CREAMS/GLEAMS is one of the most detailed field-scale models currently in use. USDA's Agriculture

Research Service (USDA-ARS) has recently developed the Soil and Water Assessment Tool (SWAT) by extending GLEAMS to basin scale.

Hydrology

The hydrology component of the model is based on a daily water balance. Surface runoff is based on the curve number method when daily rainfall data are used. If breakpoint rainfall data are used, runoff is computed using Green-Ampt infiltration and kinematic wave routing. The peak runoff rate is estimated by regression relationships (Smith and Williams 1980). Percolation is computed using a storage-routing technique to predict flow through each soil layer. Lateral subsurface flow is computed for each soil layer using a kinematic storage model starting at the top layer and progressing downward (Knisel 1993). Soil evaporation may be computed using the Priestly-Taylor method or Penman-Monteith. Plant evapotranspiration is based on the Ritchie method and requires the leaf area index depending on the stage of crop growth. Snowmelt and transmission losses are also taken into account (Knisel 1993). The CREAMS/GLEAMS models have no channel routing because they are field-scale models.

Sediment and other pollutants

Sediment yield in CREAMS is computed using detachment, deposition, and transport equations. Detachment is divided into two categories, rill and interrill. Detachment in the interrill areas is based on rainfall energy, and rill erosion is based on flow velocities. The interrill erosion is computed first; then transport capacity is computed. If transport capacity of the overland flow exceeds the interrill sediment load, rill erosion is computed. The sediment load is the lesser of transport capacity and the combined rill-interrill sediment load. If the interrill sediment load exceeds transport capacity, deposition occurs. Five particle sizes are considered for sediment transport and detachment/deposition: sand, silt, clay, small aggregates, and large aggregates.

Deposition in small impoundments and transport and deposition in terraces or small channels is also considered (Foster et al. 1980). CREAMS/GLEAMS has a welldocumented submodel for dealing with pesticides that can handle up to 20 pesticides at once (Knisel 1993). The amount of pesticide lost to runoff is computed as a soluble fraction and an adsorbed fraction of the available pesticide that has not leached, volatilized, decayed, or otherwise been lost. Different methods of pesticide application, foliar or soil incorporated, are considered, and the effects on the initial concentrations of pesticides are computed. The amount of pesticide that leaches to the groundwater may also be determined using GLEAMS (Knisel 1993). No degradation is considered in the channels because the model only looks at edge of field concentration. Nitrogen losses are considered for both nitrate and organic nitrogen. The daily soil nitrate content is computed for each soil layer. The amount of nitrate that is leached from each layer is computed and will percolate to the groundwater or may reappear with return flow. Nitrate in the runoff is computed using the nitrate in the top soil layer only. Organic nitrogen is considered with the sediment with a loading function. Crop uptake of nitrogen is also considered. The different processes that affect nitrogen are considered, mineralization, immobilization, denitrification, volatilization, and fixation (Knisel 1993). Phosphorus is mainly transported with sediment such as organic nitrogen. Soluble phosphorus transported by runoff is computed from the level of phosphorus in the top soil layer. Application of fertilizers and crop growth and residue are taken into account when computing the nutrient levels in each soil layer (Knisel 1993).

Model use

CREAMS/GLEAMS models have been widely used in many areas (Knisel 1993). Long-term studies on well-instrumented fields have shown that the methodologies used in CREAMS/GLEAMS work well. The models are readily available for PC use.

5) EPIC

Concerns over the possible decrease in agricultural productivity due to soil loss prompted the creation of the Erosion/Productivity Impact Calculator (EPIC) model. EPIC was developed to determine the long-term productivity of soil using various management strategies (Williams 1994 and Dumesnil 1993). Simulations using EPIC are usually done on small areas over a long period of time. Since the model's main purpose is to compute productivity, a greater portion of the model deals with crop growth compared with other models, but water yield, sediment production, and nutrient removal are also considered (Williams 1994).

Hydrology

The hydrology component of the model is based on a daily water balance. Surface runoff is based on the curve number method, and the peak runoff rate is estimated by the rational formula. Percolation is computed using a storage-routing technique to predict flow through each soil layer. Once water has percolated past the root zone, it is considered groundwater and lost from the model. Lateral subsurface flow is computed for each soil layer using a kinematic storage model starting at the top layer and progressing downward. Soil evaporation may be computed using either the Penman-Monteith method or the Priestly-Taylor method. Plant evapotranspiration is based on the Ritchie method and requires the leaf area index depending on the stage of crop growth. Snowmelt and transmission losses are also taken into account. Since EPIC is a small-scale model, channel routing is not considered. Irrigation of crops may be considered with the daily water balance (Williams 1994 and Sharpley and Williams 1990).

Sediment and other pollutants

Sediment yield may be computed in one of three ways specified by the user, USLE, Revised USLE (RUSLE), or the Onstad-Foster modification of the USLE. Erosion from furrow irrigation is always computed using RUSLE. The variation between these models is the energy factor used to drive erosion; USLE uses rainfall only, RUSLE uses runoff only, and Onstad-Foster uses a combination of rainfall and runoff. As sediment leaves the field, the surface layer of soil is reduced in thickness until it no longer remains. Erosion continues to move through the soil profile, allowing for soil weathering (Williams 1994 and Sharpley and Williams, 1990). Wind erosion is computed, but washoff does not affect runoff sediment loads (Sharpley and Williams 1990). Losses of nitrate are considered from the top layer of soil only. Nitrate that is adsorbed and in solution may leave with the runoff. Nitrate in solution may also leave the field though percolation or lateral subsurface flow. Loading functions for organic nitrogen are also provided. Nitrogen may be moved into the top soil layer as water in that layer evaporates and water from lower layers enters. The nitrogen cycle is simulated by the processes of mineralization, immobilization, and fixation. The denitrification, concentration of nitrogen in rainfall may also be included. Phosphorus is transported in solution or with sediment. The phosphorus cycle includes mineralization, immobilization, and mineral cycling. EPIC does not track pesticide losses (Williams 1994, and Sharpley and Williams 1990).

Other features

EPIC is able to generate long-term sediment predictions because of its built-in weather generator and weather database (Sharpley and Williams 1990). Rainfall timing is based on the probability of a wet day following a dry day and a wet day following a wet day. Daily rainfall amounts are predicted using a skewed normal distribution with the mean rainfall and standard deviation for the month. Air temperature and solar radiation are correlated with rainfall. Wind speed is predicted from a two-parameter gamma distribution, and direction is based on a cumulative probability distribution. Daily relative humidity is derived using the monthly average and a triangular distribution and adjusting
for a wet or dry day. Soil temperature and soil pH are also computed and applied to the nutrient cycle. EPIC includes a crop growth simulator to account for various stages of crop growth and their impacts such as nutrient uptake, transpiration, and soil residue. An economic section is included to further assess soil productivity (Williams 1994, and Sharpley and Williams 1990).

Model use

EPIC has been used to simulate many different things, soil productivity, crop growth, and soil degradation (Dumesnil 1993). Sharpley and Williams (1990) report on the validation of the model components and application of the complete model to differing soils and climates. Sensitivity analysis was also reported. EPIC is available for PC use and is well documented and supported by USDA-ARS.

6) SWRRB

The SWRRB (Simulator for Water Resources in Rural Basins) model was developed by the USDA-ARS to determine the effects of management practices on water and sediment yields in small ungaged rural basins (Arnold and Williams 1994). The model was developed by the USDA extending the CREAMS/GLEAMS methodology from field scale to basin scale. The major processes included in the model are surface runoff, percolation, return flow, transmission losses, pond and reservoir storage, sedimentation, pesticide fate, nutrient cycling, and crop growth. Several subbasins with varying soil, crop, and weather conditions can be simulated as part of a single watershed. The model was designed to look at long-term effects of management strategies, but single runoff events can be simulated.

Hydrology

The hydrology component of the model is based on a daily water balance. Surface runoff is based on the curve number method, and the peak runoff rate can be estimated by either the rational formula or TR-55 method. Percolation is computed using a storage-routing technique with a crack flow model to predict flow through each soil layer. Once water has percolated past the root zone, it is considered groundwater, but may appear as return flow in downstream basins. Lateral subsurface flow is computed for each soil layer using a kinematic storage model starting at the top layer and progressing downward. Soil evaporation may be computed using either the Hargreaves-Samani method or the Priestly-Taylor method. Plant evapotranspiration is based on the Ritchie method and requires the leaf area index depending on the stage of crop growth. Snow-melt and transmission losses are also taken into account (Arnold and Williams 1994). Flood routing is not performed because SWRRB is a long-term water and sediment yield predictor. Daily basin outflow is computed by summing the subbasin outflow. Farm ponds and reservoirs can be simulated with SWRRB. Irrigation of crops may be considered with the daily water balance (Arnold and Williams 1994).

Sediment and other pollutants

Sediment yield is computed for each subbasin using RUSLE. Sediment in channel routing consists of two processes operating simultaneously, deposition and degradation. Stokes' Law is applied to each sediment size for each channel reach to determine deposition. Channel degradation is a function of the stream power. Sediment is allowed to be deposited and reentrained in the channel before reaching the basin outlet. A sediment balance is maintained for ponds and reservoirs as well (Arnold and Williams 1994). SWRRB uses the same methodology as GLEAMS (Knisel 1993) to deal with pesticides. First the amount of pesticide reaching the ground is computed dependent on the stage of crop growth. The amount of pesticide that leaches to the groundwater is

computed. The amount of pesticide lost to runoff is computed as a soluble fraction and an adsorbed fraction of the available pesticide that has not leached, volatilized, decayed, or otherwise been lost. Pesticides that are adsorbed to sediment are allowed to be deposited in the channel. Soluble pesticides are considered conservative in the channel and do not degrade (Arnold and Williams 1994). Nitrogen losses are considered for both nitrate and organic nitrogen. For nitrate, the daily soil nitrate content is computed for each soil layer. The amount of nitrate that is leached from each layer is computed and will percolate to the groundwater or may reappear with return flow. Nitrate in the runoff is computed using the nitrate in the top soil layer only. Organic nitrogen is considered with the sediment with a loading function. Crop uptake of nitrogen is also considered. Phosphorus is mainly transported with sediment such as organic nitrogen. Soluble phosphorus transported by runoff is computed from the level of phosphorus in the top soil layer, but leaching is not considered. Soluble nutrients are considered conservative in the basin channels, but adsorbed nutrients may be deposited or entrained in the channel. Application of fertilizers and crop growth and residue are taken into account when computing the nutrient levels in each soil layer (Arnold and Williams 1994).

Other features

SWRRB allows the user to input the required weather data (daily rainfall and temperature), or a stochastic weather generator can simulate the weather. Solar radiation is always simulated. The probability of a rainfall event is simulated using a first-order Markov chain. The amount is simulated from a skewed normal distribution when rainfall does occur. Temperature and solar radiation are simulated using Richardson's model which correlates temperature and radiation with precipitation. Weather may be simulated for the entire basin or each subbasin individually. The parameters needed for the weather generator are included with the model for locations across the United States including

Puerto Rico (Arnold and Williams 1994). Tillage practices, crop residue, and crop growth are simulated as well as how they affect soil properties. Data for numerous soils that may be used are included with the model or may be input by the user for each subbasin. A utility program is included to assist with data entry, but the input is still in tabular form. The output is in tabular form. SWRRB has been combined successfully with a lake water quality model to simulate the end effects of management decisions (Arnold and Williams 1994).

Model use

SWRRB has been applied to predict urbanization, coastal pollution, pesticide assessment, pond irrigation, and water rights (Arnold and Williams 1994). Support and documentation for the PC version of SWRRB are available from USDA-ARS.

7) WEPP

The objective of the Water Erosion Prediction Project (WEPP) is to develop a newgeneration, process-oriented model to predict soil erosion. The WEPP model represents the start of a new generation of USDA models. It was developed for continuous simulations of small watersheds, less than 260 ha, or individual hillslopes. WEPP allows the user to look at spatial and temporal variations in sediment production. While this newly developed model uses some of the most up-to-date methodology, since some components are missing it is not a complete water quality model (Flanagan et al. 1995).

Hydrology

The hydrology of WEPP is more complex and physically based than SWRRB. The hydrology component of the model is based on a daily water balance. Surface runoff is computed as the rainfall excess, rainfall less infiltration, rather than using an empirical method. Infiltration is computed using the Green-Ampt equation as modified by Mein and Larson. Peak runoff and runoff rate are computed by routing the rainfall excess downslope using the kinematic wave approximation. Percolation is computed using methods similar to SWRRB as well as simulating flow to drain tiles and ditches. WEPP computes soil evaporation using either the Penman method or the Priestly-Taylor method. Plant evapotranspiration is based on the Ritchie method and requires the leaf area index depending on the stage of crop growth (Stone et al. 1995). Snowmelt and transmission losses are also taken into account (Savabi et al. 1995). In the watershed mode, WEPP routes hillslope runoff through channels to compute the basin outflow. Farm ponds and reservoirs can be simulated as with SWRRB (Ascough et al. 1995). Irrigation of crop may be considered with the daily water balance.

Sediment and other pollutants

WEPP computes sediment yield in a method similar to CREAMS/GLEAMS. Sediment production is divided into two parts, rill and interrill. Detachment in the interrill areas is a function of rainfall intensity, and the detachment process is dominated by raindrop impact. All interrill sediment is carried to the rills or small channels. The transport capacity of the rill is then computed, and interrill sediment is either deposited or transported. If the rill has an excess transport capacity, detachment of sediment in the rill is assumed to occur. Various soil particle sizes are considered (Foster et al. 1995). Unlike CREAMS/GLEAMS, transport capacity and shear stress is based on rill hydraulics rather than sheet flow. Sediment is allowed to be deposited and detached in the channel when using the watershed version of WEPP (Ascough et al. 1995). Unlike the other model, WEPP does not rely on the USLE to incorporate management factors, but rather focuses on the physical processes.

Other features

WEPP uses the weather generator developed for EPIC and SWRRB with some additions and refinements (Nicks, Lane, and Gander 1995). The probability of a rainfall event is simulated using a first-order Markov chain. When rainfall does occur, the amount is simulated from a skewed normal distribution. Temperature and solar radiation are simulated using Richardson's model which correlates temperature and radiation with precipitation. Dew point, wind speed, and direction are additions for use by the evapotranspiration computations. Weather may be simulated for the entire basin or each hillslope individually. The weather files included with WEPP are not as extensive as SWRRB at this time. Linking WEPP with GIS and the National Climatic Data Center is currently being explored (Flanagan et al. 1995). Tillage practices, crop residue, and crop growth are simulated as well as how they affect soil properties. Data for several soils that may be used are included with the model or may be input by the user for each subbasin. The user can use several previously developed files to create a watershed by combining soils, weather, conservation practices, slope, and channel files.

Model use

Many of the components of WEPP have been evaluated separately, but no widespread use of WEPP has been reported. The model is still under development and has yet to be fully evaluated. Components of WEPP may be used in other models. PC versions of the model, as well as documentation, support, and development, are available from the USDA-ARS National Soil Erosion Laboratory.

8) SWAT

The Soil and Water Assessment Tool (SWAT) model is the latest model developed by the USDA-ARS. Where SWRRB was an extension of CREAMS/GLEAMS from field scale to small watershed scale, SWAT is the extension of SWRRB to basin scale (Arnold et al. 1995). SWAT was developed by including ROTO (Routing Output to Outlets) with SWRBB. Complete flow and contaminant routing is accomplished as well as the inclusion of GIS interfaces, a weather generator, lake water quality, and water management options.

Hydrology

Runoff is estimated using daily rainfall data using the curve number method with peak runoff computed using a modification of the rational method. Time to concentration for both channels and overland flow is estimated using Manning's equation. Percolation and lateral subsurface flow are computed together and are based on storage routing and kinematic routing. Groundwater flow is simulated based on a shallow aquifer model with evaporation, pumping, seepage, and discharge being included. The daily water balance includes evapotranspiration based on Hargreaves-Samani, Priestly-Taylor, or Penman-Monteith equations. Plant transpiration is based on the Ritchie method. Transmission losses in channels are considered along with ponds and other small structures that will reduce runoff quantity (Arnold et al. 1995). Water may be transferred from one portion of the watershed to another to simulate pumping and irrigation.

Sediment and other pollutants

Sediment yield is based on the RUSLE. Nitrogen, phosphorus, and pesticides are simulated using the CREAMS/GLEAMS (Knisel 1993) models including biochemical processes and groundwater loading as described earlier in this report. Chemical degradation is not simulated in the channels during runoff events, but a lake water quality model has been added to simulate lake processes. Sediment-bound chemicals may settle and be detached in channels. Crop growth simulators are included to account for changing ground cover and plant uptake of nutrients. Point sources may also be included in the simulations (Arnold et al. 1995).

Other features

SWAT includes a weather generator similar to the one used in EPIC, SWRRB, and WEPP for long-term simulations and numerous weather station locations to reduce user input (Arnold et al. 1995). Weather may be simulated for the entire basin or for each subwatershed individually as is done in SWRRB (Arnold and Williams 1994). SWAT also includes an interface with GRASS (Geographic Resources Analysis Support System) GIS (Arnold et al. 1995). This allows the user to easily input data from a large heterogeneous basin. One feature in SWAT not seen in any other model is the mixing of watershed delineation techniques. A grid system, as seen in AGNPS (Agricultural Non-Point Source pollution model), may be used in areas of special interest while the rest of the basin may be simulated as more homogeneous subwatersheds. This allows detailed simulation of areas of interest without a large increase in input data (Arnold et al. 1995).

Model use

SWRRB and ROTO have both been extensively tested. SWAT has been applied to several gaged watersheds and rendered good results. PC versions of SWAT along with support and documentation are available from USDA-ARS.

9) HSPF

The Hydrologic Simulation Program—FORTRAN (HSPF) model may be one of the most complete models to deal with urban and non-urban runoff (Donigian and Huber 1990). The hydrology of HSPF is based on the Stanford Watershed Model, developed in the early 1960's. Two erosion components deal with pervious and impervious areas separately to avoid forcing one type of model to operate in an area it was not designed to simulate. HSPF contains many submodels to simulate many of the physical, chemical, and biological processes in a watershed (Bicknell et al. 1993).

Hydrology

HSPF is based on the Stanford Watershed Model. HSPF uses basic relationships to represent the physical processes. The model, like most, is based on the water balance of the soil. Rainfall rate is a user input. Rainfall is reduced by an interception rate based on the type of ground cover. Evapotranspiration is based on adjusted pan evaporation data. HSPF divides the soil into two storage zones, an upper and a lower. Evaporation computations are based on the available water in each zone. Infiltration rates are assumed to diminish linearly over time during a storm event. Interflow storage is also considered. In the impervious areas, infiltration, interflow, and soil evaporation are assumed to not occur. Channel routing and reservoir storage are accomplished by using the time-area method and summing the inputs (Bicknell et al. 1993).

Sediment and other pollutants

Sediment production is based on detachment by rainfall and transport by the overland flow in a pervious area. Scouring of the soil matrix is also considered. Sand, silt, and clay transport are modeled separately in streams. Impervious sediment loading is determined by build-up/wash-off relationships. Sediment loading in channels and reservoirs is based on the sum of the incoming loads, and settling is allowed. Scour and deposition are based on shear stress calculations. Channels and reservoirs are considered well mixed (Bicknell et al. 1993). Nitrogen, phosphorus, and three pesticides may be simulated. Constituents may move with sediment, on the surface in solution or in the groundwater in solution. Sorption may be simulated using first-order kinetics or Freundlich isotherms. HSPF also accounts for up to two degradation products of pesticides. Nutrient cycles and instream kinetics are simulated. Decay and instream kinetics include hydrolysis, oxidation, photolysis, volatilization, biodegradation, and generalized first-order decay (Bicknell et al. 1993). Other constituents that may be

simulated include water temperature, dissolved oxygen, BOD, and algal populations (benthic, phytoplankton, and zooplankton).

Model use

HSPF has been widely used in both urban and non-urban areas and is well validated in these areas (Donigian and Huber 1990). The EPA supports HSPF, and extensive documentation is available. Short courses on the use of HSPF are regularly provided as well. PC versions of the model are available and upgrades continue. The model is supported by both EPA and USGS.

10) AGNPS

Another model that was developed for agricultural watersheds is the Agricultural Non-Point Source (AGNPS) pollution model. Unlike most other models, AGNPS divides the watershed into cells based on a grid pattern. Each cell is modeled simultaneously with each other cell. The ability to set various parameters individually for each cell means better spatial description but more data input. The model was originally developed to determine the impact of feedlots on runoff quality, but it may operate with multiple point sources or as a non-point source model. The model will accommodate up to 28,000 cells ranging in size from 0.1 to 100 acres (0.0405 to 40.5 ha), but it is most commonly used for smaller watersheds (Young et al. 1994).

Hydrology

The current version of AGNPS is an event model; therefore, many of the hydrologic components normally found in other models are missing. Runoff is computed using the curve number method. Peak runoff may either be computed using TR-55 or the CREAMS method. The user must route the flow from cell to cell. Storm duration, intensity, and type must be entered for the entire watershed. The shape of the runoff

hydrograph may also be specified by the user. Once the runoff leaves a cell it is considered to flow in channels to the outlet of the watershed. The user may specify channel shapes and flow characteristics. The user may include impoundments in the channel system, and cells may have no flow outlet to simulate features such as sink holes (Young et al. 1994).

Sediment and other pollutants

Sediment production from each cell is computed using the RUSLE. Differing slopes, slope shapes, soils, and management practices can be considered for each cell. When the sediment reaches a channel, the transport capacity of the channel is computed for differing sediment sizes to determine if there will be deposition or channel detachment. The Einstein approach is used to determine transport capacity (Young et al. 1994). Nitrogen, phosphorus, pesticide, and chemical oxygen demand concentrations may be tracked from either point or non-point sources. For point sources the flow rate from the cell and the pollutant concentrations must be specified. In the case of a feedlot, runoff will be computed and pollutant loads may either be specified or computed by the model based on the size and type of feedlot. Non-point pollution loads are calculated based on the runoff and sediment loads. Nutrients are allowed to decay in impoundments and channels. The nitrogen concentration of the rainfall may be specified by the user. Fertilizer application rates, timing, and methods may be specified. If a pesticide is simulated, its concentration in solution and in the sediment is kept in equilibrium using its partition coefficient. At this time only one pesticide may be simulated for each event (Young et al. 1994).

Other features

The main drawback to a grid type model like AGNPS is the large amount of data needed to simulate a large watershed. To help alleviate this drawback, AGNPS allows the

use to set larger cell sizes and then sub-divide the cell up to 64 times to simulate specific small features without increasing the data requirements for the entire watershed. Onscreen help is available for data entry along with a routine to check the data. Work is under way to link AGNPS with ARC-INFO and GRASS GIS databases to assist with data input and output analyses (Young et al. 1994).

Model use

AGNPS is available in a PC version and is well documented. Limited support is available through USDA-ARS (Young et al. 1994). Several studies have used AGNPS to determine pollution loading from events and assist in the reduction of runoff pollution from feedlots. The current version of AGNPS is an event model, but work is continuing on producing a continuous version. Research on AGNPS has been ongoing for numerous years.

2.1.3 Discussion

Review of watershed models shows that HSPF and SWAT are the most comprehensive models. The in-stream processes are better in HSPF, but SWAT deals more completely with field processes and groundwater. Several areas could be improved in both SWAT and HSPF. Runoff in SWAT is currently based on the curve number method and the rational method to compute peak runoff rate. The use of the curve number for computing water balance is limited in its accuracy. This should be improved by simulating breakpoint rainfall and computing infiltration as in WEPP. The runoff could then be routed using kinematic wave approximations as in HSPF, WEPP, or the second option in CREAMS/GLEAMS. This could be included as a user-selected option because use of curve numbers may suffice for larger watersheds. HSPF could use updates to the hydrology section and development of an interface to improve both preprocessing and post-processing capabilities.

Current research being undertaken by the EPA focuses on the development of a GIS and pre-processor and post-processor for HSPF. The efforts of the EPA have created a software package known as Better Assessment Science Integrating a Point and Non-point Sources (BASINS). One of current limitations of the BASINS package is that the database is structured such that is not easily modified for site-specific applications. An advantage of the BASINS program is that several options are available for routing water through stream channels. Other than the HSPF routing methods, QUAL2E and TOXIROUTE are available within the system. Another system developed by the U.S. Army Engineer Waterways Experiment Station (WES) is the Watershed Modeling System (WMS). This state-of-the-art system allows for utilization of available GIS data for delineation of watershed boundaries and assignment of attributes such as land use type, soil type, etc. The WMS offers pre-processing and post-processing capabilities and the flexibility to build unique watershed databases from user provided data.

It can be seen from the review that almost every existing watershed model uses Universal Soil Loss Equation (USLE) or Revised Universal Soil Loss Equation (RUSLE) to estimate sediment production and then to estimate non-point source loading by using empirical nutrient concentrations in the runoff. It is well known that the factors used in USLE or RUSLE (e.g. erosivity index R, soil erodibility factor K, field slope S and length L, crop management factor C, and conservation practice factor P) are difficult to quantify accurately. Moreover USLE or RUSLE was developed for the estimation of annual sediment production from field-scale data, rather than daily-basis. Recently, some researchers applied Geographical Information Systems (GIS) to determine the important factors such as topographic factor, soil type and land use, etc. Application of GIS has already simplified watershed modeling, but because of the complicated processes of sedimentation and the difficulty to determine nutrient concentrations in the runoff, its accuracy is limited. In addition, the approach focuses on soil erosion and non-point source to the whole water network in the watershed, therefore it is difficult to give information for the final receiving water body. Because our study focuses on Lake Lanier water quality dynamics, we need to quantify sediment associated with nutrient loadings into Lake Lanier on a daily basis, existing watershed models are not suitable for our modeling objectives.

2.2 Review of Lake Models

2.2.1 General Review

A common cause of impairment to lake or reservoir use is eutrophication, or increase in primary productivity. Eutrophication can become a problem in reservoirs or lakes when the main tributaries import large nutrient loads over time scales that are short relative to the ability of the aquatic ecosystem to adapt to the loading. Large nutrient loads facilitate increasing populations of primary producers. Large numbers of primary producers can affect functions such as recreation and habitat maintenance or increase the cost of uses such as drinking water.

Study of the causes and consequences of eutrophication and potential mitigation actions is complex for any lake or impoundment. These studies are often accomplished with the help of models of various types. Models are essential tools in studies of large reservoirs or lakes due to their complexity in terms of morphometry, hydrology, ecology, and internal and external forcing functions.

During the early stages of development of mechanistic hydrodynamic models, Orlob (1975) stated that circulation is an important determinant of ecosystem responses. This belief was reiterated more recently (Falconer et al., 1991), reflecting its then and current role in motivating development and use of reservoir models with greater hydrodynamic

complexity. Ecological simulation models that include circulation processes seek to understand their influence on temperature zonation and vertical stratification, in-lake and outflow water quality, primary productivity, turbidity along with the light environment, habitat loss or creation, and hydraulic residence time variation as a result of sedimentation (Kim et al., 1983; Martin, 1989; Falconer et al., 1991; Okabe et al., 1993; Carrick et al., 1994; Leclerc et al., 1995; Shen et al., 1995; Ziegler and Nisbet, 1995; Bailey and Himilton, 1997; Himilton and Schladow, 1997; Schladow and Himilton, 1997; Soyupak et al., 1997).

Jorgenson (1994) reviews the role of ecological models in ecosystem understanding and environmental management. He states the case for the necessity that models increase in complexity in order to understand the system under study and its stressors. This understanding is needed to provide input to management and political decisions about actions to be taken as a response to observed or expected conditions. Straskraba (1994) discusses the management role many models can fulfill. The difference between the use of a model for ecological understanding and its use as a management or technological tool is often simply the perspective of the researcher. Ecological results may have management implications and vice versa. Thus, understanding the ecosystem of a lake or reservoir is an important aspect of research in lacustrine environments.

A detailed survey of the literature noted that many lake models applied in various regions. Lake models first arose in the 1970s. During this period, there were a large number of similar lake ecosystem models and a few unique lake models with limited applications (Anderson et al., 1976; Brylinsky and Mann, 1973; Chen and Orlob, 1972, 1973; Chen and Smith, 1976; Dillon and Rigler, 1975; Hornberger et al., 1975; Lehman et al., 1975; Scavia and Park, 1976). Table 2-1 summarizes these models in terms of various qualities. The models can be classified as four categories as to their methods: deterministic-conceptual (DC), deterministic-empirical (DE), stochastic-conceptual (SC),

and stochastic-empirical (SE). These classifications were described in detail by Clarke (1973). Deterministic models imply that the variables do not exhibit random fluctuation, while stochastic modeling includes random variation associated with some probability distribution in the model estimation procedure. Conceptual models generally imply that variables and formulations have some physical meaning. In contrast, empirical models treat the system as a *black box*, with internal variables and relationships having little or no physical interpretation.

Additional software packages of comprehensive water quality models were developed in 1980s or later (Table 2-2), such as EPA's models of WASP and CE-QUAL. Model structures made little improvement compared with 1970s models, and few people developed new models. Many researchers applied the newer versions of existing software packages (Daniel et al., 1999; Lung et al., 1993; Bierman et al., 1995; Lung and Larson, 1995).

The choice of a mathematical model to simulate water quality conditions in a lake or reservoir system depends on the characteristics of the system to be simulated, the desired level of precision, modeling objectives, and the available data. Flow conditions in the system, in general, determine the types of model structure due to advective and diffusive processes.

Generally, the types of models may be classified according to flow conditions, mass transport and chemical-biological processes. The models have different formulas due to difference between flow conditions in reservoirs and free flowing rivers. Flow velocity in a reservoir is low and the depth great. The main processes usually take place vertically. There is greater velocity in a river than in a reservoir and mass transport is produced predominantly in the longitudinal direction, with less influence from the transverse and vertical directions. Reservoir model classification may be performed according to different criteria. The classification based on spatial discretization is as follows:

(1) Zero-dimensional models: A coarse representation of the water system as a continuously stirred tank reactor (CSTR) is often sufficient for problem applications to lakes where detailed hydrodynamics are not required. No transport direction can be specified because there is only a single element in this zero-dimensional type of representation. The quantity of flow entering and leaving the system alone determines water volume changes within the element. Examples of zero-dimensional models include lake models by Vollenweider (1964); Vollenweider (1969); Vollenweider (1975).

(2) One-dimensional models: These models simulate the processes taking into account only one dimension in space. Usually longitudinal or vertical one-dimensional models are used in the studies. The former takes into account the velocity and level of concentration variation in the longitudinal direction, ignoring transverse and vertical variations. Vertical one-dimensional representations are common for lake systems with long residence times and stratification in the vertical direction. Horizontal layers are imposed and advective transport is assumed to occur only in the vertical direction, and generally the tributary inflows and outflows are assumed to enter and leave the lake at water levels of equal density. Because water is essentially incompressible inflows are assumed to generate vertical advective flow (via continuity equation) between all elements above the level of entry. The elements below this level, containing higher density water, are assumed to be unaffected. Examples of one-dimensional lake models include Lombardo (1972, 1973); Baca et al. (1976); Chen and Orlob (1975); Thomann et al. (1975); HEC (1974); Markofsky and Harleman (1973); and CE-QUAL-R1 (1982).

(3) Two-dimensional models - These are models which neglect one of the directions. The model may be two-dimensional vertically averaged model or two-dimensional laterally averaged model.

- (a) Vertically averaged, two-dimensional models have been proven to be quite useful, especially in modeling the hydrodynamics and water quality of relatively shallow and wind-driven lakes. The crucial assumption of these models is the vertically well-mixed layer that allows for vertical integration of the continuity, momentum, and mass-transport equations. Such models are frequently employed to provide the horizontal advection for water quality models since they are relatively inexpensive to operate compared to the alternatives of large scale field measurement programs or fully three-dimensional model treatments. There exist well over fifty models which would fit into the two-dimensional, vertically averaged classification. Examples of models that have been widely used and publicized include Taylor and Pagenkopf (1981); and Simons (1976).
- (b) Laterally averaged lake models have advantages when a lake exhibits significant vertical and longitudinal variations in density and water quality conditions. Two-dimensional laterally averaged models require the assumption of uniform lateral mixing in the cross channel direction. Although this simplification eliminates one horizontal dimension, the solution of the motion equations in the remaining longitudinal and vertical dimensions requires a more rigorous approach for two-dimensional vertically averaged models. Both the motion (continuity and momentum) and advective-diffusion equations must be solved simultaneously to correctly simulate the vertical effects of density gradients on the hydrodynamics and mass transport. In addition, such models must also treat the vertical eddy viscosity (momentum transfer due to velocity gradients) and eddy diffusivity (mass transfer due to concentration gradients) coefficients, which are directly related to the degree of internal mixing and the density structure over the water column. Mathematical treatment of vertical diffusion and vertical momentum

transfer varies greatly between models. Examples of laterally averaged lake models include Edinger and Buckak (1979); and Norton et al. (1973).

(4) Three-dimensional models: Fully three-dimensional and layered models have been the subject of considerable attention. Although still a developing field, a few models that have been applied to lake systems with moderate success. As with laterally averaged two-dimensional models, the main technical difficulty in this approach is in the specification of the internal turbulent momentum transfer and mass diffusivities, which are ideally calibrated with field observations, thus making availability of adequate prototype data an important consideration. An additional factor of great importance is the relatively large computational cost of running three-dimensional models, especially for long-term water quality simulations. In many cases, the effort and cost of running such models is difficult to justify from purely a water quality standpoint. However, as computational costs continue to decrease and sophistication of numerical techniques increases, such models will eventually play an important role in supplying the large scale hydrodynamic regimes in water quality simulations. Examples of the more prominent three-dimensional models include Simons (1973); and King (1982);

Water quality models initially used a simplified simulation of dissolved oxygen (Bella, 1970). The models which followed them included nitrification processes and phytoplankton dynamics. Formulae for specific problems have been developed to consider forest flooding, gas formation and some types of macrophytes. The main difficulties in these methodologies have been to identify the parameters involved and the reliability of the mathematical formulae used.

2.2.2 Review of Widely-Used Lake Models

1) CE-QUAL-W2

CE-QUAL-W2 is a longitudinal-vertical hydrodynamic and transport model developed for long-term, time-varying water quality simulations of lakes, reservoirs, and estuaries. CE-QUAL-W2 can reproduce vertical and longitudinal water quality gradients and is capable of multi-decade simulations. CE-QUAL-W2 can be used to infer changes in circulation and water quality as well as provide boundary condition data to embedded 3-D models or to near-field models such as PLUMES or CORMIX (Cornell Mixing Zone Model). It is the reservoir model of choice for the ACE, USGS, USBR, TVA, and EPA. There have been over 100 applications with the model world wide.

CE-QUAL-W2 has been under development for ACE since 1974 and has had extensive review and testing by Johnson (1981). Previous verification studies using the earlier versions LARM (Laterally Averaged Reservoir Model) and GLVHT (Generalized Longitudinal-Vertical Hydrodynamics and Transport model), and CE-QUAL-W2 have been presented by Gordon (1980, 1981 and 1983); Edinger, Buchak and Merritt (1983); Kim, Higgins and Bruggink (1983); Johnson, et al. (1981); and Martin (1988). Estuarine applications include Boatman and Buchak (1987); Buchak, et al. (1989); Buchak and Edinger (1989); Edinger, Buchak and Rives (1987); Johnson, et al. (1987); and, Johnson, et al. (1989). Lake or reservoir applications include Edinger and Buchak (1994). The model is described in Buchak and Edinger (1984) and Cole and Buchak (1993), which present formulations of the fundamental equations, the structure of the computations, and summaries of applications.

CE-QUAL-W2 presently includes water quality routines for 22 state variables: suspended solids, coliforms, total dissolved solids, labile DOM, refractory DOM, algae, detritus, phosphorous, ammonia, nitrate-nitrite, dissolved oxygen, CBOD, sediment, inorganic carbon, alkalinity, pH, carbon dioxide, bicarbonate, carbonate, iron, and a numerical tracer. Other variables and formulations can be accommodated in the modular code.

CE-QUAL-W2 is based on the laterally averaged equations of momentum, continuity, and transport. The formulation includes the vertically varying, longitudinal momentum balance, vertical momentum in the form of the hydrostatic approximation, local continuity, the free-water surface condition based on vertically integrated continuity, and longitudinal and vertical transport of any number of constituents. Constituents that determine density such as temperature and salinity are related to momentum through an equation of state. The vertically varying, longitudinal momentum balance includes local acceleration of horizontal velocity, horizontal and vertical advective momentum transfer, the horizontal pressure gradient, and horizontal and vertical shear stress. Included in the latter are the surface wind stress and the bottom stress due to friction.

The horizontal pressure gradient includes the barotropic surface slope and the baroclinic vertical integral of the horizontal density gradient which is the dominant term in density-induced, convective circulation. The time-varying solution technique of the model is based on an implicit, finite-difference scheme that results from the simultaneous solution of the horizontal momentum equation and the free-water surface equation of vertically integrated continuity. This technique results in the surface long wave equation that is solved on each time step to give the water surface profile, from which the vertical pressure distribution can be determined. The horizontal momentum is then computed, followed by internal continuity and then constituent transport.

The finite difference scheme is used for the advective processes in the constituent transport balances. Vertical turbulent transfer of momentum and constituents is determined from the vertical shear of horizontal velocity and a density gradient dependent Richardson number function. The boundary conditions at the open ends of the branches can be any combination of either flux or elevation conditions. The fluxes or elevations are specified from boundary data. The elevation boundary condition enters the formulation through the implicit long wave surface equation. Fluxes at the elevation boundary are computed from a reduced form of the longitudinal and vertical momentum equations which include the baroclinic, barotropic, vertical shear, and local acceleration terms but do not include the longitudinal spatial acceleration.

In 1998, Linmo-Tech Inc. applied CE-QUAL-W2 model to Lake Lanier (Limno-Tech, 1998). In this modeling, twelve water quality constituents were considered. The constituents and the respective internal fate pathways are listed in Table 2-3. Inflow, transport, and outflow are also pathways for all constituents. The interactions of these pathways are illustrated in Figure 2-1. The application simulated algal photosynthesis and respiration, phosphorus and nitrogen cycling, sediment-nutrient adsortion, metal (iron and manganese) – nutrient adsorption, and nutrient settling and release. pH and carbonate chemistry were not considered in this application. Nutrient release rates were estimated based on historic measurement of sediment oxygen demand (SOD) in 1991. No state variables in bottom sediment were simulated in the application, which indicates the application didn't couple water column and sediment completely. Model parameters in this application are shown in Table 2-4.

2) WASP5/DYNHYD5

(i) Modeling System

The WASP modeling system is a generalized modeling framework for contaminant fate and transport in surface waters. It can be applied in one, two, or three dimensions. Most applications are 2-D. WASP is designed to permit easy substitution of user-written routines into the program structure. Problems that have been studied using WASP include biochemical oxygen demand, dissolved oxygen dynamics, nutrients/eutrophication, bacterial contamination, and toxic chemical movement.

The WASP system consists of two stand-alone computer programs, DYNHYD and WASP, that can be run in conjunction or separately. DYNHYD is a hydrodynamics program which simulates the movement of water while the water quality program, WASP, simulates the movement and interaction of pollutants within the water. WASP is supplied with two kinetic submodels to simulate two of the major classes of water quality problems: conventional pollution (involving dissolved oxygen, biochemical oxygen demand, nutrients and eutrophication) and toxic pollution (involving organic chemicals, metals, and sediment). The linkage of either submodel with the WASP program gives the models EUTRO and TOXI, respectively.

The basic principle of both the hydrodynamics and water quality program is the conservation of mass. The water volume and water quality constituent masses being studied are tracked and accounted for over time and space using a series of mass balancing equations. The hydrodynamics program also conserves momentum, or energy, throughout time and space. The Hydrodynamic Program (DYNHYD) is a simple link-node hydrodynamic program capable of simulating variable tidal cycles, wind, and unsteady flows. It produces an output file that supplies flows, volumes, velocities, and depths (time averaged) for the WASP modeling system. The Eutrophication Model (EUTRO) combines a kinetic structure adapted from the Potomac Eutrophication Model with the WASP transport structure. This model predicts dissolved oxygen, carbonaceous biochemical oxygen demand, phytoplankton, carbon, chlorophyll-a, ammonia, nitrate, organic nitrogen, and orthophosphate in bed and overlying waters. The Toxic Chemical Model (TOXI) combines a kinetic structure adapted from the Exposure Analysis Modeling System (EXAMS) with the WASP transport structure and simple sediment

balance algorithms. TOXI predicts dissolved and sorbed chemical concentrations in the bed and overlying waters.

(ii) DYNHYD

The WASP hydrodynamics model DYNHYD is an enhancement of the Potomac Estuary hydrodynamic model which was a component of the Dynamic Estuary Model. DYNHYD solves the one-dimensional equations of continuity and momentum for a branching or channel-junction (link-node), computational network. Driven by variable upstream flows and downstream heads, simulations typically proceed at one- to fiveminute intervals. The resulting unsteady hydrodynamics are averaged over larger time intervals and stored for later use by the water quality program. The hydrodynamic model solves one-dimensional equations describing the propagation of a long wave through a shallow water system while conserving both momentum (energy) and volume (mass).

The equation of motion, based on the conservation of momentum, predicts water velocities and flows. The equation of continuity, based on the conservation of volume, predicts water heights (heads) and volumes. This approach assumes that flow is predominantly one-dimensional, Coriolis and other accelerations normal to the direction of flow are negligible, channels can be adequately represented by a constant top width with a variable hydraulic depth, i.e., rectangular, the wave length is significantly greater than the depth, and bottom slopes are moderate. Although no strict criteria are available for the latter two assumptions, most natural flow conditions in large rivers and estuaries would be acceptable. Dam-break situations could not be simulated DYNHYD nor could small mountain streams.

(iii) WASP

WASP is a dynamic compartment model that can be used to analyze a variety of water quality problems in such diverse water bodies as ponds, streams, lakes, reservoirs, rivers, estuaries, and coastal waters. This section presents the basic water quality model used to simulate dissolved, conservative chemicals such as chlorides or dye tracer. The equations solved by WASP are based on the key principle of the conservation of mass. This principle requires that the mass of each water quality constituent being investigated must be accounted for in one way or another. WASP traces each water quality constituent from the point of spatial ant temporal input to its final point of export, conserving mass in space and time. To perform these mass balance computations, the user must supply WASP with input data defining seven important characteristics: a) Simulation and output control; b) Model segmentation; c) Advective and dispersive transport; d) Boundary concentrations; e) Point and diffuse source waste loads; f) Kinetic parameters, constants, and time functions; and g) Initial concentrations.

WASP includes two water quality submodels EUTRO and TOXI. EUTRO is designed for conventional pollutants, and TOXI is designed for toxic pollutants.

a) EUTRO

Physical-chemical processes affect the transport and interaction among the nutrients, phytoplankton, carbonaceous material, and dissolved oxygen in the aquatic environment (Figure 2-2). EUTRO can be operated by the user at various levels of complexity to simulate some or all of these variables and interactions. To simulate only BOD and DO, for example, the user may bypass calculations for the nitrogen, phosphorus, and phytoplankton variables (the bypass option is documented in the User Manual). Six evels of complexity are identified in EUTRO: a) Streeter-Phelps; b) Modified Streeter-Phelps; c) Full linear DO balance; d) Simple eutrophication kinetics; e) Intermediate eutrophication kinetics; and f) Intermediate eutrophication kinetics with benthos.

EUTRO simulates the transport and transformation reactions of up to eight state variables. They can be considered as four interacting systems: phytoplankton kinetics, the phosphorus cycle, the nitrogen cycle and the dissolved oxygen balance. The general WASP mass balance equation is solved for each state variable. To this general equation, the EUTRO subroutines add specific transformation processes to customize the WASP transport equation for the eight state variables in the water column and benthos.

b) TOXI

TOXI is a dynamic compartment model of the transport and fate of organic chemicals and metals in all types of aquatic systems. It combines the hydrodynamic capabilities and the transport capabilities with the sediment balance and chemical transformation capabilities discussed. Several physical-chemical processes can affect the transport and fate of toxic chemicals in the aquatic environment. TOXI explicitly handles most of these excluding only reduction and precipitation-dissolution. If the kinetics of these reactions are described by the user, they can also be included as an extra reaction. TOXI simulates the transport and transformation of one to three chemicals and one to three types of particulate material (solid classes). The three chemicals may be independent or they may be linked with reaction yields, such as a parent compound-daughter product sequence. Each chemical exists as a neutral compound and up to four ionic species.

Neutral and ionic species can exist in five phases: dissolved, sorbed to dissolved organic carbon (DOC), and sorbed to each of the up to three types of solids. Local equilibrium is assumed so that the distribution of the chemical between each of the species and phases is defined by distribution or partition coefficients. In this fashion, the concentration of any species in any phase can be calculated from the total chemical concentration. Therefore, only a single state variable (WASP system) representing total concentration is required for each chemical. The model then is composed of up to six systems, three chemical and three solids, for which the general WASP mass balance equation is solved.

2.2.3 Major Trends

- (1) There is a tendency among some model users, and some model developers, to ascribe greater utility to models that are complex. This seems to be based on the fact that because aquatic ecosystems are complex, only complex mathematical models can be depended upon for an analysis of management issues concerning lake quality.
- (2) The spread of personal computers and the availability of workstations and supercomputers, as well as the ever escalating computing power and storage capacity of all machines, is dramatically reducing the amount of effort and computer time for designing and operating complex models. Therefore, numerous software packages of water quality models will occur on computer networks.
- (3) Model developers will address the use of automatic calibration and evaluation internal to the software to overcome the difficulties of model calibration and evaluation for users of water quality software package.
- (4) The modernization of hydro-meteorological and hydrogeochemical measurement techniques will significantly contribute to the development and application of water quality models. Increasing quantity and quality of on-site measurement data for model calibration and testing will result from modern technologies such as automation of data acquisition and transmission, and the use of chemical tracers.
- (5) Scientists will continue to advance environmental modeling as a discipline through philosophical thought and debates on (i) modeling objectives and assumptions, (ii) model design criteria and methods, (iii) scale issues, (iv) model calibration and evaluation, and (v) sensitivity and uncertainty analysis in the development and application of numerous models (Beck, 1983 and 1987; Beven, 1989; Sivapalan, 1995; Grayson et al., 1992; Jakeman and Hornberger, 1993; Wheater et al., 1993).

2.2.4 Discussion

Lake water quality modeling generally includes specifying three parts: inputs (including external and internal inputs), outputs, reactions or changes in the lake system. Among the three parts, model inputs are difficult to quantify and the reaction mechanisms in the lake system are not fully understood.

It is well known eutrophication is an important concern for many lakes, so the primary nutrient (N, P, C) loading in the input is usually considered. Nutrient loading includes point source and non-point source. In most watersheds, non-point source is more important than point source. There are three approaches to perform pollutant source evaluations: 1) Incorporating USLE or RUSLE with GIS; 2) Annual yield method based on empirical data; and 3) Rating-curve method based on intensive field data. The three approaches and the difficulty to quantify nutrient loadings have been discussed in Section 2.1.3.

Another challenge is the reaction mechanisms in the lake system which include physical and biogeochemical processes. Physical processes such as seasonal variations of temperature and lake stratification are relatively well known, but biogeochamical processes in the lake system and the effects of sediment are still uncertain. For example, diurnal variation of DO and pH in a lake is well known to be affected by algal photosynthesis and respiration. Literature review shows that conflicting mathematical formulations of photosynthesis and respiration are used. Dahl-Madsen and Strange Nielsen (1974), Patten et al. (1975), and Jørgensen (1976) expressed photosynthesis as functions of maximum growth rate, temperature, light intensity and controlling nutrients which include phosphorus, nitrogen and carbon. Other formulations of photosynthesis can be expanded to cover all three nutrients and even silicon, which must be included when diatoms are of importance for the eutrophication process (Chen, 1970; Chen and Orlob, 1975; Parker, 1972). Algal respiration was often described as first-order model reactions such as Gargas (1976) and Lehman et al.(1975). In order to determine suitable model structure of photosynthesis and respiration, Stigter and Beck (1997) used a controlled random search algorithm for calibration and a recursive prediction error algorithm as a verification tool. However, the success of this approach is greatly dependent on the pre-assumed definitions of algal photosynthesis and respiration. In my opinion, modeling of algal photosynthesis is relatively more effective than that of algal respiration.

Hypolimnetic DO can be regarded as a master indicator (Stumm and Morgan, 1996). Hypolimnetic DO is mainly influenced by algal photosynthesis and respiration, biochemical oxygen demand (BOD), benthic sediment oxygen demand (SOD), nitrification, atmospheric exchange, temperature, and diffusion. Among of these factors, respiration, exchange between atmosphere and different water layer, and benthic sediment effects are relatively not well understood. These issues will be addressed in this study.

Phosphorus (P) is considered the nutrient most frequently limiting to algal production in lakes (Carlson, 1977; Carpenter et al., 1998). Phosphorus occurs in lakes in both organic and inorganic forms. The form of phosphorus most readily available for biological uptake is dissolved inorganic phosphorus (DIP). Bioavailability of DIP is restricted by its tendency to precipitate in the presence of bivalent metal (Ca²⁺, Mg²⁺) and ferric (Fe³⁺) ions, and its tendency to sorb to clay and other amorphous inorganic particles such as aluminum and iron oxides (Parker and Rasmussen, 2001).

Phosphorus cycling in lake systems can be significantly affected by the iron cycle. Ferric oxides sorb DIP via ligand exchange. These ferric-phosphorus complexes can be transformed by reduction to the more soluble ferrous form, and the transformation releases sorbed phosphate. However, the high iron content in the soils and resident parent material of Georgia Piedmont results in significant transport of iron in runoff to receiving waterbodies. Hence the availability of inorganic phosphate is likely controlled by the iron cycle.

Conventional phosphorus cycling paradigm in lakes is based on data from systems in northern temperate regions. This paradigm involves the sinking of inorganic particulates and organic material from surface (epilimnetic) waters to the hypolimnetic waters of lakes during summer stratification. The depletion of oxygen and anoxic respiration in the hypolimnion creates reducing conditions in the buffered waters of northern-temperate lakes. As iron-phosphorus compounds are reduced and organic matter is decomposed in the anoxic hypolimnion, there is a steady increase in DIP which is circulated to the lake at fall mixis (Wetzel, 1983). This phophorus cycling paradigm fails to explain phosphorus cycling in Lake Lanier. Historical monitoring results in Lake Lanier indicate that 1) the oxidation-reduction potential never falls below 200mv, even in the presence of anoxic respiration; 2) there is no obvious phosphorus release from anoxic sediments; 3) there is no obvious increase in hypolinetic DIP; 4) there is no fall algal bloom after mixis. These characteristics in Lake Lanier indicate that our biogeochemical modeling should couple water column and benthic sediments, phopshorus and iron cycling, and nutrient-sediment adsorptions.

Reference	Туре	Dimension	Depth	System	Algae	Zooplankton	Fish	Temperature
Anderson et al. [1976]	DC	1	D	R	1	1	0	Internal
Brylinsky and Mann [1973]	SE	1	D	L	1	1	0	External
Chen and Orlob [1972]	DC	1	D	R	2	1	3	Internal
Chen and Smith [1976]	DC	1	D	L	2	1	3	Internal
Dillon and Rigler [1975]	DC	1	D	L	1	1	0	External
Fee [1973]	DC	1	D	L	1	1	0	External
Gallagher et al. [1973]	DC	2	S	L	0	0	0	Internal
Hornberger et al. [1975]	DC	0	D	L	Various	Various	1	External
Kontur [1974]	SE	1	D	L	0	0	0	External
Lehman et al. [1975]	DC	1	S	L	Various	0	0	Internal
McChesney and Edge [1976]	SC	1	D	Е	0	0	0	Internal
Newbold and Ligget [1974]	DC	1	D	L	1	1	0	External
Scavia and Park [1976]	DC	1	D	L	4	5	3	External
Simons [1972]	DC	3	D	L	0	0	0	Internal
Snodgrass and O'Media [1975]	DC	1	D	R	0	0	0	Internal
Stefan et al. [1976]	DC	1	D	L	1	1	0	Internal
Thibodeaux [1976]	DC	2	D	L, R	1	1	2	Internal
Weber [1974]	SE	1	D	L	0	0	0	External
Yang and Johnson [1974]	DC	1	S	L	1	1	3	Internal

Table 2-1 Summary of Lake Models in 1970s

Note:

Type: DC-deterministic-conceptual; SE-stochastic-empirical; SC-stochastic-conceptual

Depth: D-deep; S-shallow

System: R-reservoir; L-lake; E-estuary

Water Ouality	1-D Models					
Considerations	WQRRS	CE-QUAL-R1	RMA-1	DYRESM	MS-CLEANER	
Constituents:	-	-				
Coliform Bacteria						
Algae	\checkmark	\checkmark		\checkmark		
Organic Matter	\checkmark				\checkmark	
Suspended Solids						
Temperature						
DO						
BOD	Ń	Ń	Ń	Ń	Ń	
Phosphorus	Ń	Ń	Ń	V	Ń	
Nitrate-N	Ń	V	1	V	N	
Ammonia-N	Ń	Ń	J	Ń	N	
TDS	1	V	N	N	N	
Hydrodynamics Formulation	•	v	v	v	v	
Black Box	•				V	
N-S Equations	V		N		v	
Configured to Simulate:	v	Ŷ	•	,		
Multiple tributaries	N	N	N	N	N	
Selective withdrawal	Ń	Ń	,	,	v	
Inflow mixing and placement	1	Ŷ	2	2		
Biochemical process formula	v ations:		V	v		
Empirical	ations.					
Process-oriented	\checkmark					
Application:	•	,	,	•	,	
Previous Application						
Manual and	Ń	V	,	,	V	
Documentation	·	Ŷ			v	
Updates and Maintenance	\checkmark					
Public Distribution	V					
PC Compatible	Ń	Ń		Ń	Ń	
Graphical Output	•	V	•	V	V	
Personnel Requirements	М	Ň	М	Ň	Ņ	
Data Requirements	M	M	M	M	M	
(parameter/coefficients)					111	
User - Friendly	R	R	R	R	R	
Management Use	V					
Post-Audit Evaluation		Ň	,		, V	
Uncertainty Estimates						

 Table 2-2
 Summary of Lake and Reservoir Model Software

Note:

R = Reasonable; M = Moderate; E = Extensive; D = Difficult

Water Quality	2-D Models			3-D Models		
Considerations	CE-OUAL-W2	BETTER	RMA-2	WASP5	GL-3	
Constituents:	Ľ					
Coliform Bacteria						
Algae		\checkmark	V	\checkmark	\checkmark	
Organic Matter	Ń		V		V	
Suspended Solids		\checkmark			V	
Temperature		V	V		V	
DO		V	V	\checkmark	V	
BOD					V	
Phosphorus	Ń	Ń	Ń		Ń	
Nitrate-N	Ń	Ń	Ń		Ń	
Ammonia-N		V	V		V	
TDS	Ń	Ń	Ń	,	Ń	
Hydrodynamics Formulation						
Black Box						
N-S Equations			\checkmark	\checkmark	\checkmark	
Configured to Simulate:						
Multiple tributaries		\checkmark	\checkmark	\checkmark		
Selective withdrawal	\checkmark					
Inflow mixing and placement	\checkmark					
Biochemical process formula	ations:					
Empirical						
Process-oriented		\checkmark	\checkmark	\checkmark	\checkmark	
Application:						
Previous Application		\checkmark	\checkmark			
Manual and		\checkmark		\checkmark	\checkmark	
Documentation						
Updates and Maintenance		\checkmark	\checkmark		\checkmark	
Public Distribution		\checkmark		\checkmark	\checkmark	
PC Compatible	\checkmark	\checkmark		\checkmark	\checkmark	
Graphical Output	\checkmark	\checkmark	\checkmark		\checkmark	
Personnel Requirements	М	М	М	М	Е	
Data Requirements	М	М	М	Е	Е	
(parameter/coefficients)						
User - Friendly	М	М	М	М	D	
Management Use	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	
Post-Audit Evaluation						
Uncertainty Estimates						

 Table 2-2
 Summary of Lake and Reservoir Model Software (Con't)

Note:

R = Reasonable; M = Moderate; E = Extensive; D = Difficult

Constituents	Internal Source Modeled	Internal sink Modeled		
Temperature	Atmospheric heat exchange	Atmospheric heat exchange		
Suspended solids	None	Settling		
Labile dissolved organic	Algae mortality/excretion	Decomposition		
matter (LDOM)				
Refractory dissolved	Decomposition of LDOM	Decomposition		
organic matter (RDOM)				
Algae	Algal growth	Algal respiration, excretion,		
		mortality and settling		
Particulate organic	Algal mortality	Settling,		
matter (POM)		decomposition		
Phosphate	Algal respiration,	Algal growth,		
	decomposition of LDOM,	adsorption onto suspended		
	RDOM, POM,	solids		
	and sediment release			
Ammonia	Sediment release,	Algal growth,		
	algal respiration,	nitrification		
	decomposition of LDOM,			
	RDOM, and POM			
Nitrate + Nitrite	Nitrification	Algal growth		
Dissolved oxygen	Surface exchange,	Surface exchange,		
	algal growth	algal respiration,		
		nitrification, decomposition		
		of POM, LDOM, RDOM,		
		sediment oxygen demand		
Iron	Sediment release	Settling		
Manganese	Sediment release	Settling		

Table 2-3 Constituents Modeled and Internal Fate Pathways(Limno-Tech, 1998)

Parameter	Value
Extinction for water, m ⁻¹	0.30
Extinction due to inorganic suspended solids, m ³ m ⁻¹ g ⁻¹	0.01
Extinction due to organic suspended solids, m ³ m ⁻¹ g ⁻¹	0.10
Fraction of incident solar radiation absorbed at water surface, mday ⁻¹	0.36
Inorganic suspended solids settling rate, mday ¹	0.25
Algal growth rate, day^{-1}	2.30
Algal mortality rate, day ⁻¹	0.10
Algal excretion rate, day ⁻¹	0.04
Algal dark respiration rate, day ⁻¹	0.10
Algal settling rate, mday ¹	0.30
Saturation intensity at maximum photosynthetic rate, Wm ⁻²	100.0
Fraction of algal biomass lost by mortality to detritus	0.25
Lower temperature for maximum algal growth, °C	25.0
Lower temperature for algal growth, °C	5.0
Upper temperature for maximum algal growth, °C	33.0
Upper temperature for algal growth, °C	40.0
Fraction of algal growth rate at ALGT1	0.10
Fraction of maximum algal growth rate at ALGT2	0.99
Fraction of maximum algal growth rate at ALGT3	0.99
Fraction of algal growth rate at ALGT4	0.10
Labile DOM decay rate, day ¹	0.30
Labile to refractory decay rate, day ⁻¹	0.01
Maximum refractory decay rate, day ¹	0.01
Detritus decay rate, day ⁻¹	0.00
Detritus settling rate, mday ¹	0.30
Lower temperature for organic matter decay, °C	0.01
Lower temperature for maximum organic matter decay, °C	30.0
Fraction of organic matter decay rate at OMT1	0.10
Fraction of organic matter decay rate at OMT2	0.99

Table 2-4 Parameters of CE-QUAL-W2 Used in Lake Lanier Modeling (Limno-Tech, 1998)

Parameter	Value
Fraction inflow unavailable P as RDOM, days 150-250	0.25
Fraction inflow unavailable P as detritus, days 150-250	0.10
Sediment release rate of ammonia (fraction of SOD)	0.04
Ammonia decay rate, day ⁻¹	0.20
Algal half-saturation constant for ammonia	0.014
Lower temperature for ammonia decay, °C	5.0
Lower temperature for maximum ammonia decay, °C	25.0
Fraction of nitrification rate at NH4T1	0.10
Fraction of nitrification rate at NH4T2	0.99
Coefficient	1991
Nitrate decay, day ⁻¹	0.00
Lower temperature for nitrate decay, °C	5.0
Lower temperature for maximum nitrate decay, °C	25.0
Fraction of denitrification rate at NO3T1	0.10
Fraction of denitrification rate at NO3T2	0.99
Sediment release rate of iron (fraction of SOD)	0.1
Iron settling rate, mday-1	0.5
Sediment release rate of manganese (fraction of SOD)	0.1
Manganese settling rate, mday ⁻¹	0.5
Oxygen stoichiometric equivalent for ammonia decay	4.57
Oxygen stoichiometric equivalent for organic matter decay	1.4
Oxygen stoichiometric equivalent for dark respiration	1.1
Oxygen stoichiometric equivalent for algal growth	1.4
Stoichiometric equivalent between organic matter and phosphorus	0.011
Stoichiometric equivalent between organic matter and nitrogen	0.24
Stoichiometric equivalent between organic matter and carbon	0.45
Dissolved oxygen concentration at which anaerobic processes begin, gm ⁻³	1.0
Fraction of SOD	1.0

 Table 2-4
 Parameters of CE-QUAL-W2 Used in Lake Lanier Modeling (con't)


Figure 2-1 Water Quality Kinetic Pathways in CE-QUAL-W2 (Limno-Tech, 1998)



Figure 2-2 State Variable Interactions in EUTRO of WASP5

CHAPTER 3

WATERSHED AND LAKE WATER QUALITY CHARACTERIZATION

In this chapter, we include a description of Lake Lanier watershed, Lake Lanier water quality issues and characteristics, and introduce an application using principal components analysis and cluster analysis to: 1) classify correlated tributary water quality parameters into parameter categories that have similar temporal characteristics, 2) group tributaries into spatial categories that have similar water quality parameter characteristics, and 3) provide long-term water quality monitoring strategies. Principal components analysis of the water quality data set (from 1996/97) indicates that variability of suspended sediment concentration, total phosphorus, orthophosphate, total Kjeldahl nitrogen, ammonia, total organic carbon, dissolved organic carbon, iron and manganese in the tributaries of Lake Lanier are strongly correlated and dominated by non-point source model by using rating-curve methods. The non-point source model will be introduced in detail in next chapter. Lake water quality issues and characteristics are the important considerations for model development.

3.1 Description of Lake Lanier and Its Watershed

3.1.1 General

Lake Lanier is a reservoir located 40 miles northeast of Atlanta, Georgia (Fig.3-1). It is the largest impoundment in the Atlanta metropolitan area. The reservoir, when full,

covers 38,542 acres and has a total storage of 2,064,600 acre-feet (Hatcher et al., 1998). The reservoir is used for water supply, hydroelectric power generation, flood control, navigation, and recreation. Long-term average outflows from the watershed are approximately 2,074 cubic feet per second. Of this flow, approximately 70% are contributed from the two largest tributaries, the Chattahoochee and Chestatee Rivers. The Lake Lanier watershed covers 1040 mi², and includes land in Forsyth, Habersham, Hall, Lumpkin, White, Dawson, Gwinnett and Union Counties (Figure 3-1). Table 3-1 summarizes the distributions of tributary drainage areas. Detailed characteristics of Lake Lanier are provided in Table 3-2. The reservoir morphometric attributes and order of magnitude estimates are shown in Table 3-3.

3.1.2 Elevation, Slope, Soils and Land use

Land slope is an important factor in determining watershed sedimentation and nonpoint source loading. Figure 3-2 indicates the watershed elevation which was obtained from 1993 Georgia GIS Data Clearinghouse DEM data:

http://www.gis.state.ga.us/clearinghouse/clearinghouse.html

The slope of the watershed shown in Figure 3-3 was derived from the DEM data by using Arcview tools. Most areas of the watershed have elevations of $300 \sim 400$ m with slope less than 5%. The elevation is highest in north and northwest part of the watershed with a maximum 1300 m.

The basic nature of the underlying soils can play a large role in determining the amount of runoff and erosion from a particular piece of land. A depiction of the GIS soils coverage is shown in Figure 3-4 which was also obtained from 1993 Georgia Clearinghouse data STATSGO with the same website as above.

Land cover/use information was obtained in GIS format by using 1989 LANDSAT data which was classified by the Georgia Department of Natural Resources. The entire Lanier watershed was divided into fifteen land cover classes. Titles for the classes represent the majority of the land cover making up the classes. The land cover/use are shown in Figure 3-5. 1989 Land cover distribution in Lake Lanier watershed is: 77% forest, 9% pasture, 6% open water, 4% crops, 3% urban, and 1% others.

3.1.3 Water pollutant sources

Water quality degradation is a long-term concern of the communities surrounding the reservoir. Threats include both point- and non-point sources of pollution. Point sources within the Lake Lanier watershed include 13 municipal wastewater treatment facilities (Figure 3-6) and 33 private and industrial dischargers (Figure 3-7). Several point sources are directly discharged into Lake Lanier, and these discharges are listed in Table 3-4 (Hatcher, 1998). Non-point sources are ubiquitous, and include eight landfills, numerous septic tanks, dairy and poultry wastes, as well as stormwater runoff from rapidly expanding urban sources.

3.2 Watershed Water Quality Characterization

3.2.1 Introduction

The cornerstone of lake water quality management is monitoring data. Unfortunately, effective watershed water quality monitoring is expensive, timeconsuming, labor intensive, and spatially extensive. A well-designed water-quality monitoring plan should preserve scarce resources by minimizing the number of monitoring stations and the types of variables monitored, while at the same time maintaining the information quality of the collected data.

We apply both the principal components and cluster analysis methods to Lake Lanier tributary water quality data. Data for this study were collected as part of a lake water quality monitoring program that was funded by the Upper Chattahoochee Basin Group, an organization made up of cities and counties within the Lake Lanier watershed. The purpose of the monitoring program was to provide data for the development and application of watershed loading and lake water quality response models for Lake Lanier.

Principal components analysis is one method of data interpretation that can be used to understand the structure of collected data (Schoer, 1985; Buckley and Winters, 1992; Padro et al., 1993). In many cases, issues of data structure arise because of correlations between individual parameters. While not commonly used in water quality analysis, a few researchers have employed factor analysis to identify sources of contamination. Borovec (1996) used principal components analysis to extract dominant types of heavy metals in river sediments. The study was able to specify three parameter groups, which were then used to identify the sources of contamination. Principal components analysis is also used to find associations between parameters so that the number of measured parameters can be reduced. Known associations are then used to predict unmeasured water quality parameters.

Cluster analysis is another data reduction method that is used to group together entities with similar properties. The cluster analysis method divides a large number of objects into a smaller number of homogeneous groups on the basis of their correlation structure (Hartigan, 1975). Again, few water quality studies have employed this approach to assist in the design of water quality monitoring programs. Salmaso (1996) applied cluster analysis in a phytoplankton community study to identify similar algal groups.

3.2.2 Water Quality Monitoring Data

Water quality monitoring data were collected between March 1996 and March 1997 by a private consultant under contract from the Upper Chattahoochee Basin Group. The monitoring sites were located upstream of the mouths of ten significant tributaries to Lake Lanier and at 17 points within the reservoir. Monitored parameters are provided in Table 3-5 and the locations of tribuatry sampling stations are shown in Figure 3-8. The tributary water quality monitoring stations include two major stations on the Chattahoochee and Chestatee Rivers, and eight minor stations at the other tributaries. Routine tributary monitoring was conducted twice-monthly at the major stations and monthly at the minor stations.

Lake sampling was conducted twice-monthly during the April-October growing season and monthly during the non-growing season. Non-growing season samples were collected just below the lake surface and one meter above the lake bottom and analyzed for all lake water quality parameters. Growing-season samples were collected at approximately five depths at each station. Samples at the middle of the epilimnion and hypolimnion were analyzed for all lake parameters, while the remaining three samples were analyzed for nutrients and chlorophyll *a* (shown in Table 3-5).

3.2.3 Principal Components Analysis

Principal components analysis is a form of factor analysis that is routinely used as a data reduction method to reduce the number of observed variables. The method uses the correlation matrix of observations, X, to estimate a sorted vector of eigenvalues, λ , and corresponding eigenvectors (also called factor loadings), V. The eigenvalue equation is:

$$[X - \lambda I]V = 0 \tag{3-1}$$

where each eigenvalue, λ_i , is associated with an eigenvector, V_i , and I is a unitary matrix. The largest eigenvalue, λ_i , accounts for the largest explanatory capability, with additional eigenvalues accounting for smaller amounts of explanatory capability. The last eigenvalue may contribute little to the explanatory capability of the data. Guidelines have been developed for determining how many eigenvectors to use and how many to ignore (Browne, 1968; Hakstian, Rogers and Cattell, 1982; Linn, 1968; Tucker, Koopman and Linn, 1969). The most widely used method is the *Kaiser criterion* (Kaiser, 1960) which retains only those eigenvectors with eigenvalues greater that one. This means that each retained eigenvector provides as much explanatory capability as one original variable. The *scree test* (Cattell, 1966) identifies the useful eigenvectors as those whose eigenvalues are substantially larger than subsequent eigenvalues.

Table 3-6 provides the eigenvalues and the explanatory capability for the Lake Lanier water quality data. There are 13 eigenvectors because there are 13 water quality variables. The first factor accounts for approximately 59% of the total water quality variability, the first two account for 75%, while the first three account for 84%. According to the Kaiser criterion, only the first three factors should be used, because subsequent eigenvalues are all less than one. The scree test would recommend the first four factors (Figure 3-9), because subsequent eigenvalues do not decrease substantially. We use the Kaiser criterion to explain a large proportion of the observed water quality variability in Lake Lanier tributaries using just three factors.

Factor loadings (i.e., the eigenvectors for each eigenvalue) reflect the correlations between the variables and the extracted factors. Figure 3-10 presents the factor loading scatterplot between the first two factors. Each variable is presented as a point in these plots. Factor loadings are shown without rotation. It is possible to rotate the axes in any direction without changing the relative locations of the points to each other. The purpose of factor rotation is to yield a factor structure that is simpler. A *simple structure* was coined by Thurstone (1947) to describe a condition when factor loadings score highly only on one axis. The most standard computational method of rotation to obtain a simple structure is the *varimax* rotation (Kaiser, 1958). Others that have been proposed are

quartimax, *biquartimax*, and *equamax* (Harman, 1967). We have no need to rotate because none of our factor loadings plot highly on more than one axis.

Factor loadings for the three retained eigenvalues are shown in Table 3-7. The first factor is strongly correlated with most of the water quality variables, including suspended sediment concentration, both phosphorus species, total Kjeldahl nitrogen and ammonia, both organic carbon species, and total iron and manganese. Suspended sediment concentrations, *SSC*, have previously been shown to be highly correlated with discharge, Q, in the Upper Chattahoochee River basin (Holmbeck-Pelham and Rasmussen, 1997). This relationship is:

$$SSC = 16.5 \left(\frac{Q}{Q_0}\right)^{1.6}$$
(3-2)

where Q_o is the average discharge. Unfortunately, discharge during sampling was not monitored, so no direct correlation with streamflow can be made. Regardless, it is known that increases in discharge and suspended sediments are consistent with storm runoff. We thus suggest that storm runoff is the predominant cause of elevated concentrations of water quality parameters correlated to the first factor. This one factor accounts for 59% of the total water quality variability of tributaries to Lake Lanier.

It is interesting to note that alkalinity, nitrite plus nitrate, and total nitrogen are not strongly correlated with the stormwater runoff factor. Instead, nitrite plus nitrate and total nitrogen are better correlated with the second factor, accounting for 16% of the total variability. In the Georgia Piedmont, oxidized forms of nitrogen are more commonly associated with point-source discharges and land-application facilities. This is because organic forms of nitrogen have been converted to oxidized forms as part of the wastetreatment process, and there are few natural sources of oxidized nitrogen species. Total nitrogen is also correlated with the second factor due to the large contribution of nitrate plus nitrite to the calculated value of total nitrogen.

Alkalinity is correlated with the third factor, and accounts for only 9% of the total variability. We infer that this factor accounts for those waters with higher carbonate concentrations. These waters with higher carbonate may result from geologic conditions, or perhaps from industrial or municipal discharges.

3.2.4 Cluster Analysis

The principal components analysis described in the previous section focused on combining water quality parameters into homogeneous groups. We now wish to evaluate whether water quality samples at various locations can be combined into homogeneous regions so that the number of sampling sites can be reduced. Cluster analysis is one way of identifying homogeneous units. While we focus on tree clustering in this paper, other clustering methods (including block and k-means clustering) are also possible.

The purpose of tree clustering is to join together objects into successively larger clusters using a distance measure. A typical result of tree clustering is a hierarchical tree which is a nested sequence of partitions showing how similar the objects are. Clustering proceeds using a series of successive linkages with the final outcome being a single group of all objects separated by distances. Each object is initially represented by its own cluster. Distances between objects are defined using a distance measure (Table 3-8 presents a variety of distance measures). A linkage or amalgamation rule is then used to determine whether two objects are sufficiently close to be linked together. If the objects are sufficiently close, then they are linked together, and the distances between the linked objects is computed. Remaining clusters are then recursively tested to determine whether they should be linked or not.

The distance measure can be based on a single dimension or multiple dimensions and there are several measurement methods. The *single linkage* (or nearest neighbor) method uses the distance between two clusters. This rule forms clusters that are shaped as long *chains* (Sokal and Sneath, 1963; Johnson and Wichern, 1982). The *complete linkage* (or furthest neighbor) method uses the greatest distance between any two objects in the different clusters (i.e., by the furthest neighbors). The *unweighted pair-group average* method uses the average distance between all pairs of objects in the different clusters (Sneath and Sokal, 1973). The *weighted pair-group average* method is identical to the unweighted method, except that in the size of the respective clusters (i.e., the number of objects contained in them) is used as a weight (Sneath and Sokal, 1973).

The *unweighted pair-group centroid* method uses the centroid of a cluster (i.e., the average point in the multidimensional space defined by the dimensions) to define its center of gravity (Sneath and Sokal, 1973). The *weighted pair-group centroid* method is identical to the unweighted method, except that weighting is introduced using the number of objects contained in the cluster (Sneath and Sokal, 1973). *Ward's* method is distinct from other methods because it uses an analysis of variance approach to evaluate the distances between clusters. Ward's method minimizes the sum of squares of any two (hypothetical) clusters that can be formed at each step (Ward, 1963). In general, this method is regarded as very efficient, however, it tends to create clusters of small size. The Ward's method is selected in our study.

Figure 3-11 presents the results of cluster analysis for water quality monitoring data from the tributaries to Lake Lanier. Two associations are evident. The association between E. Fork Little River and Flat Creek North is most significant, with bonds to Wahoo Creek, and, to a lesser degree, Balus Creek, then to W. Fork Little River. These are small streams with large nonpoint source pollution inputs.

A second group of tributary water quality associations was found between the Chestatee and Chattahoochee Rivers. These rivers are the two largest inputs to the reservoir and these linkages appear to confirm the simularity in water quality between these two sources. There is a weak association between the Limestone Creek, Six Mile Creek and Flat Creek South, both mutual and with the other main groups. These three streams, especially Flat Creek South, receive more point sources inputs than the other tributaries.

3.2.5 Summary and Recommendations

We used principal components analysis to identify sources of water quality inputs into Lake Lanier. The largest inputs appear to be from nonpoint sources associated with stormwater inflows. Water quality parameters associated with stormwater inflows appear in the first factor, explaining 59% of the total water quality variation. Stormwater inflows estimated here contain increased concentrations of suspended sediments, total phosphorus, soluble reactive phosphorus, total Kjeldahl nitrogen, ammonia, total organic carbon, dissolved organic carbon, total iron, and total manganese. Increases in organic forms of nutrients, sediments, and metals are likely caused by overland flow and soil erosion associated with stormwater runoff.

Additional inputs from point sources appear in the second factor, accounting for 16% of the total water quality variability. This second factor is associated with high concentrations of oxidized forms of nitrogen (i.e., nitrite plus nitrate) resulting from wastewater treatment. Elevated nitrate concentrations are observed below wastewater treatment and land application facilities. A final factor, accounting for 9% of the total water quality variability, is correlated to alkalinity. Alkalinity has both natural and anthropogenic sources.

Cluster analysis was used to characterize the spatial variability of water quality data. The ten tributaries to Lake Lanier that were monitored in this study can be divided into five homogeneous groups: 1) Small Upper Basin Streams (including the East Fork of the Little River, Flat Creek North, Wahoo Creek, Balus Creek, and the West Fork of the Little River); 2) Large Upper Basin Streams (including the Chestatee and Chattahoochee Rivers); 3) Limestone Creek; 4) Six Mile Creek; 5) Flat Creek South.

A monitoring station should be situated on the largest tributary in the first group (Wahoo Creek) to track the behavior of those streams. Notwithstanding the fact that the Chestatee and Chattahoochee Rivers have much in common, they should both be monitored because they are the largest tributaries to Lake Lanier. Although the remaining three tributaries (Limestone Creek, Six Mile Creek, and Flat Creek South) are small, they behave sufficiently differently from the other tributaries and monitoring with one station is suggested. In all, water quality monitoring in six tributaries to Lake Lanier is recommended.

Because the bulk of nutrient inputs appears to be from stormwater, stage-dependent sampling is recommended. Water quality sampling should be concomitant with discharge measurements over a wide range of discharges (e.g., at 10% exceedence frequency intervals). Additional sampling for nitrates should focus on those tributaries where wastewater treatment and land application facilities are located. Sampling should be performed during average and below average flow conditions to avoid the influence of stormflow dilution.

3.3 Lake Water Quality Characterization

3.3.1 Lake Water Quality Issues

The primary management objective of this study is to simulate and predict water quality in Lake Lanier. This objective requires specification of the water quality parameters of potential concern. Selection of water quality concerns to be addressed by this study was dictated by: (1) problems to be most significant for Lake Lanier, and (2) problems most relevant to basin-wide water resources planning in the area. From a previous study on Lake Lanier water quality (Kathryn Hatcher, 1998), the water quality issues include:

- (a) Eutrophication: Loading of nutrients (primarily phosphorous) to Lake Lanier was identified as primary water quality concern. Increases in nutrient loading will cause an increase in aquatic plants, a decrease in water clarity, and a decrease in dissolved oxygen in certain areas of the lake.
- (b) Dissolved oxygen: Another water quality concern is depression of dissolved oxygen in the lake due to temperature stratification that isolates bottom waters of the lake from atmosphere sources of oxygen.
- (c) Bacteria: Pathogenic bacteria were identified as a water quality concern due to high recreational use of the lake. Elevated concentrations of bacteria have been observed in many lake tributaries, although the surface waters of the lake itself have remained in compliance with water quality standards.
- (d) Aquatic toxicity: Toxicity of the reclaimed water discharges in the direct vicinity of wastewater outfalls was identified as a concern by the public due to constituents such as ammonia, chlorine, metals, and organic toxicants.
- (e) Sedimentation: Accelerated sedimentation of Lake Lanier due to loading of eroded soils was identified as potential concern.
- (f) Temperature/stratification: The effect of reclaimed water discharges on thermal stratification of Lake Lanier also is a concern, in that it could introduce nutrient laden bottom waters of the lake to the lake surface, where they could trigger additional algal growth.

During this research period, an extensive survey about environmental concerns of the public was conducted. Some results are shown in Table 3-9. Based on the sum of *very concerned* and *somewhat concerned* is more than 80%, all of the three groups are concerned about *brown water*, *green water* and *nutrient levels* in the near future. In addition, most of stakeholders and scientists are concerned about *bacteria levels* and *pesticides and other chemicals*. In the long run, *brown water*, *green water*, *nutrient levels*, *bacteria levels* and *water unsafe for swimming* are concerned by stakeholders, scientists and decision-makers.

Green water results from algal growth. Excessive algae and aquatic plant growths are highly visible and can interfere significantly with the uses and aesthetic quality of a waterbody. One consequence of such growths can be the production of taste and odor problems in drinking water drawn from a water body, even though the water may be treated and filtered prior to use. The water treatment process itself can become more expensive and time-consuming for eutrophic waters. The water transparency may be greatly reduced. There are also significant ecological consequences related to cultural entrophication. As algal population die and sink to the bottom of a water body, their bacterially mediated decay can reduce oxygen concentrations in bottom waters to levels which are too low to support fish life, resulting in fish kills. Such oxygen-deficient conditions can also result in excessive levels of iron and manganese in the water, which can interfere with drinking water treatment. There are also potential health effects, especially in tropical regions, related to such parasitic diseases as schistosomiasis, onchocerchiasis and malaria, all of which can be aggrevated by cultural eutrophication, and which can enhance the appropriate habitats for these organisms. Algal photosynthesis and respiration will affect CO₂ concentration and then affect pH and carbonate species.

Brown water is mainly generated by colloids from runoff. For Southeastern lakes (or reservoirs), the region's warm climate, highly erodible and deeply weathered soils, and

increasing land development, present a challenging environment for water management, since the watershed with these characteristics will deliver a lot of colloids to the lake water during storm events. Colloids consist of a number of chemicals. Among them nutrients (including organic and inorganic nutrients) are an important threat to lake eutrophication. Nutrients delivered in storm runoff are usually considered as non-point source, and are associated with sediment erosion. Colloids discharged into lake water will increase water turbidity and decrease water clarity. The increase of water turbidity will increase extinction of sunlight in the water column, which will impact the available light for photosynthetic use by aquatic plants and algae. In addition, because of the long residence time of Lake Lanier (about 495 days at normal water level) and low flow velocity, colloids discharged into the lake will deposit to the bottom. This is called sedimentation and is a potential concern for lake management.

As stated above, nutrient concentrations pose a potential threat to lake eutrophication. For example, the loss of bioavailable phosphorus (BAP) in both soluble (SP) and particulate (BPP, bioavailable particulate phosphorus) forms in agricultural runoff, can accelerate the eutrophication of surface waters, because bioavailable phosphorus is potentially available for algal uptake (Andrew, 1992). Eutrophication of lakes and reservoirs is ranked as one of the most widely-spread water quality problems around the world. The effects of eutrophication on a water body can render the water unsuitable for many uses, or else require that the water be treated (often expensive and time-consuming) prior to use by humans. Eutrophication can also result in detrimental effects on the biological stability of a lake or reservoir ecosystem, affecting virtually all the biological populations and their interactions in the water body. Consequently, eutrophication of lakes and reservoirs can have significant negative ecological, health, social, and economic impacts on man's use of a primary and finite resource. Fecal coliform bacteria are present in the intestines or feces of warm blooded animals in normal numbers of about a million per gram of feces. Fecal coliforms are used as the primary indicator for determining whether the water is contaminated by animal or human waste. Although fecal coliforms do not normally cause illness in humans, their presence suggests that other potentially dangerous pathogens could also be present. A fecal coliform standard of less than 2000 colonies per 100 mL has been established for non-contact recreation sports such as sailing. A standard of less than 200 colonies per 100 mL was established for contact recreation such as swimming. Fecal coliform counts below 14 colonies per 100 mL comprise the standard for shellfish harvesting.

Dissolved oxygen (DO) is the traditional and ubiquitous concern of aquatic health. It determines the ability of aerobic organisms to survive, and in most cases higher dissolved oxygen is better. The concentration of dissolved oxygen depends upon temperature (an inverse relationship), salinity, wind and water turbulence, atmospheric pressure, the presence of oxygen-demanding compounds and organisms, algal photosynthesis and respiration. Of these, DO is introduced into the water column principally through reaeration (simple mechanical agitation by wind), and through photosynthesis. Dissolved oxygen deficit is the difference between the capacity of the water to hold oxygen and the actual amount of DO in the water. A large deficit is an indicator of some oxygen demanding stress on natural waters, while a low deficit is an indicator of generally unstressed conditions. A DO saturation greater than 100 percent can occur when the water is supersaturated with oxygen, a temporary condition that typically results from rapid photosynthesis.

For a deep lake like Lake Lanier, the vertical thermal regime has due significance to the water quality. First, temperature has direct importance because it influences the rates of chemical and biochemical reactions (such as algal photosythesis and respiration, equilibrium among carbonate species, etc.). Second, the effect of reclaimed water discharges on the thermal stratification of Lake Lanier is also a concern, in that it could introduce nutrient laden bottom waters of the lake to the lake surface, where they could trigger additional algal growth. Moreover, lake thermal stratification leads to the seasonal isolation of hypolimnetic water, which then becomes anoxic over time due to the decay and respiration of organic matter.

3.3.2 Cluster Analysis

Cluster analysis is used in this chapter to 1) group regions within the lake into spatial categories that have similar water quality parameter characteristics, and 2) provide long-term water quality monitoring strategies for the lake. The sampling data in 1996/97 is used for the analysis (Figure 3-12 shows the monitoring stations in 1996/97). Figure 3-13 presents the cluster analysis results for lake water quality stations. The association between Stations 4 and 5 is most significant, with bonds to Stations 2 and 3, and to a lesser degree, Station 1. These stations are located in the lowest part of the lake nearest the dam and are currently remote from most point and non-point source inputs.

A second association is between Stations 8 and 9, associated with Station 6, then to Station 10 and 7. This group of association is almost at the same level of significance as the first group. The second group is located in the central part of the lake, intermediate between the deep part of the lake near the dam and the shallow parts near the tributary inputs.

A third association exists between Stations 12 and 13, and associated with Stations 14, 15, and 17. This group indicates that the lake in the region of the Chestatee and Chattahoochee River inputs have similar water quality patterns, which conforms with tributary data analyses. Station 11 has a weak association with above three groups, which means the water quality at this location is different. Station 11 is the near Flat Creek South, which receives substantial point and nonpoint source inputs.

Based on the analysis here, we recommend the initial use of four zones: 1) the lowest part of the lake near the dam (Stations 1-5); 2) the central part of the lake (Stations 6-10); 3) the upper part of the lake (Stations 12-17) nearest the influent tributaries; and 4) the embayment near Flat Creek - South (Station 11). In all, a minimum of water quality monitoring at four lake stations is recommended. Additional sampling should be performed as resources become available.

3.3.3 Trophic Classification

There are three general classifications of lakes, one is based on the productivity of the lakes or on the relative nutrient richness of the lake. This is the trophic basis of classification which includes oligotrophy, mesotrophy and eutrophy and its basis is a continuous scale. The second lake classification is based on the times during the year that the water of a lake becomes mixed and the extent to which the water is mixed. The third system is based on the fish community of lakes.

The average values and the range of values for phosphorus and chlorophyll concentrations and Secchi disk depth characteristic of oligotrophic, mesotrophic and eutrophic lakes given in Table 3-10 were taken from Wetzel (1983). It is apparent from Table 3-10 that there are no fixed values of phosphorus or chlorophyll concentration or of Secchi disk depth which can be used to differentiate mesotrophic lakes, oligotrophic lakes and eutrophic lakes.

Lake Lanier's concentrations of TP, Chlorophyll *a* and Secchi disc depth are about 13 μ g/L, 1.5 μ g/L and 2.8 m respectively. Compared with Table 3-10, Lake Lanier can be classified as a *mesotrophic lake*.

3.3.4 Water Quality Characteristics

Based on the analysis of the following existing data sets (Table 3-11 summarizes the sampling stations in 1966, 1973 and 1991, Figure 3-14 presents the sampling locations at different time, Figure 3-12 shows the monitoring stations in 1996/97): 1) Holder (1966/67, monthly), 2) EPA's National Eutrophication Survey (1973), 3) EPA's Clean Lake Study (1991, monthly), 4) Upper Chattahoochee River Basin Group's Study (monthly and biweekly, 1996/97), and 5) Supplementary sampling data in August and December 1999. The following water quality characteristics can be identified:

- (a) Lake Lanier water temperature, pH, and dissolved oxygen concentration distribution are uniform horizontally (Figure 3-15a, b, c), but highly variable in the vertical direction (Figures 3-17 to 3-23). No clear long-term changes are apparent (Figure 3-16a, b).
- (b) TSS, turbidity, and secchi disc depth are spatially variable, with higher TSS and turbidity values near tributaries and lower values downstream. Secchi disc depth has the reverse distribution (Figure 3-15d). No clear long-term changes are apparent, other than small changes in the seasonal distribution.
- (c) The concentrations of chlorophyll *a* and algal biomass have variable spatial distribution, higher in the upper portions of the lake and lower in the lower lake (Figure 3-15d). This distribution has not changed markedly during the past thirty years of study.
- (d) During the growing season (or stratification period), the highest DO concentration and pH occur at around the thermocline because of the photosynthetic activity of phytoplankton setting from the photic zone (Figures 3-18 to 3-19).

	Area		
Tributaries	(acres)	(%)	
Chattahoochee River	275,200	41.4	
Chestatee River	151,680	22.8	
Wahoo Creek	16,000	2.4	
W. Fork Little River	11,520	1.7	
Flat Creek North	11,520	1.7	
E. Fork Little River	10,240	1.5	
Four Mile Creek	5,120	0.8	
Flat Creek South	3,840	0.6	
Balus Creek	3,840	0.6	
Limestone Creek	2,560	0.4	
Squirrel Creek	1,920	0.3	
Six Mile Creek	1,920	0.3	
Smaller Tributaries	130,560	19.6	
Lake Surface	38,542	5.8	
Total	664,462	100.0	

 Table 3-1
 Lake Lanier Tributary Drainage Areas

Elevation of dam	1106 feet	337 m
Length of dam	1630 feet	497 m
Size of drainage area	1040 mi ²	2662 km ²
Normal water level elevation	1070 feet	326 m
Flood level elevation	1085 feet	331 m
Normal surface area	38500 acre	156 km ²
Flood surface area	47000 acre	191 km ²
Volume at normal level	1917000 acre ft.	$2.37*10^9 \text{ m}^3$
Volume at flood level	2554000 acre ft.	3.16*10 ⁹ m ³
Length of shoreline at normal level	540 mi.	864 km
Length of shoreline at flood level	670 mi.	1072 km
Length of reservoir along major axis	54 mi.	86 km
Maximum depth at normal level	151 feet	46 m
Annual average discharge	1918 cfs.	54 m ³ /s

 Table 3-2 Physical Characteristics of Lake Lanier

Reservoir Attributes		Value	Unit
Volume	V	2.36*10 ⁹	m ³
Surface area	As	155.8	10^{6} m^{2}
Watershed area	A_w	2696	10^{6} m^{2}
Length	L	86.9	km
Length of shoreline	L _s	869	km
Mean width	$W = A_s/L$	1.8	km
Maximum depth	Z _m	46	m
Mean depth	$Z = V/A_s$	15.1	m
Average inflow	Q	58.7	m^3/s
Largest daily inflow on record	Qs	1556.5	m^3/s
Average secchi disc depth	Zs	2.8	m
Order of Magnitude Estimates		Value	Unit
Relative depth (1)	Z/Z _m	0.328	-
Relative depth (2)	$50Z_{m}^{*}(\pi/A_{s})^{1/2}$	0.326	-
Drainage area/surface area	A_w/A_s	17.3	-
Aspect ratio	L/W	48.3	-
Shoreline development ratio	$L_{s}/[2*(*(\pi A_{s})^{1/2})]$	19.6	-
Residence time	V/Q	1.35	year
Single storm flushing ratio	Q_s/V	0.06	1/day
Photic zone depth	$lnZ_{1\%} = 1.362 + 0.745 \ lnZ_s$	8.5	m

 Table 3-3
 Lake Lanier Morphometric Attributes and Order of Magnitude

 Estimates

Municipal Wastewater Treatment Facilities					
Facility Name NPDES Permit # Type of Operation Permitted Flow(!					
Flowery Branch WPCP	GA0031933	Activated sludge	0.20		
Gainesville #2 Linwood	GA0020168	Trickling filter	3.10		
Lake Lanier Islands GA004911		Activated sludge	0.35		
Privat	te and Industrial	Development			
Site Name	NPDES Permit#	Type of Operation	Permitted Flow(MGD)		
Lanier Beach South WWTP	GA0031674	Activated sludge	0.0380		
Chattahoochee Bay	GA0024189	STSF	0.0004		
Chattahoochee Country Club WPCP	GA0022471	STSF	0.0100		
Cinnamon Cove Condos WPCP	GA0049051	Activated sludge	0.0700		

 Table 3-4 Lists of Point Sources Discharged Directly into Lake Lanier

Note: STSF – Septic Tank Sand Filter

		Tributary	Lake Sta	ations
	Variables	Stations	"A"	"В"
TDS	Total Dissolved Solids	Х	Х	
SSC	Suspended Sediment Concentration	Х	Х	
Cha	Chlorophyll a		Х	Х
ТР	Total Phosphorus	Х	х	Х
SRP	Soluble Reactive Phosphorus	х	х	Х
TKN	Total Kjeldahl Nitrogen	х	х	Х
NH ₃	Ammonia	х	х	Х
NOn	Nitrite plus Nitrate	Х	х	Х
ТОС	Total Organic Carbon	Х	X	
DOC	Dissolved Organic Carbon	Х	X	
TFe	Total Iron	Х	х	
TMn	Total Manganese	Х	Х	
ALK	Alkalinity	Х	Х	

Table 3-5Lake Lanier Water Quality Parameters Sampled from March 1996through March 1997

[†] "A" Lake Stations are sampled at two depths (monthly at 1 m below the surface and 1 m above the bottom during the non-growing season and twice-monthly at the mid-depths of the epilimnion and hypolimnion during the growing season).

"B" Lake Stations are sampled at three depths twice-monthly during the growing season.

_	Eigenvalue		Varian	ce (%)
Factor	Individual	Cumulative	Individual	Cumulative
1	7.6	7.6	58.6	58.6
2	2.1	9.7	16.0	74.6
3	1.2	10.9	8.9	83.6
4	0.5	11.4	4.0	87.6
5	0.5	11.9	3.7	91.2
6	0.4	12.3	3.4	94.6
7	0.3	12.6	2.0	96.6
8	0.2	12.7	1.3	97.9
9	0.1	12.8	0.8	98.8
10	0.1	12.9	0.5	99.2
11	0.1	13.0	0.4	99.7
12	0.0	13.0	0.2	99.8
13	0.0	13.0	0.2	100.0

Table 3-6	Eigenvalues of Lake Lanier Tributary Data
(Ca	Iculated Using Principal Components Technique)

			Factor	
	Variable	1	2	3
ALK	Alkalinity	-0.131	-0.026	-0.930
ТР	Total Phosphorus	<u>0.948</u>	0.157	0.014
SRP	Soluble Reactive Phosphorus	<u>0.795</u>	-0.083	-0.004
TKN	Total Kjeldahl Nitrogen	<u>0.958</u>	0.018	0.006
NH3	Ammonia	<u>0.813</u>	-0.196	0.036
NOn	Nitrite plus Nitrate	0.142	<u>-0.931</u>	0.161
TN	Total Nitrogen	0.613	<u>-0.744</u>	0.142
SSC	Suspended Sediment Concentration	<u>0.901</u>	0.220	0.078
TDS	Total Dissolved Solids	0.433	-0.611	-0.418
ТОС	Total Organic Carbon	<u>0.943</u>	0.174	-0.051
DOC	Dissolved Organic Carbon	<u>0.887</u>	0.189	-0.217
TFe	Total Iron	<u>0.904</u>	0.282	-0.022
TMn	Total Manganese	<u>0.777</u>	0.160	0.120

Table 3-7 Unrotated Factor Loadings for Lake Lanier Tributary Data
(Loadings greater than ± 0.7 are bold and underlined)

Distance	Expressions
Euclidean [†]	$\sqrt{\sum (x_i - y_i)^2}$
Squared Euclidean	$\sum (x_i - y_i)^2$
Manhattan	$\sum x_i - y_i $
Chebychev	$\max x_i - y_i $
Power [‡]	$\sqrt{\sum x_i - y_i ^p}$
Disagreement	$\frac{count\left(x_{i}\neq y_{i}\right)}{n}$

 Table 3-8 Types of Distance Measures

Notes: [†] Most common type of distance chosen. [‡] p and r are user-defined

Indicators	Decision-maker		Stakeholder	
	Very	Somewhat	Very	Somewhat
	concerned	concerned	concerned	concerned
	Short-tern	п		
Brown water	69.2%	23.1%	70%	21%
Green water	30.8%	50%	49%	31%
Nutrient levels	46.2%	42.3%	52%	28%
Zooplankton levels	19.2%	34.6%	33%	25%
Bacteria levels	38.5%	30.8%	84%	10%
Pesticides and other chemicals	30.8%	30.8%	70%	21%
Water unsafe for drinking	38.5%	11.5%	65%	24%
Water unsafe for swimming	38.5%	30.8%	76%	17%
Fish unsafe for eating	34.6%	11.5%	64%	23%
Water unsuitable as fish habitat	38.5%	30.8%	68%	21%
Non-native species	26.9%	38.5%	38%	28%
	Long-tern	n		
Brown water	73.2%	19.2%	79%	13%
Green water	57.7%	30.8%	66%	20%
Nutrient levels	65.4%	30.8%	67%	18%
Zooplankton levels	23.1%	50%	51%	18%
Bacteria levels	46.2%	42.3%	86%	7%
Pesticides and other chemicals	50%	26.9%	79%	12%
Water unsafe for drinking	50%	26.9%	78%	13%
Water unsafe for swimming	53.8%	26.9%	83%	9%
Fish unsafe for eating	42.3%	34.6%	76%	14%
Water unsuitable as fish habitat	61.5%	26.9%	77%	13%
Non-native species	46.2%	26.9%	52%	20%

Table 3-9 Investigation Results about Water Quality Indicators

Note: The row in which the sum of "very concerned" and "somewhat concerned" is more than 80% for every group is shaded.

Indicators	Scientist				
Indicators	Verv	Somewhat			
	concerned	concerned			
Short-term					
Brown water	71.4%	14.3%			
Green water	14.3%	85.7%			
Nutrient levels	14.3%	85.7%			
Zooplankton levels	0%	57.1%			
Bacteria levels	57.1%	28.6%			
Pesticides and other chemicals	28.5%	42.9%			
Water unsafe for drinking	28.6%	28.6%			
Water unsafe for swimming	42.9%	14.2%			
Fish unsafe for eating	14.3%	42.9%			
Water unsuitable as fish habitat	28.6%	28.6%			
Non-native species	14.3%	57.1%			
L	long-term				
Brown water	71.4%	14.3%			
Green water	42.9%	57.1%			
Nutrient levels	42.9%	57.1%			
Zooplankton levels	14.3%	42.8%			
Bacteria levels	71.4%	14.3%			
Pesticides and other chemicals	57.1%	14.3%			
Water unsafe for drinking	57.1%	28.6%			
Water unsafe for swimming	57.1%	42.9%			
Fish unsafe for eating	42.9%	28.5%			
Water unsuitable as fish habitat	42.8%	28.6%			
Non-native species	57.1%	28.6%			

Table 3-9 Investigation Results about Water Quality Indicators (Con't)

Note: The row in which the sum of "very concerned" and "somewhat concerned" is more than 80% for every group is shaded.

Measured Par	rameter	Oligotrophic	Mesotrophic	Eutrophic
Total Phosphorus	Average	8	26.7	84.4
(µg/L)	Range	3.0-17.7	10.9-95.6	16-386
Chlorophyll a	Average	1.7	4.7	14.3
(µg/L)	Range	0.3-4.5	3-11	3-78
Secchi disc depth	Average	9.9	4.2	2.45
(m)	Range	5.4-28.3	1.5-8.1	0.8-7.0

 Table 3-10
 Lake Classification Based on Trophic Concept

	Station							
Year	1	2	3	4	5	6	7	8
1966	1-1	1-2	1-3	1-4	1-5	1-6	-	-
1973	2-1	2-2	2-3	2-4	2-5	2-6	2-7	2-8
1991	3-1	3-2	3-3	3-4	3-5	3-6	3-7	3-8

 Table 3-11
 Lake Sampling Stations in 1966, 1973, 1991



Figure 3-1 Location of Lake Lanier and Its Watershed



Figure 3-2 Elevation



Figure 3-3 Slope



Figure 3-4 Soils


Figure 3-5 Land Cover/Use



Figure 3-6 Locations of Municipal Wastewater Treatment Plants



Figure 3-7 Locations of Industrial Facilities



Figure 3-8 Tributary Monitoring Sites in 1996/97



Figure 3-9 Plot of Eigenvalues



Figure 3-10 Factor Loadings, Factor 1 vs. Factor 2



Note: five groups

- 1) Chestatee R. and Chattahoochee R.
- 2) Wahoo Creek, E. Fork Little R., Flat Creek North, Balus Creek, and W. Fork Little R.
- 3) Limestone Creek
- 4) Six Mile Creek
- 5) Flat Creek South

Figure 3-11 Tree Diagram of the 10 Tribuatries



Figure 3-12 Lake Sampling Locations in 1996/97



Note: four groups

1). The lowest part of the lake near the dam (Stations 1, 2, 3, 4, 5)

2). The central part of the lake (Stations 6, 7, 8, 9, 10)

3). The upper part of the lake (Stations 12, 13, 14, 15, 16, 17)

4). The embayment near Flat Creek South (Station 11)

Figure 3-13 Tree Diagram of Lake 17 Stations (1996/97)



Figure 3-14 Lake Sampling Locations in 1966, 1973 and 1991









Figure 3-15 Spatial (at Surface) Distribution of Lake Water Quality



Figure 3-16 Comparison of Surface Water Quality at Different Time



Figure 3-16 Comparison of Surface Water Quality at Different Time (Con't)



Figure 3-17 Vertical Temperature Profile of Lake Lanier (Aug. 1999)



Figure 3-18 Vertical DO Profile of Lake Lanier (Aug. 1999)



Figure 3-19 Vertical pH Profile of Lake Lanier (Aug. 1999)



Figure 3-20 Vertical Temperature Profile of Lake Lanier (Dec. 1999)



Figure 3-21 Vertical DO Profile of Lake Lanier (Dec. 1999)



Figure 3-22 Vertical pH Profile of Lake Lanier (Dec. 1999)



Figure 3-23 Vertical Profile of Alkalinity, DIC and pCO₂ (Dec. 1999)

CHAPTER 4

WATERSHED NUTRIENT LOADING ANALYSIS AND LAKE NUTRIENT BUDGET

Lake Lanier is the primary drinking water supply for the Altanta Metropolitan Area. Burgeoning growth within the lake's watershed and beyond is placing new burdens on the reservoir in the form of increased municipal and industrial wastewater discharges, agricultural waste inputs, and urban stormwater inflows. Of primary concern to the local community is the need to develop a watershed model that properly accounts for nutrient loading information and the need to provide effective control strategies for the purpose of maintaining current lake uses. As discussed in Chapter 2, we need to develop a watershed nutrient load model that meets our lake modeling objectives on a daily basis. Chapter 3 indicates that it is feasible to build a rating-curve model based on the analysis of water quality characteristics of Lake Lanier watershed. In this chapter, the rating-curve model is developed, and nutrient loads from Lake Lanier watershed (including short-term and long-term inputs) are estimated using the rating-curve model for riverine and shoreline inputs. The modeling results (non-point source) together with other sources (such as point sources and atmospheric deposition which are also discussed in this chapter) are intended to provide inputs needed for lake water quality model application in Chapter 7.

4.1 Watershed Nutrient Loading Analysis

4.1.1 Introduction

Lake water quality can be degraded by the excessive accumulation of nutrients derived from both agricultural and municipal development within the lake's catchment

(Carpenter et al., 1998). Such a problem is usually referred to as cultural eutrophication and is most approximately interpreted as an artificial acceleration of a slow natural, geochemical aging process (Beck, 1985). The increased availability of nutrients in the lake, particularly phosphorus (P), nitrogen (N) and carbon (C) compounds, creates conditions ripe for the explosive transient growth of micro-organism (phytoplankton) populations which occupy a position at the base of the lake food web. Cultural *entropphication* results in a temporarily unbalance in the lake ecosystem during certain periods of the annual cycle, and also can result in gradual changes - from year to year - in terms of species abundance and diversity. Large growths of phytoplankton blooms can be unsightly, and can be linked to taste and odor problems, fish kills, and a loss of regional income from tourism around the lake. In addition, phytoplankton blooms can also markedly increase the costs of treating the lake's water if it is used for drinking water supply. Therefore it is important to make accurate quantitative estimates of nutrient loadings among different types from different sources (Beck, 1982). Accurate estimation of nutrient loadings is the foundation of lake eutrophication control strategies. Different pollutant sources need different control strategies. Therefore accurate estimation of nutrient loadings not only serves as reliable inputs for our water quality modeling of Lake Lanier, but also provides important information for lake water quality management.

4.1.2 Approach

Nutrient loadings and their distributions within the lake watershed are difficult to quantify. There are three approaches for performing pollutant source evaluations. The first approach is to consider all emissions (fertilizers, liquid manure, sewage discharges, etc.) and transmission processes in the watershed that contribute to the lake's external nutrient load. The reviewed watershed models in Chapter 2 can be regarded as this approach. When using this approach, USLE (or RUSLE) and GIS are usually used to

estimate sediment and nutrient loadings. This approach has three disadvantages which has been discussed in Chapter 2: 1) USLE or RUSLE was developed for the estimation of annual sediment production, rather than daily; 2) nutrient concentrations in the runoff and parameters in USLE or RUSLE are very difficult to identify accurately; 3) the estimation result of this approach is for the whole water network of the watershed, not for the final receiving waterbody. Limno-Tech Inc. (1998) estimated nutrient loadings to Lake Lnaier using the first approach and GIS. Limno-Tech selected the Generalized Watershed Loading Functions (GWLF) model which is based on USLE to estimate nutrient loadings.

The second approach uses an annual yield method which is based on empirical nutrient yielding data expressed as $M/L^2/T$ (i.e. kg/ha/yr) and watershed area to estimate pollutant loading. This approach is simple but rough.

The third approach uses the rating curve method which is based on an evaluation of data (nutrient concentrations vs. stream flow) from the monitoring networks of loadings (tributaries, sewage discharges, atmospheric pollution, etc.) entering the lake directly. The rating curve approach is straightforward but does not provide information on the origin of the nutrients in question. In addition, the rating-curve method is seldom used in practice due to a lack of monitoring data.

The rating curve approach is superior to other sediment and nutrient models (e.g., the Universal Soil Loss Equation, yield method) because the seasonal and annual estimates provided by these alternative approaches are not compatible with the need to model lake water quality dynamics on a daily basis. However, it is possible to use the results from the rating curve approach to calibrate parameters used by the other two approaches.

4.1.3 Short-Term Analysis

Nutrient loadings from tributaries are estimated by using a discharge-sedimentnutrient model (e.g. rating curve method). Based on the principal components analysis results in Chapter 3, we believe that tributary nutrient loading is associated with sediment erosion, and that sediment erosion is associated with storm runoff. This conclusion is also proved by current research (Zeng, 2000). Therefore it is necessary to find relationships between these environmental variables.

Principal components analysis results (Figure 3-10 in Chapter 3) indicate that in tributaries (excluding Flat Creek South), suspended solids concentration (SSC), total phosphorus (*TP*), soluble reactive phosphorus (*SRP*), total organic carbon (*TOC*), dissolved organic carbon (*DOC*), ammonium (*NH*₃) and total Kjeldahl nitrogen (*TKN*) are primarily affected by the first factor which we interpret as nonpoint source storm runoff factor, and nitrite plus nitrate (NO_2+NO_3) and total nitrogen (*TN*) are mainly affected by the secondary factor which we interpret as a point source discharge factor. The relationships among these parameters can be expressed as in Table 4-1 (see also Figure 4-1).

Because the field monitoring in 1996/97 was conducted monthly and biweekly during growing season, the water quality data should contain samples collected during periods of storm runoff. Therefore the water quality at the tributary mouth embodies the ultimate contributions of point and non-point pollutant sources from the tributary subwatersheds.

Previous research by Holmbeck-Pelham and Rasmussen (1997) has established the following functional equation:

$$SSC(t) = SSC_0 \left[\frac{Q(t)}{Q_0}\right]^b$$
(4-1)

where SSC(t) and Q(t) are the average suspended sediment concentration and discharge on *t*th day respectively, Q_0 is the long-term annual mean discharge, b is equal to 1.6 \pm 0.05 for the four USGS stations in the Upper Chattahoochee River watershed and Chestatee River watershed, and SSC₀ is the suspended sediment concentration at mean discharge for each site.

USGS sediment and stream discharge data for the Lake Lanier watershed indicate an approximate value of 16.5 mg/L for SSC_0 (Holmbeck-Pelham and Rasmussen, 1997). So equation (4-1) is:

$$SSC(t) = 16.5 \left[\frac{Q(t)}{Q_0} \right]^{1.6}$$
 (4-2)

We next calculate nutrient concentrations for different nutrient species ($C_i(t)$) using equation (4-2) and equations in Table 4.1. The nutrient loading of *i*th species on *t*th day ($W_i(t)$) is estimated using equation (4-3).

$$W_{i}(t) = \left[\sum_{j} Q_{j}(t)\right] \cdot C_{i}(t) = Q_{T}(t) \cdot C_{i}(t)$$
(4-3)

where $Q_j(t)$ is the discharge of *j*th tributary on *t*th day, $Q_T(t)$ is the total inflow of the watershed on *t*th day.

Equation (4-3) estimates daily loads by multiplying the continuous daily concentration and continuous daily stream flow. It is particularly important to know the average daily concentration and average daily flow, especially for high-flow days. From Figure 4-2, the measured maximum concentrations of SSC in Chattahoochee River and Chastatee River are about 120 mg/L, which indicates that the estimated average daily concentration of SSC by Equation (4-2) can be set to 120 mg/L when it exceeds this value. Otherwise the loads may be overestimated if Equation (4-2) is applied to all high-flow events.

The average daily concentrations of SSC in small streams may exceed 120 mg/L, but will likely have a minor effect because their loads are much less than those from the Chattahoochee River and the Chestatee River watersheds.

Estimated nutrient loads based on Equation (4-2) and (4-3) are shown in Figure 4-3.

Applying Equation (4-3) to an entire year, the total nutrient loading of *i*th species (W_{Ti}) in the watershed can be expressed as follows:

$$W_{Ti} = \sum_{t=1}^{365} W_i(t) = \sum_{t=1}^{365} [Q_T(t) \cdot C_i(t)] = k_i \overline{Q}_T \overline{C}_i$$
(4-4)

Where \overline{Q}_{T} is the annual mean inflow of the watershed which is 2704 ft³/s in 1996 excluding inflow of Flat Creek South (65.72 ft³/s), \overline{C}_{i} is the concentration of *i*th species at annual mean flow, k_{i} is a rating-curve bias correction factor for *i*th species. The estimated results of \overline{C}_{i} and k_{i} are shown in Table 4-2. k_{i} was set to 1.00 for TN and (NO₂+NO₃) because they are primarily affected by point sources.

It is necessary to note that the water quality of Flat Creek South behaves very differently from other tributaries as indicated by the tree diagram Figure 3.11 in Chapter 3, so the nutrient loading of this tributary is estimated separately. The load of this tributary is estimated by multiplying measured annual concentration, discharge and the derived correction factor k_i .

4.1.4 Long-Term Analysis

Equation (4-1) was obtained based on statistical analysis of a 20-year USGS daily data. The equation can be used for short-term analysis of sedimentation as well as for an evaluation of long-term change when daily data are available. When only annual inflow data are available, Equation (4-5) and sediment-nutrient relationships are a simple way to estimate the long-term sediment production and nutrient loading. Figure 4-4 is the long-

term annual inflow data. The estimated long-term loadings are shown in Figure 4-5. Figure 4-6 is the estimation results using Equation (4-2) and Equation (4-4) based on historical inflow into Lake Lanier from 1979-1999. The results coincide well ($R^2 = 0.909$, t-stat = 28.17). Figure 4-7 is the estimation of annual deposition thickness based on annual sediment loading analysis. Sediment deposition is approximately 0.4-0.8 mm/yr for the last 20 years. Figure 4-8 indicates that the trend of the long-term estimation result is similar to the observed trend.

4.1.5 Discussion

Knowledge of the temporal variability of sediment and nutrient loads into Lake Lanier from the principal tributaries (e.g., the Chattahoochee River and Chestatee River) is crucial to evaluation of the future response of the lake to changes in these inputs. The rating-curve method is shown to adequately simulate patterns of sediment and nutrient loadings. It is also shown that a rating-curve bias correction factor k (which is different for different species) should be applied when using annual mean inflow and mean concentrations of suspended sediment and nutrients to estimate annual loads. Annual loads are underestimated when the rating-curve bias correction factor is not used.

4.2 Lake Nutrient Budget

4.2.1 Approach

A nutrient budget is the comparison between all nutrient sources and sinks. Although a nutrient budget is not an exact formula for nutrient analysis, it is one macroscopic method for evaluating nutrient sources and sinks. This analysis can be used to assess nutrient categories and to identify potential sources or sinks especially internal nutrient sources or sinks. Nutrient sources include nutrient inflow from tributary mouths, point sources directly into the lake, atmospheric deposition, and nutrient release from bottom sediment. Nutrient sinks include outflow and nutrient settling into bottom sediment. Other poorly identified sources or sinks include exchanges between surface water and groundwater, plant uptake, fish consumption and excretion, etc. A schematic of the Lake Lanier nutrient budget is shown in Figure 4-9.

4.2.2 Sediment-Water Interaction Model

Nutrient settling and release are estimated using following equations:

$$J_s = \mathbf{v}_s A_w C_w \tag{4-5}$$

$$J_r = v_r A_m C_m \tag{4-6}$$

Where:

 J_s — nutrient settling (kg/yr)

 J_r — nutrient release (kg/yr)

 v_s — burial flux of solid matter (m/yr)

- v_r flux of the feedback of nutrient from sediments (m/yr)
- A_w lake surface area (m²)
- A_m interface area between water and sediment (m²)
- C_w nutrient concentration in water (mg/L)
- C_m nutrient concentration in sediment (mg/kg)

Mass balances for water column and mixed sediment nutrient concentrations yield the following coupled differential equations:

$$V_{w} \frac{dC_{w}}{dt} = W_{in} + v_{r} A_{m} C_{m} - v_{s} A_{w} C_{w} - W_{out} - E V_{w} C_{w}$$
(4-7)

$$V_m \frac{dC_m}{dt} = -v_r A_m C_m + (1 - f_b) v_s A_w C_w - k_m V_m C_m$$
(4-8)

Where:

subscripts w and m — water and surface sediments, respectively

 v_s — burial flux of solid matter (m/yr)

 v_r — flux of feedback of nutrient from the sediments into the water column (m/yr)

 f_b — the fraction of nutrient buried directly to the lake's deep sediments

C — nutrient concentration (mg/L)

 W_{in}, W_{out} — nutrient inflow and outflow respectively

 C_w — water volume (m³)

 V_m — sediment mixing volume (m³).

 $V_m = A_m H$, H is mixing depth which is approximately 0.1 m (Somlybody, 1986)

 k_m — decay coefficient in sediment (1/yr)

E — Coefficient of other sources and sinks (1/yr), including exchange with ground water, fish consumption, plant uptake, etc.

Assuming $A_w = A_m = A$, at steady state, the solutions are as follows:

$$C_{w} = \frac{(W_{in} - W_{out})(v_{r}A + k_{m}V_{m})}{(v_{s}A + EV_{w})(v_{r}A + k_{m}V_{m}) - v_{r}A(1 - f_{b})v_{s}A}$$
(4-9)

$$C_{m} = \frac{(W_{in} - W_{out})(1 - f_{b})v_{s}A}{(v_{s}A + EV_{w})(v_{r}A + k_{m}V_{m}) - v_{r}(1 - f_{b})v_{s}A^{2}}$$
(4-10)

The coefficients of v_s , v_r and f_b for phosphorus used by Lorenzen (1976) in Lake Washington are 36 m/yr, 0.0012 m/yr and 0.6 respectively. We think v_s is strongly related to sediment settling because of sediment-nutrient adsortion, it can be regarded as a physical parameter, so the settling rate of phosphorus can be assumed as the same as that

of nitrogen. Moreover, we assume v_r and f_b for phosphorus are similar among large lakes.

Nitrogen (N) can be lost from the sediment by diffusion of gaseous N formed by denitrification. Gaseous N can be considered as inert:

$$5CH_2O + 4NO_3^- + 4H^+ \to 5CO_2 + 2N_2 + 7H_2O \tag{4-11}$$

Phosphorus (P) can not be lost by any process other than transportation. Therefore k_m is zero for P. k_m is of the order of 0.1 /yr (Somlybody, 1986) for N. As a result, there are four parameters to be calibrated: v_s , E for phosphorus, E for nitrogen, and v_r for nitrogen. If we separate Equations (4-9) and (4-10) for phosphorus and nitrogen, four equations will appear, so the four parameters can be calibrated.

Analysis of Lake Lanier data in 1996/7 showed that the average concentrations of *TP*, *TN* and *TOC* in water are about 13 μ g/L, 0.6 mg/L and 1.8 mg/L respectively, the concentrations of *TP* and *TN* in lake bottom sediment are 334 mg/kg and 828 mg/kg respectively. Based on these data, the parameters v_s , v_r , f_b and *E* are calibrated as in Table 4-3.

4.2.3 Tributary inflows

Water quality characteristics of Flat Creek South are very different from other tributaries based on the results of cluster analysis in Chapter 3, so nutrient input evaluation from this creek is separated from other tributaries. Pollutant inputs from it can be estimated by multiplying average concentrations and inflows because Flat Creek South receives nutrient from multiple point sources. Other tributary inflows of nutrients have been evaluated using rating-curve method.

4.2.4 Lake inputs

Lake inputs were determined by multiplying effluent and nutrient concentrations in the effluent. The data for these calculations are presented in Table 4-4. The data were obtained from Clean Lakes Program (Hatcher, 1998) which was originally collected from EPD discharge monitoring reports.

4.2.5 Atmospheric deposition

Atmospheric deposition can be estimated based on lake surface area (38,500 acres), total rainfall and the average deposition of PO_4^{3-} (0.336 kg/ha/yr) and $NH_4^{+}+NO_3^{-}$ (12 kg/ha/yr) in rainfall from 1978-1989 as reported by Malker and Melin (1991). The total rainfall in 1996 is 4.159 feet.

4.2.6 Nutrient outflow from Buford Dam

Nutrient outflow can be calculated by multiplying discharge and nutrient concentration in the outflow. The average outflow of 1996 is 2701.43 ft³/s, the average concentrations of *TP*, *SRP*, *TN*, *TKN*, *NH*₃, *NO*₂+*NO*₃, *TOC*, and *DOC* are shown in Table 4-5.

4.2.7 Results and Discussion

The estimation results are shown in Table 4-6 and Table 4-7. It shows that total phosphorus settling is 154,230 kg in 1996, it is about 54.4% of total accumulation in the lake. Total nitrogen settling is 6,865,982 kg, it is about 158.4% of total accumulation. Table 4-6 shows that about 191,044 kg total phosphorus lost in 1996 except settling and release, while about 965,018 kg total nitrogen went into the lake water. Figure 410 and Figure 4-11 depict different sources and sinks for total phosphorus and total nitrogen respectively. To close the phosphorus budget, it is necessary to measure the concentrations of surrounding ground water and determine the exchange between lake water and ground water. Analysis results indicate that non-point source is a dominant

nutrient source into Lake Lanier, so it is very important to control non-point pollutants from the watershed.

Expression	R^2
$TP = 0.002 \cdot SSC + 0.006$	0.8262
$SRP = 0.4506 \cdot TP$	0.9144
$TKN = 2.6801 \cdot TP + 0.152$	0.9136
$NH_3 = 0.27 \cdot TKN$	0.7563
$TOC = 0.02 \cdot SSC + 1.8$	0.6816
$DOC = 0.6069 \cdot TOC$	0.6473
$Fe = 0.0298 \cdot SSC + 0.6$	0.8984
$NO_{2} + NO_{3} = 0.8763 \cdot TN$	0.9333
$TN = TKN + NH_3 + (NO_2 + NO_3)$	

Table 4-1Results of Correlation Analysis
(excluding Flat Creek South)

Parameters	\overline{C}_i (mg/L)	k_i
SSC	25.220	1.95
ТР	0.050	1.95
SRP	0.023	1.95
TN	1.390	1.00
TKN	0.286	1.45
NH ₃	0.077	1.45
<i>NO</i> ₂ + <i>NO</i> ₃	0.930	1.00
ТОС	2.508	1.35
DOC	2.041	1.20

Table 4-2 Estimated mean concentration \overline{C}_i and rating curve bias coefficient k_i for
different species

	\mathcal{V}_{s}	f_b	V_r	Е
Phosphorus	77.1 m/yr	0.6	0.0012 m/yr	+7666 /yr
Nitrogen	77.1 m/yr	0.6	0.0123 m/yr	-839 /yr

 Table 4-3 Parameterization for Sediment-Water Interaction Model

Note: • Carbon is not calibrated due to a lack of lake sediment concentration data. • In column E, "+" means sink, "-" means source

Municipal Wastewater Treatment Facilities								
Facility Name	TP (kg/yr)	TN (kg/yr)	NH ₃ (kg/yr)	BOD ₅ (kg/yr)				
Flowery Branch WPCP	101	1,470	102	804				
Gainesville #2 Linwood	10,123	60,583	24,659	36,143				
Lake Lanier Islands	271	14,508	1,088	893				
Private and Industrial Development								
Site Name	TP (kg/yr)	TN (kg/yr)	NH ₃ (kg/yr)	BOD ₅ (kg/yr)				
Lanier Beach South WWTP	15	179	14	54				
Chattahoochee Bay	1	5	2	4				
Chattahoochee Country Club WPCP	14	117	55	21				
Cinnamon Cove Condos WPCP	96	816	384	120				
Total	10.621	77,678	26,304	38.039				

Table 4-4 List of Lake Inputs
Parameter	Concentration
	(mg/L)
TP	0.005
SRP	0.001
NH_3	0.060
TKN	0.206
TN	0.600
$NO_2 + NO_3$	0.334
TOC	1.790
DOC	1.660

 Table 4-5
 Outflow Concentrations From Buford Dam

Inflow:	Phosphorus (kg/yr)		Nitrogen (kg/yr)				Carbon (kg/yr)	
	TP	SRP	TN	TKN	NH ₃	NO ₂ +NO ₃	TOC	DOC
Tributary inflows	234,779	105,791	4,996,229	997,077	269,211	3,729,941	8070616	5869003
Flat Creek (South) inflow	43,805	19,787	704,188	100,355	8,505	595,328	414,917	293,500
Lake inputs	10,621	10,621	77,678	/	26,304	51,374	38,039	38,039
Atmospheric deposition	5,242	5,242	186,984	/	/	186,984	/	/
Subtotal	294,447	143,441	5,780,322	1,097,432	304,020	4,378,870	8523572	6200542
Outflow from Buford Dam	10,849	2,411	1,446,565	496,654	144,657	805,257	4315600	4002177
Total accumulation	283,598	139,030	4,333,757	600,778	159,363	3,573,613	4207992	2198365
Settling	154,230		6,865,982					
Release	61,676		1,567,207					
Others	191,044		-965,018					
Annual budget	0		0					

 Table 4-6 Annual Nutrient Budget of Lake Water in 1996

 Table 4-7 Annual Nutrient Budget of Lake Bottom Sediment in 1996

	Phosphorus (kg/yr)		Nitrogen (kg/yr)				Carbon (kg/yr)	
	ТР	SRP	TN	TKN	NH_3	NO ₂ +NO ₃	TOC	DOC
Settling	154,230		6,865,982					
Release	61,676		1,567,207					
Into deep sediment	92,554		4,119,589					
Decay	0		1,179,186					
Annual budget	0		0					





Figure 4-1 Correlation Analysis





Figure 4-1 Correlation Analysis (Con't)





Figure 4-1 Correlation Analysis (Con't)





Figure 4-1 Correlation Analysis (Con't)





Figure 4-2 Q and SSC in Large Tributaries





Figure 4-3 Short-Term Pollutant Loading Estimation Results -1996





Figure 4-3 Short-Term Pollutant Loading Estimation Results –1996 (Con't)





Figure 4-3 Short-Term Pollutant Loading Estimation Results –1996 (Con't)





Figure 4-3 Short-Term Pollutant Loading Estimation Results –1996 (Con't)



Figure 4-4 Long-Term Annual Inflow





Figure 4-5 Long-Term Pollutant Loading Estimation Results





Figure 4-5 Long-Term Pollutant Loading Estimation Results (Con't)





Figure 4-5 Long-Term Pollutant Loading Estimation Results (Con't)





Figure 4-5 Long-Term Pollutant Loading Estimation Results (Con't)



Figure 4-6 Comparison between Daily and Annual Estimation



Figure 4-7 Estimated Annual Sediment Deposition Thickness



Figure 4-8 Comparison between Estimated and Observed Trend



Figure 4-9 Scheme of Nutrient Budget



Figure 4-10 Annual Budget of TP in 1996



Figure 4-11 Annual Budget of TN in 1996

CHAPTER 5

THERMAL MODELING FOR STRATIFIED DEEP LAKES

Existing temperature models estimate the heat balance at the air-water interface to determine the vertical distribution of temperature in stratified lakes. A simplified model is presented in this chapter that is useful for avoiding a complicated heat balance at the interface. The observed water surface temperature is represented using a sinusoidal curve and is directly regarded as the upper boundary of the model, the observed thermocline variation is utilized to quantitatively determine the position which separates the epilimnion and the hypolimnion. Monte Carlo simulation with heat dispersion coefficients at different time periods (transition and stratification periods) is used in model calibration. Temperature modeling results of Lake Lanier are used for determining the chemical reaction kinetics for the biogeochemical model application in Chapter 7, and the calibrated vertical heat dispersion coefficients are used for the estimation of vertical mass exchange coefficients. In this chapter, we first introduce previous modeling of temperature changes in stratified deep lakes and thermal regimes of Lake Lanier, and then introduce our thermal model development based on thermal transport physics and observed temperature data.

5.1 Introduction

Many of the physical, biological and chemical characteristics of surface water are dependent on temperature. Temperature affects the solubility of oxygen in water, the rate of photosynthesis by algae and larger aquatic plants, the metabolic rates of aquatic organisms and the sensitivity of organisms to toxic wastes, parasites and diseases. Aquatic organisms exhibit a species specific tolerance range for temperature, when the water temperature falls outside of the range for a particular species, it dies.

In stratified deep lakes, the creation of vertical gradients in the water column is inextricably tied to the lake's biology and chemistry. Dynamic changes of deep lake temperature include water temperature profile, depth of epilimnion, and length of stratification period. All of these characteristics of thermal stratification may have profound effects on the cycling and partitioning of matter between components of the lake ecosystem.

Formal mathematical modeling of temperature changes in stratified deep lakes or reservoirs has been conducted by both the Tennessee Valley Authority (TVA) and the California Department of Fish and Games (CDFG). The latter agency was concerned with the effects of large lakes or reservoirs on salmon migration. In 1965, CDFG contracted with Water Resources Engineers, Inc. to develop a predictive model (Orlob, 1965). In the following year TVA and WRE collaborated in developing the model. TVA quantified heat exchange phenomena and conducted field studies on several of its reservoirs to provide data for model calibration and validation (Elder and Wunderlich, 1968). This combined effort culminated in a working model that was first applied to Fontana Reservoir in the TVA system (WRE, Inc., 1968). It was later revised as a result of experience with several reservoirs in United States (WRE, Inc., 1969). The characteristics of the model and preliminary test results were first reported by Orlob and Selna (1967, 1970). Subsequently, it was documented for the Environmental Protection Agency (Gaume and Duke, 1975). It is currently being used in various forms by many United States governmental agencies.

In a parallel research and development effort, spanning the same period in the late 1960s and also in collaboration with the TVA Engineering Laboratory, D.R.F. Harleman and his co-workers at Massachusetts Institute of Technology (MIT) developed a comparable one-dimensional temperature simulation model (Huber et al., 1972). The development effort at MIT focused more strongly at first on fundamental heat transfer mechanisms, utilizing laboratory models as prototypes for mathematical development (Dake and Harleman, 1966). Subsequently, however, the MIT model was extended to simulation of actual reservoirs, e.g. Fontana Reservoir.

The MIT model, which has also been well documented and tested, is presently used by TVA and other United States governmental agencies. Apart from some refinements in treating inflow and withdrawal processes, the MIT model is substantially equivalent in performance to the WRE model.

A one-dimensional temperature model designed for deep, stratified lakes was developed at the Cornell Aeronautical Laboratory (Sundaram et al., 1969) and applied to Cayuga Lake in upper New York State in a study of power plant cooling water discharges. The model is based on the one-dimensional diffusion equation and is limited by assumption of a constant cross-sectional area (horizontal plane), absorption of all incoming heat energy in the surface layer, and neglect of heat advected either laterally or vertically in the water column, except that associated with power plant withdrawals or discharges. Wind effects are included. Apparently, because of its case-specific nature, the model has been applied only to Cayaga Lake.

Other significant developments in mathematical modeling of temperature in deep, stratified lakes or reservoirs include several attempts to extend the one-dimensional concept to segmented, weakly stratified reservoirs. Water Resources Engineers, Inc. (1968) modeled Lake Roosevelt as a six-segment system and Baca et al. (1974), using a modification of the WRE model, simulated American Falls Reservoir with a three-segment system. In each instance, model results compared favorably with observation of the lake or reservoir, but difficulties were experienced in the interfacing of segment

according to the densimetric criteria used for introducing advective flows into the water column.

5.2 Thermal Regimes of Lake Lanier

The temperature model requires data to determine initial conditions, thermocline variations, surface temperature changes, and to calibrate the model. These data were obtained from the 1996-97 monitoring program. This program was conducted primarily to collect data required for development and application of watershed loading and lake water quality response models for Lake Lanier. Monitoring began in March 1996 and ended in March 1997. A total of 17 stations were monitored for the lake water quality. Figure 6-2 in Chapter 6 shows the locations of each of these stations. Lake sampling was conducted on a bi-weekly basis during the growing season (April-October) and a monthly basis during all other times. At each station, in-situ measurements were collected for temperature, DO, specific conductivity, and pH at one-meter intervals from the surface to the bottom. The monitoring results of the temperature profile in the dam pool (station 1) and central lake (station 7) are shown in Figure 5-1(a) and Figure 5-1(b) respectively.

The thermal regimes in Lake Lanier (Figure 5-1) are primarily the result of the interplay of two processes: (i) heat and momentum transfer across the lake's surface and (ii) the force of gravity acting on density differences within the lake. Depending on the season of the year, heat transfer tends to either raise or lower the temperature at the lake's surface as a consequence of a number of factors, including the magnitude of solar radiation, air temperature, relative humidity, wind speed and cloud cover. Wind blowing across the lake's surface tends to mix the surface waters and transfer heat and momentum down though the water column. The extent of this mixing is, in turn, inhibited by buoyancy (and sometimes rotational) effects. These relate to the fact that the density of

water varies over the range of temperatures encountered in lakes. Therefore, denser waters accumulate at the lake's bottom and are overlain with lighter waters.

During the spring, the whole lake water temperature is in the range of 7.5°C-15°C. At this temperature range, heating or cooling of the lake's surface results in very small density differences, and consequently, only a small amount of wind stress is required to keep the water column well mixed. As spring progresses, solar radiation increases, air temperature rises, and thermal stratification is established in the near surface waters. However, density gradients are neither large enough nor deep enough to prevent mixing of the water column by major storms.

At the end of spring and the beginning of summer, surface heating increases to the point that mixing is confined to the upper layer (i.e. the epilimnion). The fluid has reached the point where the density gradient is sufficient for stable stratification. The attainment of persistent stratification in the lake leads to the three regimes: the upper (epilimnion) and lower (hypolimnion) layers separated by a narrow region (i.e. metalimnion).

During the midsummer, he net daily heat flux at the surface is low and, although the thermocline deepens gradually, the density gradient between epilimnion and hypolimnion remains strong and stable. Although transport of heat and energy across the thermocline occurs, it is at a low level and exchange between the upper and lower layers is at a minimum.

In late summer and fall, loss of heat due largely to falling air temperature results in a net heat loss from the lake. Surface waters become denser as they cool and mix with underlying deeper epilimnion water. Because this is an unstable situation, strong vertical convective mixing occurs. Together with increased winds during fall, the processes erode the metalimnion from above, resulting in a sinking thermocline. As the lake cools further, a point is reached at which the deepened surface layer becomes denser than the bottom layer and complete mixing of the water column occurs. The lake continues to be wellmixed and to lose heat as air and water temperatures drop in winter.

In summary, the seasonal changes of the lake can be idealized in both time and space. Temporally, the cycle consists of two stages: a summer period of strong stratification and a non-stratified period of intense vertical mixing. Spatially, the summer stratified period can be treated as consisting of two layers separated by an interface of minimal vertical mixing.

5.3 Temperature Modeling

5.3.1 Governing equations

The developed temperature model for stratified lakes is a one-dimensional, deterministic, process-oriented, dynamic model. In the model, the lake is described by a series of horizontal layers, each of which is assumed to be well mixed in the horizontal dimension. Vertical transport of heat is described by a diffusion equation. Unlike existing models, the model does not regard the air-water interface as the upper boundary. The surface layer of the water column is the upper boundary. This treatment avoids a complicated heat balance computation across the air-water interface. The governing equations are:

$$\frac{\partial T}{\partial t} = D_z \frac{\partial^2 T}{\partial z^2}$$
(5-1)

$$T(z=0, t) = T_{0,t}$$
(5-2)

$$\frac{\partial T}{\partial z}\Big|_{z=H} = 0 \tag{5-3}$$

$$T(z, t=0) = T_{z,0}$$
(5-4)

Where:

T — water temperature

 D_z — vertical heat dispersion coefficient

 $T_{0, t}$ — specified upper boundary temperature at time t

 $T_{z,0}$ — specified initial temperature at depth Z

H— lake depth

While some heat loss into the lake bottom may be present, the temperature profile in the bottom layer of the water column (shown in Figure 5-1) is almost straight, which means that it is reasonable to treat the heat flux in the bottom as zero as in equation (5-3).

The vertical heat dispersion coefficient D_z can be estimated using water temperature measurements. However, this parameter estimation does not reflect the average heat dispersion in the whole year. Therefore it is better to use the model to calibrate the vertical heat dispersion coefficient D_z directly.

5.3.2 Numerical solution

The Crank-Nicholson method is used to discretize the differential equation (5-1):

$$\frac{T_{i,j+1} - T_{i,j}}{\Delta t} = D_z \frac{T_{i-1,j+1} - 2T_{i,j+1} + T_{i+1,j+1} + T_{i-1,j} - 2T_{i,j} + T_{i+1,j}}{2\Delta z^2}$$
(5-5)

Let $k = \Delta t$, $h = \Delta c$, $r = D_z k/h^2$, then we can obtain:

$$-T_{i-1,j+1} + (\frac{2}{r} + 2)T_{i,j+1} - T_{i+1,j+1} = (\frac{2}{r} - 2)T_{i,j} + T_{i-1,j} + T_{i+1,j}$$
(5-6)

for i=2,3,...,n-1. The boundary conditions are used in the first and last equations. The above equations form a tridiagonal matrix for AX=B:

$$\begin{bmatrix} r_{1} & -1 & & & \\ -1 & r_{1} & -1 & & 0 & \\ & -1 & \mathbf{O} & & & \\ & & r_{1} & -1 & & \\ & & & -1 & \mathbf{O} & & \\ & & & r_{1} & -1 & \\ & & & & -1 & \mathbf{O} & & \\ & & & & & r_{1} & -1 & \\ & & & & & -1 & r_{1} \end{bmatrix} \begin{bmatrix} T_{2,j+1} \\ T_{3,j+1} \\ \mathbf{M} \\ T_{i,j+1} \\ \mathbf{M} \\ T_{n-2,j+1} \\ T_{n-1,j+1} \end{bmatrix} = \begin{bmatrix} r_{2}T_{2,j} + T_{1,j} + T_{3,j} \\ r_{2}T_{3,j} + T_{2,j} + T_{4,j} \\ \mathbf{M} \\ r_{2}T_{i,j} + T_{i-1,j} + T_{i+1,j} \\ \mathbf{M} \\ r_{2}T_{n-2,j} + T_{n-3,j} + T_{n-1,j} \\ r_{2}T_{n-1,j} + T_{n-2,j} + T_{n,j} \end{bmatrix}$$

Here $r_1 = 2/r+2$, $r_2 = 2/r-2$.

5.3.3 Upper Boundary Condition – Surface Temperature

In this model solar radiation is not included at the right side in equation (5-1) because surface temperature is chosen as the upper boundary condition. The surface temperature of Lake Lanier in 1996/97 is shown in Figure 5-2.

In temperate lakes, the annual variation of water temperature typically follows a sinusoidal cycle:

$$T_{0,t} = A\sin(\omega t + \varphi) + B \tag{5-7}$$

where:

 $T_{0,t}$ — water surface temperature.

A— annual amplitude.

B — annual average temperature at water surface.

 ω — frequency.

 φ — phase angle.

Equation (5-7) can be expressed as follows:

$$T_{0t} = A(\cos \omega t \sin \varphi + \sin \omega t \cos \varphi) + B$$
(5-8)

letting $a = A \sin \varphi$, $b = A \cos \varphi$, then we obtain

$$T_{0,t} = a\cos\omega t + b\sin\omega t + B \tag{5-9}$$

where:

$$A = \sqrt{a^2 + b^2} \tag{5-10}$$

$$\tan \varphi = \frac{a}{b} \tag{5-11}$$

The constants a, b and B can be determined by using linear regression, then amplitude A and phase φ can be calculated by using equation (5-10) and (5-11) respectively.

$$a = -9.19 \pm 0.35$$

$$b = -5.06 \pm 0.34$$

$$B = 18.10 \pm 0.24$$

$$A = \sqrt{a^2 + b^2} = 10.49$$

$$\varphi = a \tan(a/b) = -2.08 \approx -2\pi/365 \times 121$$

The regression result is shown in Figure 5-2.

5.3.4 Treatment of surface mixed depth

The surface mixed depth is difficult to simulate directly. Instead observed data are used to determine the surface mixed depth. Figure 5-3 shows the variation of surface mixed depth at the center of Lake Lanier in 1996/97. The lake is almost completely mixed around mid-January. Stratification is not apparent from mid-January to early-May. The lake begins stratification in early May, and the surface mixed depth increases with time. Full mixing occurs around mid-January.

5.3.5 Selection of initial conditions

Lake Lanier is assumed to be completely mixed by January 15. This is a reasonable assumption given the sampling data in 1996/97. The uniform temperature profile is selected as the initial condition. Because of the characteristics of a sinusoidal cycle of surface temperature, the computation period is chosen from January 15, 1996 to January 14, 1997, and the simulation results from January 1 to January 14 in 1997 are regarded as the same as the same period in 1996. After this treatment, the simulation results for the whole year of 1996 can be obtained.

5.4 Model Calibration

By specifying the upper boundary condition and the initial vertical temperature profile, temperatures at different depths for additional time periods can be simulated by the governing equations.

In this model, there is only one parameter (heat dispersion coefficient D_z) which needs to be calibrated. This will greatly decrease model calibration difficulty and increase modeling reliability.

Uncertainty commonly exists in model parameters. Monte Carlo simulation handles this situation by randomly choosing parameters at the start of the simulation (from specified probability distribution) and keeps them fixed for the duration of the simulation. This is certainly appropriate in situations where the parameters are thought to be constant through the time but the precise values are not known with certainty. If any of the parameters vary through time in the real system, however, it is intuitively appealing to allow the model parameters to vary by resampling at intervals during the simulation.

In this model calibration, the heat dispersion coefficient D_z is considered different at the transition period and stratification period. Therefore Monte Carlo simulation was used to randomly generate a set of 200 parameters to calibrate the model (assuming uniform probability density distribution). Calibration results indicate that D_z is about 0.35 nf/day in Lake Lanier during the stratification period (Figure 5-4), while D_z at the transition period is not sensitive to model calibration (Figure 5-5). The minimum root mean square error of simulated temperature is 0.97 °C when D_z at transition period is chosen as 1.35 m²/day.

5.5 Results and Discussion

The Thermocline is usually defined as the depth where the temperature drops 1 °C or more in 1 meter of depth. From Figure 5-1 it appears that the thermocline exists from early May to early November, which means the lake is stratified at this time period.

Comparisons between simulations with the calibrated model and measured temperature profiles for Lake Lanier are shown in Figure 5-6, which indicate that the modeling results fit the measured data quite well (root mean square error for the entire year is $0.97 \,^{\circ}$ C). The modeling result in the whole year of 1996 is shown in Figure 5-7.

Model calibration results indicate that the vertical heat dispersion coefficient D_z at stratification period is about 0.35 m²/day, while D_z at transition period is not sensitive to the model calibration because temperature variations with time and depth are relatively small at transition period. Lierature values of maximum hypolimnetic eddy diffusivity are $0.086 - 8.64 \text{ m}^2/\text{day}$ (Hondzo and Stefan, 1993).

This model is developed primarily based on field measurement to determine surface temperatures and thermocline depth. Meteorological data are not used, therefore the model can be used for temperature interpolation for the whole year rather than prediction for the future.





Figure 5-1 Temperature Profile of Lake Lanier in 1996/97



Figure 5-2 Surface Temperature of Lake Lanier in 1996/97






Figure 5-4 Monte Carlo Simulation with Heat Dispersion Coefficient at Stratification Period



Figure 5-5 Monte Carlo Simulation with Heat Dispersion Coefficient at Transition Period



Figure 5-6 Simulation Results of Temperature Profile



Figure 5-6 Simulation Results of Temperature Profile (con't)



Figure 5-6 Simulation Results of Temperature Profile (con't)



Figure 5-6 Simulation Results of Temperature Profile (con't)



Figure 5-6 Simulation Results of Temperature Profile (con't)



Figure 5-6 Simulation Results of Temperature Profile (con't)



Figure 5-6 Simulation Results of Temperature Profile (con't)



Figure 5-6 Simulation Results of Temperature Profile (con't)



Figure 5-7 Simulation Results of Temperature Profile in 1996

CHAPTER 6

LAKE WATER QUALITY MODEL DEVELOPMENT AND TESTING IN A SMALL POND

Water quality model development needs to consider water quality characteristics, water quality concerns, modeling objectives, and data availability. Review of existing lake water quality models in Chapter 2 indicates that it is necessary to build a new biogeochemical model to meet our modeling objectives. Water quality characteristics discussed in Chapter 3 indicate that our model development needs to focus on vertical distributions. In this chapter, a 1-D vertical biogeochemical model is developed, and the model structure is tested with real-time monitoring data in a small pond. The reason to study the pond is that a small-scale waterbody is easier to monitor and manipulate.

6.1 Introduction

Later Lanier water temperature, dissolved oxygen concentration, pH distributions are uniform horizontally, but highly variable in the vertical direction (as discussed in Chapter 3). This indicates a 1-D vertical distribution model is needed to study the ecosystems. In addition, considering the fact that the residence time of the reservoir is relatively long (about one and a half years), our water quality model development does not include hydrodynamic transport effects.

Most current water quality models for impounded water bodies (Kayombo et al., 2000; Chapelle et al., 2000; Hamilton and Schladow, 1997; Schladow and Hamilton, 1997; Ambrose et al., 1993) do not simulate carbonate chemistry and *pH*. However algal photosynthesis and respiration will affect both O_2 and *pH*. Algal photosynthesis produces

 O_2 and consumes CO_2 , while algal respiration produces CO_2 and consumes O_2 . In natural waters, pH is usually dominated by carbonate chemistry (Langmuir, 1997). Cai et al. (1995) listed some equations of the pore water inorganic carbon system. Chapra (1983) introduced some major ordinary differential equations of carbonate species. In this dissertation, we present a biogeochemical model that is used to simulate temporal dynamics and vertical variations of DO, algae, nutrients (P, N, C), pH, total iron and bottom sediment effects. It is well known that both O_2 and CO_2 have exchanges between atmosphere and water, but the exchange processes are different. The exchange of O_2 is mainly a physical process, while the exchange of CO_2 involves fast carbonate reactions in the water column. Therefore it necessary to simulate and calibrate both DO and pH. The biogeochemical model will be more reliable if DO and pH can be calibrated simultaneously. In addition, pH-dependent charge of soils is highly related with pH, this charge affects cation exchange capacity (CEC) and sediment adsorption capacity with respect to ammonium ions. Modeling pH is therefore essential to accurately simulate sediment-nutrient adsorption process.

6.2 Water Quality Indicators

Water quality characteristics, water quality indicators, water quality issues or concerns, modeling objectives, and data availability are the important considerations for water quality model development or model selection. The following is a brief summary of water quality indicators.

(1) Dissolved Oxygen (DO)

Dissolved oxygen is an essential element for the maintenance of healthy lakes and rivers. Most aquatic plants and animals require a minimum concentration of oxygen dissolved in water for survival. Some aquatic organisms such as trout require medium to high levels of dissolved oxygen to live. Waters of consistently high dissolved oxygen are usually considered healthy. A healthy water body provides a stable aquatic ecosystem capable of supporting many different kinds of aquatic organisms. The atmosphere, algae, and vascular aquatic plants are the primary sources of dissolved oxygen in lakes and rivers, while the accumulation of organic wastes depletes dissolved oxygen. The dissolved oxygen deficit is the difference between the equilibrium of O_2 with the atmosphere and the actual amount of DO in the water. A large deficit is an indicator of oxygen stress on natural waters, while a low deficit is an indicator of generally unstressed conditions. A DO concentration greater than 100 percent saturation can occur when the water has a higher concentration than what would be in equilibrium with oxygen, a temporary condition that typically results from rapid photosynthesis.

(2) Carbonaceous Biochemical Oxygen Demand (CBOD)

Carbonaceous biochemical oxygen demand measures the amount of organic material in the water. Organic material is fed upon by aerobic bacteria which require oxygen. In this process, organic matter is broken down and oxidized. Therefore *CBOD* is also a measure of the quantity of oxygen used by these microorganisms in the aerobic oxidation of organic matter.

(3) Water Temperature

Many of the physical, biological and chemical characteristics of surface water are dependent on temperature. Temperature affects the solubility of oxygen in water, the rate of photosynthesis by algae and larger aquatic plants, the metabolic rates of aquatic organisms and the sensitivity of organisms to toxic wastes, parasites and diseases. For example, aquatic organisms will die when the water temperature falls below a certain level (e.g., 0°C for most species) or when it exceeds a maximum value (about 35°C for many finfish).

(4) *pH*

pH is a measure of the state of equilibrium between water (H_2O) and its ions (H^+) and (OH) and is determined by various dissolved compounds in water, including salts and gasses. When compounds having ionizable (H^+) or (OH) groups dissolve in water, the equilibrium between H_2O , (H^+) , and (OH) shifts and the pH value increases (becomes more basic) or decreases (becomes more acidic). pH reflects the reactivity of water with various pollutants, and therefore the toxicity of those pollutants. Most valuable species, such as brook trout, are sensitive to changes in pH; immature stages of aquatic insects and immature fish are extremely sensitive to low pH values. Very acidic lakes and streams cause leaching of heavy metals into the water.

(5) Turbidity

Turbidity is the converse of water clarity and refers to interference with the passage of light by suspended matter, soluble colored organic compounds, or plankton in the water. The measurement of turbidity is used as an indirect indicator of the concentration of suspended matter, and also is important for evaluating the available light for photosynthetic use by aquatic plants and algae. One method of measuring turbidity uses an electronic transmissiometer, which measures light attenuation in water optically, yielding a percent transmittance. A much simpler, traditional method is use of a Secchi disc (a Secchi disc is a black and white disc which is lowered in water to the point where it is just barely visible in order to measure the depth of light penetration). When turbidity is high, water loses its ability to support a diversity of aquatic organisms. Oxygen levels decrease in turbid water as they become warmer as the result of heat absorption from the sunlight by the suspended particles and with decreased light penetration resulting in decreased photosynthesis. Suspended solids can clog fish gills, reduce growth rates and disease resistance, and prevent egg and larval development.

(6) Total Suspended Solids (TSS)

Total suspended solids refers to the concentration of suspended solid matter in water. *TSS* is measured by weighing the undissolved material trapped on a 450nm filter after filtration. The constituents that pass through the filter are designated total dissolved solids (*TDS*) and are comprised mainly of ions and colloids such as iron, chloride, sodium, sulfate, etc. It should be noted that there is a direct proportional relationship between suspended solids and turbidity. The solids in suspension may include sediment or detrital particles and plankton.

(7) Chlorophyll-a

Chlorophyll-*a* reflects the concentration of the principal pigment in green plants responsible for photosynthesis. As such, this parameter is a surrogate indicator of phytoplankton biomass, the amount of unattached algae that is present in the water.

(8) Fecal Coliform Bacteria

Fecal coliform bacteria are derived from the feces of humans and other warmblooded animals. These organisms enter rivers through direct discharge from mammals and birds; from agricultural and storm runoff containing mammal and bird wastes; and from sewage discharge. Even though fecal coliform bacteria are not pathogenic, they occur along with pathogenic organisms; therefore, their presence suggests the occurrence of disease-causing organisms. When fecal coliform counts are greater than 200 colonies/100 mL of water sample there is a greater chance that the disease-causing organisms are present. Possible diseases and illnesses carried by such waters are typhoid fever, hepatitis, gastroenteritis, dysentery, swimmers itch, and ear infections. A fecal coliform standard of less than 2000 colonies per 100 mL has been established for non-contact recreation sports such as sailing. A standard of less than 200 colonies per 100 mL was established for contact recreation such as swimming. Fecal coliform counts below 14 colonies per 100 mL comprise the standard for shellfish harvesting.

(9) SpecificConductance

Specific conductance measures the electrical conductants in the water. This is an indication of the quantity of dissolved inorganic acids, bases and salts in the water. The specific conductance to TDS ratio varies as a function of the cations and anions present in the water.

(10) Total Phosphorus (TP)

Total phosphorus includes organic phosphorus and inorganic phosphate. Organic phosphorus is a part of living plants and animals. It is attached to particulate organic matter composed of once-living plants and animals. Inorganic phosphates comprise the ions bonded to soil particles and phosphates present in laundry detergents. Some inorganic phosphorus is bounded to iron, calcium, etc. Phosphorus is an essential element for life; it is a plant nutrient needed for growth and a fundamental element in metabolic reactions of plants and animals. In many lakes, phosphorus functions as a *growth-limiting* factor because it is usually present in very low concentrations. This scarcity of phosphorus is attributed to its relationship with organic matter and soil particles. Any unattached or *free* phosphorus, in the form of inorganic phosphates, is rapidly taken up by algae and larger aquatic plants. Because algae only require small amounts of phosphorus to live, excess phosphorus causes extensive algal growth called algal blooms. Algal

blooms color the water and can be seen as a classic symptom of cultural eutrophication. Sources of phosphorus are human wastes, animal wastes, industrial wastes, and human disturbance of the land and its vegetation.

(11) Nitrate and Nitrite

Nitrate and nitrite are inorganic forms of nitrogen in the aquatic environment. Nitrate along with ammonia are the forms of nitrogen used by plants. Nitrates and nitrites are formed through the oxidation of ammonia by nitrifying bacteria, a process known as nitrification. In turn they are converted to other nitrogen forms by denitrification and plant uptake. Nitrogen, in its various forms is usually more abundant than phosphorus in the aquatic environment. Sources of nitrates are the atmosphere, inadequately treated wastewater from sewage treatment plants, agricultural runoff, storm drains, and poorly functioning septic systems.

(12) Benthic Macroinvertebrates

Benthic macroinvertebrates are bottom dwelling organisms that live in, crawl on or attach themselves to the bottom. These are visible with the naked eye. Macroinvertebrates are good indicators of aquatic health because they are sensitive to pollution; they reside in the water through the year, can not easily escape pollution as a fish can, and can easily be collected.

6.3 Model Development

Based on the analysis of water quality indicators, possible important chemical reactions, water quality concerns, modeling objectives, and the availability of data for Lake Lanier, suspended solids, phytoplankton, dissolved oxygen, carbonaceous biochemical oxygen demand, organic phosphorus, orthophosphate, organic nitrogen,

ammonia, nitrate, pH, iron, sediment oxygen demand, and sediment organic matter were selected as state variables in the model. Table 6-1 shows the symbols of the state variables and their units. Figure 6-1 indicates the state variable interactions.

(1) Suspended solids

Suspended solids are important in water quality simulations because of their influence on density, light penetration, and nutrient availability. Increased solids concentrations reduce light penetration in the water column thus affecting temperature which in turn affects biological and chemical reaction rates. Nutrient concentrations are also affected by solids through adsorption and settling. Light and nutrient availability largely control algal production.

$$\frac{\partial[SS]}{\partial t} = \frac{W_{SS}}{V} + D_z \frac{\partial^2[SS]}{\partial z^2} - \omega_{SS} \frac{\partial[SS]}{\partial z} - \frac{Q_{out} \cdot [SS]_{out}}{V}$$
loading diffusion settling outflow
(6-1)

where:

[SS] = suspended solid concentration (mg/L).

 W_{SS} = loading of suspended solids (g/day).

V =water volume (m³).

 D_z = vertical diffusion coefficient (m²/day).

 ω_{SS} = settling velocity of suspended solids (m/day).

 $Q_{out} = \text{outflow} (\text{m}^3/\text{day}).$

 $[SS]_{out}$ = outflow concentration of suspended sediment (mg/L).

Settling velocity can be set within the range of Stoke's velocity corresponding to the suspended particle size distribution:

$$\omega_{ss} = \frac{8.64g}{18\mu} (\rho_s - \rho_w) d_d^2$$
(6-2)

where:

 ω_{SS} = Stoke's velocity (m/day).

 $g = \text{acceleration of gravity (9.81 m/s^2)}.$

- μ = viscosity of water (about 10⁻³ N·s/m² at 20°C).
- ρ_s = density of the solid (g/cm³).
- ρ_w = density of water (g/cm³).
- d_P = particle diameter (mm).

Table 6-2 lists values of ω_{ss} for a range of particle sizes and densities.

(2) Phytoplankton

Phytoplankton is mainly affected by four processes: phytoplankton growth, phytoplanton respiration, phytoplankton death, and settling.

• Phytoplankton growth:

$$106CO_{2} + 16NO_{3}^{-} + HPO_{4}^{2^{-}} + 122H_{2}O + 18H^{+}(+energy) \leftrightarrow C_{106}H_{263}O_{110}N_{16}P + 138O_{2}$$
(6-3)

The forward reaction describes photosynthesis, and the backward reaction describes respiration. A byproduct of photosynthetic carbon fixation is the production of dissolved oxygen. The rate of oxygen production (and nutrient uptake) is proportional to the growth rate of the phytoplankton since its stoichiometry is fixed. Thus, for each unit of phytoplankton carbon produced by growth, (138*32)/(106*12) units of O_2 are produced.

• Phytoplankton respiration and death

Oxygen is diminished in the water column as a result of phytoplankton respiration, which is basically the reverse process of photosynthesis. Thus for every unit of phytoplankton carbon consumed by respiration, (138*32)/(106*12) units of oxygen are also consumed. The death of phytoplankton provides organic carbon, which can be

oxidized. The kinetic expression recycles phytoplankton carbon to *CBOD* using a first order death rate and the stoichiometric oxygen to carbon ratio 32/12.

Mass balance equation for phytoplankton:

$$\frac{\partial [PHYT]}{\partial t} = D_z \frac{\partial^2 [PHYT]}{\partial z^2} + K_{ag} [PHYT] - K_{ar} [PHYT] - K_{ad} [PHYT] - \omega_a \frac{\partial [PHYT]}{\partial z}$$

diffusion growth respiration death settling
(6-4)

Where:

[PHYT] = phytoplankton concentration (mg C/L).

 K_{ag} = phytoplankton growth rate (day⁻¹).

 K_{ar} = phytoplankton respiration rate (day⁻¹).

 K_{ad} = phytoplankton death rate (day⁻¹).

 ω_t = phytoplankton settling rate (m/day)

From Figure 3-18 and Figure 3-19 in Chapter 3, we can see DO and pH are both highest around the thermocline during the growing season. This phenomenon can be explained by the fact that when the increased phytoplankton in the epilimnion settle down to the thermocline, it will stop settling because of very low temperature and high water density in the hypolimnion. Phytoplankton settling rate can be set to be proportional to the difference between phytoplankton density and water density:

$$\omega_a = c \frac{\rho_a - \rho_w}{\rho_w} \tag{6-5}$$

In which:

- c coefficient (m/day).
- ρ_a phytoplankton density (g/cm³).
- ρ_w density of water (g/cm³).

The density of water varies at different temperatures (Figure 6-2):

$$\rho_w = 0.00002T - 0.0059T^2 + 0.0174T + 1000 \tag{6-6}$$

Where T = water temperature.

Phytoplankton growth rate is computed by modifying a maximum growth rate affected by temperature, light, and nutrient availability (Chen et al., 1975; Scavia, 1980; Ambrose, 1993):

$$K_{ag} = K_{agMax} f(T) f(I) \cdot \min(\frac{[PO_4]}{k_P + [PO_4]}, \frac{([NO_3^-] + [NH_3])}{k_N + ([NO_3^-] + [NH_3])}, \frac{TIC}{k_C + TIC})$$
(6-7)

where:

 K_{agMax} = maximum growth rate of phytoplankton.

f(T) = function of water temperature. Here $f(T) = \theta^{T-20}$ is selected (Chen and Orlob, 1975).

f(I) = function of light.

 k_P , k_N , k_C = half-saturation constant for phosphorus, nitrogen and carbon respectively.

TIC = Total inorganic carbon.

Algal respiration rate is computed using following equation (Ambrose, 1993; Cole, 1995):

$$K_{ar} = K_{arMax} f(T) \tag{6-8}$$

where K_{arMax} = maximum respiration rate of phytoplankton.

Temperature factor f(T) for algal respiration is assumed the same as that for algal growth, and phytoplankton death is assumed independent of temperature (Bierman, 1976).

(3) Dissolved Oxygen

Dissolved osygen (*DO*) has been modeled for over 70 years. The basic steady-state equations were developed and used by Streeter and Phelps (1925). Subsequent development and applications have added terms to their basic equation and provided for time-variable analysis. The equations implemented here are fairly standard.

Seven state variables can participate directly in the *DO* balance: phytoplankton, ammonia, nitrate, carbonaceous biochemical oxygen demand, sediment oxygen demand, sediment organic matter, and dissolved oxygen. The reduction of dissolved oxygen is a consequence of the aerobic respiratory processes in the water column and the anaerobic processes in the underlying sediments. Because both of these sets of processes can contribute significantly, it is necessary to formulate their kinetics explicitly.

• Reaeration:

Reaeration is the process of oxygen exchange between the atmosphere and a water body in contact with the atmosphere. Typically, the net transfer of oxygen is from the atmosphere and into the water, since dissolved oxygen levels in most natural waters are below saturation. However, when photosynthesis produces supersaturated dissolved oxygen levels, the net transfer is back into the atmosphere.

The reaeration process is modeled as the product of a mass-transfer coefficient multiplied by the difference between dissolved oxygen saturation and the actual dissolved oxygen concentration. The mass-transfer coefficient is a function of the average water velocity, depth, wind, and temperature. Here a single reaeration rate constant K_{O2} is specified:

$$Flux = K_{O2}(DO_s - DO) \tag{6-9}$$

where DO_s is saturation concentration of dissolved oxygen expressed as follows (Bowie et al., 1985).

$$DO_{s} = 14.5412 - 0.3928T + 0.007323T^{2} - 0.00006629T^{3}$$
(6-10)

in which, *T* is water temperature.

• Photosynthesis and respiration:

See Equation (6-3).

• Carbonaceous oxidation:

$$C_x H_y O_z + O_2 \rightarrow CO_2 + H_2 O \tag{6-11}$$

• Nitrification:

$$NH_{4}^{+} + 2O_{2} \rightarrow NO_{3}^{-} + H_{2}O + 2H^{+}$$
(6-12)

Thus for every unit of ammonia nitrogen oxidized, 2 (32/14) units of oxygen are consumed.

• Sediment oxygen demand and decay of sediment organic matter

$$CH_2O + O_2 \to CO_2 + H_2O \tag{6-13}$$

Therefore mass balance equation for dissolved oxygen is as follows:

$$\frac{\partial DO}{\partial t} = D_z \frac{\partial^2 DO}{\partial z^2} + K_{O2}(DO_s - DO) - k_{BOD} \Theta_{BOD}^{T-20} BOD - \frac{64}{14} k_{NI} \Theta_{NI}^{T-20} \left(\frac{DO}{K_{NIT} + DO}\right) [NH_3] \cdot f(pH)$$
diffusion reaeration oxidation nitrification
$$-\frac{SOD}{D_w} \Theta_{SOD}^{T-20} + \frac{138 * 32}{106 * 12} K_{ag} [PHYT] - \frac{138 * 32}{106 * 12} K_{ar} [PHYT] - \frac{32}{12} k_{SOM} \Theta_{SOM}^{T-20} [SOM]$$
sediment demand growth respiration SOM decay
$$(6-14)$$

where:

 $k_{BOD} = BOD$ decay rate (1/day).

 Θ_{BOD} = temperature factor for *BOD*.

 k_{NI} = nitrification rate (1/day).

 Θ_{NI} = temperature factor for nitrification.

 K_{NIT} = half-saturation constant for oxygen limitation in nitrification (mg N/L).

SOD = sediment oxygen demand (g/m²-day).

 D_w = depth of water segment (m).

 Θ_{BOD} = temperature factor for SOD.

[SOM] = concentration of sediment organic matter (mg/L).

 k_{SOM} = sediment organic matter decay rate (1/day).

 Θ_{SOM} = temperature factor for sediment organic matter decay.

f(pH) = function of pH for nitrification, which will be explained in the part of nitrogen cycle.

(4) Carbonaceous Biochemical Oxygen Demand (CBOD)

The long history of applications have focused primarily on the use of *BOD* as the measure of the quantity of oxygen demanding material and its rate of oxidation as the controlling kinetic reaction. This has proven to be appropriate for waters receiving a heterogeneous combination of organic wastes of municipal and industrial origin since an aggregate measure of their potential effect is a great simplification that reduces a complex problem to one of tractable dimensions.

The oxidation of carbonaceous material is the classical *BOD* reaction. Internally the model uses ultimate carbonaceous biochemical oxygen demand (*CBOD*) as the indicator of equivalent oxygen demand for the carbonaceous material. A principal source of *CBOD*, other than man-made sources and natural runoff, is detrived phytoplankton carbon, produced as a result of algal death. The primary loss mechanism associated with *CBOD* is oxidation:

• Carbonaceous oxidation:

See equation (6-11).

• Phytoplankton death:

The death of phytoplankton provides organic carbon, which can be oxidized. The kinetic expression recycles phytoplankton carbon to *CBOD* using a first order death rate and the stoichiometric oxygen to carbon ratio 32/12.

- Settling of organic matter
- Denitrification:

Under low DO conditions, the denitrification reaction provides a sink for CBOD:

$$5 CH_2O + 5 H_2O + 4 NO_3^{-} + 4 H^{+} \rightarrow 5 CO_2 + 2 N_2 + 12 H_2O$$
(6-15)

Thus for each unit of nitrate nitrogen reduced, 5/4 (12/14) units of carbon are consumed, which reduces *CBOD* by 5/4 (32/14) units. Denitrification is not a significant loss in the water column, but can be important when simulating anaerobic benthic conditions.

Mass balance equation for CBOD is:

$$\frac{\partial BOD}{\partial t} = \frac{W_{BOD}}{V} + D_z \frac{\partial^2 BOD}{\partial z^2} - k_{BOD} \Theta_{BOD}^{(T-20)} BOD + \frac{32}{12} K_{ad} [PHYT] - \frac{Q_{out} \cdot BOD_{out}}{V}$$

$$loading \quad diffusion \quad oxidation \quad death \quad outflow$$

$$-\frac{5}{4} \frac{32}{14} k_{DN} \Theta_{DN}^{(T-20)} \left(\frac{K_{NO3}}{K_{NO3} + DO}\right) [NO_3^-] - v_s (1 - c_{BOD}) \frac{\partial BOD}{\partial z}$$

$$denitrification \quad settling$$

where:

BOD = BOD concentration (mg/L).

 $W_{BOD} = BOD$ loading (g/day).

 $k_{BOD} = BOD$ decay coefficient (day⁻¹)

 $Q_{out} =$ outflow (m3/day).

 BOD_{out} = outflow concentration of BOD (mg/L).

 K_{DN} = denitrification rate (1/day).

 K_{ad} = algal death rate (1/day).

 Θ_{DN} = temperature factor for denitrification.

 K_{NO3} = half-saturation constant of nitrate for oxygen limitation (mg N/L).

 v_s = organic matter settling velocity (m/day).

 c_{BOD} = fraction of dissolved *CBOD*.

(5) Sediment Oxygen Demand (SOD) and Sediment Organic Matter (SOM)

The decomposition of organic material in benthic sediment can have profound effects on the concentrations of oxygen in the overlying waters. The decomposition of organic material results in the exertion of an oxygen demand at the sediment-water interface. As a result, the areal fluxes from the sediment can be substantial oxygen sinks to the overlying water column.

Sediment oxygen demand is influenced by two different phenomena. The first is the rate at which oxygen diffuses into the bottom sediments and is then consumed. The second is essentially the rate at which reduced organic substances in sediment are conveyed into the water column, and are then oxidized (Bowie et al., 1985).

$$SOD = \frac{E_{SOD}}{D_m} \left(DO_w - DO_m \right) \tag{6-17}$$

$$\frac{\partial [SOM]}{\partial t} = \frac{\omega_a}{\Delta z} [PHYT] + \frac{12}{32} v_s (1 - c_{BOD}) \frac{BOD}{\Delta z} - k_{SOM} \Theta_{SOM}^{T-20} [SOM]$$
phytoplankton settling BOD settling decay
$$(6-18)$$

where:

SOD = sediment oxygen demand (g/m²-day).

 E_{SOD} = diffusive exchange coefficient of SOD (m²/day).

 D_m = depth of benthic sediment layer (m).

 DO_w = dissolved oxygen concentration in the water column (mg/L).

 DO_m = dissolved oxygen concentration in the sediment layer (mg/L).

[SOM] = concentration of sediment organic matter (mg/L).

 k_{SOM} = sediment organic matter decay coefficient (1/day).

 Θ_{SOM} = temperature factor.

 ω_t = phytoplankton settling velocity (m/day).

 v_s = organic matter settling velocity (m/day).

(6) Nitrogen cycle

Three nitrogen variables are modeled: organic nitrogen, ammonia, and nitrate.

Phytoplankton Growth

Dissolved inorganic nitrogen is taken up and incorporated into biomass as phytoplankton grow. For every unit of phytoplankton carbon produced, a_{NC} units of inorganic nitrogen are taken up. Both ammonia and nitrate are available for uptake and use in cell growth by phytoplankton. However, for physiological reasons, the preferred form is ammonia nitrogen. The ammonia preference term P_{NH3} is given (Thomann et al. 1982; O'Connor et al. 1981; Ambrose et al., 1993):

$$P_{NH3} = \left(\frac{[NH_3][NO_3^-]}{(K_{mN} + [NH_3])(K_{mN} + [NO_3^-])}\right) + \left(\frac{K_{mN}[NH_3]}{([NH_3] + [NO_3^-])(K_{mN} + [NO_3^-])}\right) (6-19)$$

The behavior of this equation, for a Michaelis value, K_{mN} , is 25 µg N/L (Ambrose et al., 1993). The behavior of this equation is sensitive at low values of ammonia or nitrate. For a given concentration of ammonia, as the available nitrate increases above approximately the Michaelis limitation, the preference for ammonia reaches an asymptote. Also, as the concentration of available ammonia increases, the plateau levels off at values closer to unity, i.e., total preference for ammonia.

Phytoplankton Respiration

Living organic material is recycled to nonliving organic and inorganic matter as phytoplankton respire. For every unit of phytoplankton carbon consumed or lost, a_{NC} units of nitrogen is released. During phytoplankton respiration, a fraction of the cellular nitrogen f_{ON} is organic, while $(1 - f_{ON})$ is in the inorganic form of ammonia nitrogen. The fraction recycled to the inorganic pool for Great Lakes models has been assigned at 50% (Di Toro and Matystik, 1980).

• Mineralization

Nonliving organic nitrogen may undergo mineralization or bacterial decomposition into ammonia nitrogen before utilization by phytoplankton. In this model, the first order, temperature-corrected rate constant is modified by a saturated recycle term k_{mPc} . This mechanism slows the mineralization rate if the phytoplankton population is small, but does not permit the rate to increase continuously as phytoplankton increases (Ambrose et al. 1993).

• Settling and release

Particulate organic nitrogen settles according to velocity and particulate fraction,

and some ammonia nitrogen will be released when sediment organic matter decays.

• Nitrification

Ammonia nitrogen, in the presence of nitrifying bacteria and oxygen, is converted to nitrate nitrogen (nitrification). The process of nitrification in natural waters is carried out by aerobic autotrophs; *Nitrosomonas* and *Nitrobacter* predominate in fresh waters. It is a two-step process with *Nitrosomonas* bacteria responsible for the conversion of ammonia to nitrite and *Nitrobacter* responsible for the conversion of nitrite. Essential to this reaction process are aerobic conditions. Also this process appears to be affected by

high or low values of pH that inhibit *Nitrosomonas* growth, particularly for pH below 4 and greater than 9 (Ambrose et al. 1993). As with phytoplankton, the nitrifying bacterial populations are sensitive to flow. During periods of high flow or storm runoff, upstream bacteria may be advected downstream, with some lag time after a flow transient before they can build up to significant levels again.

The process of nitrification in natural waters, then, is complex, depending on dissolved oxygen, pH, and flow conditions, which in turn leads to spatially and temporally varying rates of nitrification. To properly account for this complex phenomenon in the modeling framework would be difficult and would require a data base that is usually unavailable. In this modeling, only pH is considered for nitrification process.

• Denitrification

Denitrification refers to the reduction of nitrate (or nitrite) to N_2 and other gaseous products such as N_2O and NO. This process is carried out by a large number of heterotrophic, facultative anaerobes. Under normal aerobic conditions found in the water column, these organisms use oxygen to oxidize organic material. Under the anaerobic conditions found in the sediment bed or during extremely low oxygen conditions in the water column, however, these organisms are able to use nitrate as the electron acceptor.

• Sediment adsorption for ammonium ions

Soil minerals can exibit constant charge and variable charge or pH-dependent charge. The negative charge results from isomorphous substitution, and the variable charge results from deprotonation of functional groups (Sparks, 1995). The negative surface charge is balanced by positive charge such as ammonium ions in the form of exchangeable cations. Sediment-ammonium adsorption is affected by pH.

Mass balance equations:

$$\frac{\partial [ON]}{\partial t} = \frac{W_{ON}}{V} + \frac{16*14}{106*12} K_{ar} f_{ON} [PHYT] - k_{ON} \Theta_{ON}^{T-20} \left(\frac{[PHYT]}{K_{mPc} + [PHYT]} \right) [ON]$$

loading respiration mineralization (6-20)

$$+ D_{z} \frac{\partial^{2}[ON]}{\partial z^{2}} - v_{s}(1 - c_{ON}) \frac{\partial[ON]}{\partial z} - \frac{Q_{out} \cdot [ON]_{out}}{V}$$

diffusion settling outflow

AMMONIA NITROGEN :

$$\frac{\partial [NH_3]}{\partial t} = \frac{W_{NH3}}{V} + D_z \frac{\partial^2 [NH_3]}{\partial z^2} + \frac{16*14}{106*12} K_{ar} (l - f_{ON}) [PHYT] + k_{ON} \Theta_{ON}^{T-20} \left(\frac{[PHYT]}{K_{mPc} + [PHYT]} \right) [ON]$$
loading diffusion respiration mineralization

$$-\frac{16*14}{106*12}K_{ag}P_{NH3}[PHYT] - k_{NI}\Theta_{NI}^{T-20}\left(\frac{DO}{K_{NIT}+DO}\right)[NH_3] \cdot f(pH)$$
growth
nitrification

$$+\frac{16*14}{106*12}k_{SOM}\Theta_{SOM}^{T-20}[SOM] - \frac{P_{N}\{\boldsymbol{\omega}_{SS}[SS]\}}{\Delta z}[NH_{3}] - \frac{Q_{out}\cdot[NH_{3}]_{out}}{V}$$
release adsorption outflow
(6-21)

NITRATE NITROGEN :

$$\frac{\partial [NO_3^-]}{\partial t} = \frac{W_{NO_3^-}}{V} + D_z \frac{\partial^2 [NO_3^-]}{\partial z^2} + k_{NI} \Theta_{NI}^{T-20} \left(\frac{DO}{K_{NIT} + DO}\right) [NH_3] \cdot f(pH)$$

loading diffusion nitrification

$$-\frac{16*14}{106*12}K_{ag}(1-P_{NH3})[PHYT] - k_{DN}\Theta_{DN}^{T-20}\left(\frac{K_{NO3}}{K_{NO3}+DO}\right)[NO_{3}^{-}] - \frac{Q_{out}\cdot[NO_{3}^{-}]_{out}}{V}$$
growth
denitrification
outflow
(6-22)

where:

 f_{ON} = fraction of organic nitrogen in phytoplankton.

 k_{mPc} = saturated recycle constant for mineralization.

 v_s = organic matter settling velocity (m/day).

 c_{ON} = fraction of dissolved organic nitrogen.

 k_{NI} = nitrification rate (1/day).

 Θ_{NI} = temperature factor for nitrification.

 K_{NIT} = half-saturation constant for oxygen limitation in nitrification (mg N/l).

 K_{DN} = denitrification rate (1/day).

 Θ_{DN} = temperature factor for denitrification.

 K_{NO3} = half-saturation constant of nitrate for oxygen limitation (mg N/l).

 P_{NH3} = ammonia preference term for phytoplankton growth.

 P_N = adsorption coefficient for NH_3 (m³/g).

f(pH) = function of pH expressed as follows (Darrah et al., 1986):

$$f(pH) = \begin{cases} 35.019 - 24.538 \, pH + 6.147 \, pH^2 - 0.647 \, pH^3 + 0.02435 \, pH^4 & 4 \le pH \le 9\\ 0 & pH < 4 \text{ or } pH > 9 \end{cases}$$
(6-23)

Equation (6-23) was obtained from pore water experiment data shown Figure 6-3.

(7) Phosphorus Cycle

Phosphorus is an important element in aquatic ecosystems since it serves as one of the primary nutrients for phytoplankton growth. In many fresh waters, phosphorus is considered to be the nutrient limiting maximum production of phytoplankton biomass.

Phosphorus is assumed to be completely available as orthophosphate (PO_4) for uptake by phytoplankton. Measurements of soluble reactive phosphorus are closest to the bioavailable form. In this model, two phosphorus variables are modeled: organic

phosphorus, and inorganic (orthophosphate) phosphorus. Organic phosphorus is divided into particulate and dissolved concentrations by spatially variable dissolved fractions. Inorganic phosphorus also is divided into particulate and dissolved concentrations by spatially variable dissolved fractions, reflecting sorption.

• Phytoplankton growth

As phytoplankton grow, dissolved inorganic phosphorus is taken up, stored and incorporated into biomass. For every mg of phytoplankton carbon produced, a_{PC} mg of inorganic phosphorus is taken up.

• Phytoplankton respiration and death

As phytoplankton respire and die, biomass is recycled to nonliving organic and inorganic matter. For every mg of phytoplankton carbon consumed or lost, a_{PC} mg of phosphorus is released. A fraction f_{OP} is organic, while $(1 - f_{OP})$ is in the inorganic form and readily available for uptake by other viable algal cells. In work on the Great Lakes, f_{OP} was assigned at 50% (Di Toro and Matystik, 1980).

• Mineralization

Nonliving organic phosphorus must undergo mineralization bacterial or decomposition into inorganic phosphorus before utilization by phytoplankton. In the work on Lake Huron and Saginaw Bay, Di Toro and Matystik (1980) proposed a nutrient recycle formulation that was a function of the localized phytoplankton population. This proposal was based on both an analysis of available field data and the work of others (Hendry, 1977; Lowe, 1976; Henrici, 1938; Menon, 1972; and Rao, 1976) that indicated bacterial biomass increased as phytoplankton biomass increased. This model uses a saturating recycle mechanism, a compromise between conventional first-order kinetics and a second order recycle mechanism wherein the recycle rate is directly proportional to had been indicated in pure the phytoplankton biomass present, as culture, bacteria-seeded, laboratory studies (Jewell and McCarty, 1971).

Saturating recycle permits second order dependency at low phytoplankton concentrations, when $P_c \ll K_{mPc}$, where K_{mPc} is the half-saturation constant for recycle, and permits first order recycle when the phytoplankton greatly exceed the half-saturation constant. Basically, this mechanism slows the recycle rate if the phytoplankton population is small, but does not permit the rate to increase continuously as phytoplankton increase. The assumption is that at higher population levels, recycle kinetics proceeds at the maximum first order rate (Di Toro and Matystik, 1980).

• Settling and release

Particulate organic and inorganic phosphorus settles according to settling velocity and particulate fraction, and some inorganic phosphorus will release when sediment organic matter decays.

• Sediment-phosphorus adsorption and iron-phosphorus binding

There is an adsorption-desorption interaction between dissolved inorganic phosphorus and suspended particulate matter in the water column. The subsequent settling of the suspended solids together with the sorbed inorganic phosphorus can act as a significant loss mechanism in the water column and is a source of phosphorus to bottom sediment.

The complex interactions between iron and phosphorus play an important role in the availability of phosphorus in surface waters. Ferric oxides sorb dissolved inorganic phosphorus via ligand exchange. In Georgia piedmont impoundments, iron-phosphorus binding is an important sink for dissolved inorganic phosphorus because of iron-rich soils (Parker and Rasmussen, 2001).

ORGANIC PHOSPHORUS :

$$\frac{\partial [OP]}{\partial t} = \frac{W_{OP}}{V} + D_2 \frac{\partial^2 [OP]}{\partial z^2} + \frac{31}{106*12} K_{ar} f_{OP} [PHYT] - \frac{Q_{out} \cdot [OP]_{out}}{V}$$

$$loading diffusion respiration outflow (6-24)$$

$$-k_{OP} \Theta_{OP}^{T-20} \left(\frac{[PHYT]}{K_{mPc} + [PHYT]} \right) [OP] - v_s (1 - c_{OP}) \frac{\partial [OP]}{\partial z}$$

$$mineralization settling$$

$$\frac{\partial [PO_4]}{\partial t} = \frac{W_{PO4}}{V} + D_z \frac{\partial^2 [PO_4]}{\partial z^2} + \frac{31}{106*12} K_{ar} (1 - f_{OP}) [PHYT] + k_{OP} \Theta_{OP}^{T-20} \left(\frac{[PHYT]}{K_{mPc} + [PHYT]} \right) [OP]$$

$$loading diffusion respiration mineralization - \frac{31}{106*12} K_{ag} [PHYT] - \frac{P_p \{\Theta_{SS}[SS] + \Theta_{Fc}[Fe]\}}{\Delta z} [PO_4] + \frac{31}{106*12} k_{SOM} \Theta_{SOM}^{T-20} [SOM]$$

$$growth adsorption release$$

$$- \frac{Q_{out} \cdot [PO_4]_{out}}{V}$$

(6-25)

where

 f_{OP} = fraction of organic phosphorus in phytoplankton.

 k_{mPc} = saturated recycle constant for mineralization.

 v_s = organic matter settling velocity (m/day).

 c_{OP} = fraction of dissolved organic phosphorus.

 K_{OP} = mineralization rate for organic phosphorus (1/day).

 Θ_{OP} = temperature factor for mineralization.

 ω_{ss} = settling velocity of suspended solids.

- ω_{Fe} = settling velocity of iron.
- P_p = adsorption coefficient for phosphorus (m³/g).
- Δz = thickness of water segment.

(8) Total iron

Total iron is included in the model primarily because of the its effect on nutrient concentrations through adsorption and settling. Iron is commonly released from anoxic sediments and may also contribute to dissolved oxygen depletions, but the model does not presently include these effects. Iron sediment release is modeled as a zero-order process.

$$\frac{\partial [Fe]}{\partial t} = \frac{W_{Fe}}{V} + D_z \frac{\partial^2 [Fe]}{\partial z^2} + \frac{S_{Fe}}{D_w} \Theta_{Fe}^{(T-20)} - \omega_{Fe} \frac{\partial [Fe]}{\partial z} - \frac{Q_{out} \cdot [Fe]_{out}}{V}$$
(6-26)
loading diffusion release settling outflow

Where:

[Fe] – concentration of total iron in the water column.

 W_{Fe} – loading of total iron.

 S_{Fe} - release rate of total iron from sediment (g/m²-day). It is assumed proportional to sediment oxygen demand (Cole, 1995).

 D_w - water depth.

 ω_{Fe} – settling rate of total iron.

(9) pH

The pH is computed based on the equilibrium among carbonate species which include carbon dioxide, bicarbonates and carbonate. Carbon dioxide enters and leaves the
inorganic carbon pool via two major pathways: atmospheric and biological exchange processes. Other heterogeneous reactions such as calcium carbonate dissolution and precipitation are neglected.

• Atmospheric exchange

$$W_{atm} = K_{CO2}\{[CO_2(aq)]_{s} - [CO_2(aq)]\}$$
(6-27)

Where:

 W_{atm} --rate of mass transfer of CO_2 across the air-water interface (mol/L)

 K_{CO2} -mass transfer coefficient for CO_2 (day⁻¹)

 $[CO_2(aq)]$ --concentration of dissolved carbon dioxide in the lake (mol/L)

 $[CO_2(aq)]_s$ --concentration of dissolved carbon dioxide at saturation (mol/L)

$$CO_2(g) + H_2O = H_2CO_3$$
 (6-28)
 $[CO_2(aq)]_s = K_H P_{CO2}$

where:

 K_H —Henry's constant. At standard condition (1 atm, 25°C), K_H =10^{-1.47}

 P_{CO2} -partial pressure of CO_2 (atm)

• Photosynthesis/Respiration

The chemical reaction is the same as equation (6-3).

• Dissociation of carbonate dioxide and bicarbonate ion

$$H_2CO_3^{*} \stackrel{k_3}{\longleftrightarrow} H^+ + HCO_3^{-} \qquad (6-29)$$

Equilibrium constant:

$$K_{1} = \frac{k_{3}}{k_{4}} = \frac{[H^{+}][HCO_{3}^{-}]}{[H_{2}CO_{3}^{*}]}$$
(6-30)

$$HCO_{3}^{k_{5}} \leftrightarrow H^{+} + CO_{3}^{2} \qquad (6-31)$$

$$k_{6}$$

Equilibrium constant:

$$K_{2} = \frac{k_{5}}{k_{6}} = \frac{[H^{+}][CO_{3}^{2-}]}{[HCO_{3}^{-}]}$$
(6-32)

At standard condition, $K_1 = 10^{-6.35}$, $K_2 = 10^{-10.33}$

Therefore mass balance equations for carbonate species can be obtained as follows:

$$\frac{d[H_2CO_3^*]}{dt} = D_z \frac{\partial^2 [H_2CO_3^*]}{\partial z^2} + K_{CO2} \{ [CO_2(aq)]_s - [H_2CO_3^*] \} - K_{ag} [PHYT] + K_{ar} [PHYT]$$

diffusion atmospheric exchange growth respiration

$$+K_{BOD}\Theta_{BOD}^{(T-20)} \cdot BOD + \frac{5}{4}\frac{12}{14}k_{DN}\Theta_{DN}^{(T-20)}\left(\frac{K_{NO3}}{K_{NO3} + DO}\right)NO_{3}^{-}] - \{k_{3}[H_{2}CO_{3}^{*}] - k_{4}[H^{+}][HCO_{3}^{-}]\}$$

oxidation denitrification

$$+ k_{SOM} \Theta_{SOM}^{T-20} [SOM]$$
SOM decay
(6-33)

$$\frac{d[HCO_3^-]}{dt} = D_z \frac{\partial^2 [HCO_3^-]}{\partial z^2} + \{k_3 [H_2 CO_3^*] - k_4 [H^+] [HCO_3^-]\} - \{k_5 [HCO_3^-] - k_6 [H^+] [CO_3^{2-}]\}$$

(6-34)

$$\frac{d[CO_3^{2^-}]}{dt} = D_z \frac{\partial^2 [CO_3^{2^-}]}{\partial z^2} + \{k_5 [HCO_3^-] - k_6 [H^+] [CO_3^{2^-}]\}$$
(6-35)

$$\frac{d[H^+]}{dt} = D_z \frac{\partial^2 [H^+]}{\partial z^2} - \frac{18}{106} \frac{1}{12} (K_{ag} - K_{ar}) [PHYT] + \frac{2}{14} k_{NI} \Theta_{NI}^{T-20} \left(\frac{DO}{K_{NIT} + DO}\right) [NH_3]$$

+ {
$$k_{3}[H_{2}CO_{3}^{*}] - k_{4}[H^{+}][HCO_{3}^{-}]$$
} + { $k_{5}[HCO_{3}^{-}] - k_{6}[H^{+}][CO_{3}^{2^{-}}]$ } (6-36)

$$Alk = [HCO_3^-] + 2[CO_3^{2-}] + [OH^-] - [H^+] = [HCO_3^-] + 2[CO_3^{2-}] + \frac{K_{\omega}}{[H^+]} - [H^+]$$
(6-37)

$$pH = -\log_{10}[H^+] \tag{6-38}$$

Because the reactions between the inorganic carbon species are much faster than the gains and losses due to atmospheric and biotic exchange, a local equilibrium assumption can be made (Di Toro, 1976). Therefore equations (6-33) through (6-35) can be combined to yield:

$$\frac{dCT}{dt} = D_z \frac{\partial^2 CT}{\partial z^2} + K_{CO2} \{ [CO_2(aq)]_s - [H_2 CO_3^*] \} - K_{ag} [PHYT] + K_{ar} [PHYT] + K_{ar} [PHYT] + K_{BOD} \Theta_{BOD}^{(T-20)} \cdot BOD + \frac{5}{4} \frac{12}{14} k_{DN} \Theta_{DN}^{(T-20)} \left(\frac{K_{NO3}}{K_{NO3} + DO} \right) NO_3^-] + k_{SOM} \Theta_{SOM}^{T-20} [SOM]$$

$$(6-39)$$

Where *CT* is the concentration of total carbon:

$$CT = H_2 CO_3^* + HCO_3^- + CO_3^{2-}$$
(6-40)

Equation (6-39) allows computation of the dynamics of total inorganic carbon as a function of biotic and atmospheric interactions. As such, it effectively connects the organic carbon system with the food chain.

Theoretically the above mass balance equations can be implemented with numerical methods designed to solve sets of nonlinear simultaneous equations. But this is difficult to implement because the reaction rate constants k_3 , k_4 , k_5 and k_6 are greatly dependent on temperature and difficult to estimate. A simpler and less costly alternative is to solve the equations directly by assuming that hydrogen and hydroxyl ions have negligible effect on alkalinity. For such cases, the equation (6-37) can be replaced by:

$$A_c = [HCO_3^-] + 2[CO_3^{2-}]$$
(6-41)

Where A_c is carbonate alkalinity. The change of CO_2 due to photosynthesis and respiration has no effect on carbonate alkalinity (Cai et al.1995), because:

$$H_2O + CO_2 + CO_3^{2-} \leftrightarrow 2HCO_3^{-} \tag{6-42}$$

The direct method is to compute total inorganic carbon *CT* dynamically first, then at each time step, connections of equation (6-41), (6-42), (6-30) and (6-32) can be solved simultaneously for the four unknowns $[H^+]$, $[H_2CO_3^*]$, $[HCO_3^-]$ and $[CO_3^{2-}]$ at different layers:

$$[H^{+}] = \frac{-(K_{1}A_{c} - K_{1} \cdot CT) + \sqrt{(K_{1}A_{c} - K_{1} \cdot CT)^{2} - 4A_{c}(K_{1}K_{2}A_{c} - 2K_{1}K_{2} \cdot CT)}}{2A_{c}}$$
(6-43)

$$[H_2 CO_3^*] = \frac{[H^+]^2}{[H^+]^2 + K_1[H^+] + K_1K_2} \cdot CT$$
(6-44)

$$[HCO_{3}^{-}] = \frac{K_{1}[H^{+}]}{[H^{+}]^{2} + K_{1}[H^{+}] + K_{1}K_{2}} \cdot CT$$
(6-45)

$$[CO_{3}^{2-}] = \frac{K_{1}K_{2}}{[H^{+}]^{2} + K_{1}[H^{+}] + K_{1}K_{2}} \cdot CT$$
(6-46)

Figure 6-4 indicates the concentrations of carbonate species at different pH.

6.4 Identification of Important Parameters

(1) Maximum growth rate of algal biomass

Usually there exist different dominant algae in waters such as diatoms, blue-green algae, and green algae, etc. Different algae have very different maximum growth rate at different temperatures (Bowie et al., 1985, Zheng et al.1994). However, we choose a total growth rate in this model, see equation (6-7).

(2) Respiration/death rate of algae

Respiration rate of algae is the rate at which the algae oxidize their organic carbon to carbon dioxide per unit weight of algal organic carbon. Respiration is the reverse of the photosynthesis process. If the respiration rate of the algae as a whole is greater than the growth rate, there is a net loss of algae carbon or biomass. Algal respiration rate is temperature dependent (Riley et al., 1949) and will be determined by equation. Reported values of algal respiration rate at 20°C vary from 0.02/day to 0.6/day, with most values falling between 0.05/day to 0.35/day (Bowie et al., 1985).

(3) Light limiting factor

The Steele (1965) equation is selected to estimate f(I) (shown in Figure 6-5):

$$f(I) = \frac{I}{I_s} \exp(1 - \frac{I}{I_s})$$
(6-47)

where:

 I_s = saturating light intensity at maximum photosynthetic rate.

I = available light intensity.

Equation (6-54) allows for simulation of photoinhibition at light intensities greater than the saturation value. However, light penetration decreases with depth:

$$I = (1 - \beta)I_0 e^{-\alpha z}$$
(6-48)

in which:

 I_0 = solar radiation at the water surface.

 α = attenuation coefficient.

z = depth.

 β = fraction of solar radiation absorbed at the water surface.

Equation (6-47) and (6-48) can be combined to yield an equation for the growth rate reduction as a function of light attenuated to a given depth:

$$f[I(z)] = \frac{(1-\beta)I_0 e^{-\alpha z}}{I_s} \left[1 - \frac{(1-\beta)I_0 e^{-\alpha z}}{I_s}\right]$$
(6-49)

To use equation (6-49) in the present mathematical model, it must be averaged in space and time. The former can be done by integrating over the depth of the layer. The temporal averaging must take into account the fact that light varies through the course of a day. This can be approximated as

$$I_0(t) = I_a 0 < t < f (6-50)$$

$$I_0(t) = 0 f < t < 1 (6-51)$$

where:

f = daylight fraction of the day, or photoperiod.

 I_a = average incident solar radiation during the daylight period.

The photoperiod f and average incident solar radiation I_a are shown in Figure 6-6.

The integration over depth and photoperiod can be represented as follows (Reckhow, 1983):

$$f(I) = \frac{1}{z_2 - z_1} \int_{z_1}^{z_2} \frac{1}{T} \int_{0}^{f} f[I(z)] dt dz$$
(6-52)

where:

 z_1 = depth of the top of the layer where depth increases downward.

 z_2 = depth of the bottom of the layer.

The result of the integration for each layer is

$$f(I) = \frac{ef}{O(z_2 - z_1)} [e^{-\gamma_2} - e^{-\gamma_1}]$$
(6-53)

Where:

$$\gamma_1 = \frac{(1 - \beta)I_0}{I_s} e^{-\alpha z_1}$$
(6-54)

$$\gamma_2 = \frac{(1 - \beta)I_0}{I_s} e^{-\alpha z_2}$$
(6-55)

(4) Equilibrium constants K_H , K_1 and K_2

The equilibrium constants K_H , K_1 and K_2 for CO_2 , H_2CO_3 , and HCO_3^- dissolution, respectively, are affected by temperature. The relationship between the equilibrium constant and temperature is given by van't Hoff equation:

$$\frac{d(\ln K)}{dT} = \frac{\Delta H_r^0}{RT^2}$$
(6-56)

Where:

K--equilibrium constant

T--absolute temperature ($^{\circ}K$)

R--gas constant which is 8.3145 J K⁻¹mol⁻¹

 ΔH_r^0 --reaction enthalpy at standard condition (KJ mol⁻¹)

The van't Hoff equation is easily integrated if ΔH_r° is a constant, independent of temperature *T*. The integrated result is:

$$\ln K_{T_2} - \ln K_{T_1} = -\frac{\Delta H_r^0}{R} (\frac{1}{T_2} - \frac{1}{T_1})$$
(6-57)

 ΔH_r^0 can be calculated from the following equation:

$$\Delta H_r^0 = \Sigma \mathcal{M}_f^0 (\text{Products}) - \Sigma \mathcal{M}_f^0 (\text{Reactants})$$
(6-58)

where the terms on the right side are the standard formation enthalpies of the products and reactants weighted by the stoichiometric coefficients v in the chemical equation. The standard formation enthalpies of the considered species are shown in Table 6-3.

From the known values of K_H , K_1 and K_2 at standard condition, using equations (6-57) and (6-58), we can calculate K_H , K_1 and K_2 at different temperatures which are shown in Figure 6-7, Figure 6-8, Figure 6-9.

(5) Other parameters

Other parameters are shown in Table 6-4.

6.5 Model Testing in a Small Pond

6.5.1 Data collection

Current studies on Lake Lanier have identified requirements which include a more detailed understanding of basic lake ecosystem behavior, the role of the microbial food web, and limnetic geochemistry. Prior to embarking on a large scale and expensive sampling schedule, good scientific method requires economical field experiments to provide sufficient data to verify complex model structures. Until recently, scientists were confronted with two data problems: (a) data poor due to high information costs associated with quantitative sampling beyond the mesocosm scale - a problem which certainly affects our ability to build a reliable model suitable for ecosystems of lake scale; (b) data rich but information poor due to most of data collection not meeting the requirements of mathematical modeling. The intensive data collection was carefully designed and conducted at a small impoundment in the Southeastern Piedmont from August 12 through November 14, 1998 (95 days). The pond has about 2000 m³ water volume and about 7000 m² drainage area. It is within Whitehall Experimental Forest, near the campus of the University of Georgia, Athens, Georgia, U.S.A. (83°24'W, 33°54'N). The pond is situated down slope of the main timber plots and wildlife pens of the experimental forest, adjacent to the Oconee River, with all surface flow supplied by a first-order perennial stream. Water depth of the pond was measured, with a minimum depth of 42 cm at the headwater and a maximum depth of 3 m at the levee.

The University of Georgia's Environmental Process Control Laboratory (EPCL) was deployed on-site at two locations (upstream and downstream, see Figure 6-10) to automatically sample, measure and record ammonia (NH_3-N) , nitrite (NO_2-N) , nitrate $(NO_3 - N)$, total oxidized nitrogen (TON), total organic carbon (TOC), orthophosphate (PO_4) , dissolved oxygen (DO), and temperature at 15 minute intervals. Water samples were pumped from 0.5 m depth of the pond. To accommodate sample return to the pond and reduce sampling error, a submerged drain baffle was constructed at a point equidistant from each sampling intake. It is worth noting that the EPCL is the core facility of the Environmental Informatics and Control Program at the University of Georgia, commissioned in 1997. It comprises two mobile trailers, each trailer can sample from three locations for a total of six locations. Each trailer houses an on-line respirometer capable of monitoring and examining microbial activity at the same variety of locations, day-in, day-out, over extended periods. Not only can biochemical transformations of carbon-, nitrogen-and phosphorus-bearing materials be monitored simultaneously at designed time intervals, but also supplementary sensors can be incorporated into the sampling streams, notably Turner fluorometers, acquired for tracking algal population dynamics.

Oxidation-reduction potential (*ORP*), *pH*, specific conductivity, Photosynthetically Active Radiation (*PAR*), dissolved oxygen (*DO*) and temperature were measured at 15 minute intervals independently of the EPCL, with two hydrolabs at the same locations as the EPCL intakes (see Figure 6-10).

Chlorophyll *a* was measured by fluorometer in situ at 15 minute intervals via continuous flow from the depth of 0.5m. Rainfall was collected by rain gage and water level was measured by pressure transmitter.

EPCL data were calibrated with calibration curves generated in Minworth Systems Limited GFX software, independent measurements, and by cross-checking data with stated sampling instruments. Hydrolabs were checked and calibrated approximately every week.

In order to understand the detailed diurnal dynamics of the interaction between phytoplankton and their environments, the pond was enriched in three treatments with 8L of commercially available 11-37-0 (*N-P-K*) liquid fertilizer on August 21, September 13, and October 24, 1998;

Figure 611 shows the monitoring results of DO and pH at the downstream location. Because there are some data missing during the sampling period, Figure 6-11 does not show all of the monitoring results of DO and pH of the entire monitoring period. From Figure 611 it can be seen that during the period from September 30 to October 14 DOand pH are apparently lower than that of other periods respectively. This phenomenon results from the fact that the water surface was covered with duckweed during this period. Therefore data from September 14 to 24 and data from October 25 to November 6 were selected for the following model calibration and evaluation respectively.

6.5.2 Model equations

The pond is small and shallow, if we neglect stratification during the growing season and consider the pond as a continuouly stired tank reactor (CSTR), then the previous equations which are designed for stratified lakes should be modified for the pond.

Suspended Solids (SS):

$$\frac{\partial [SS]}{\partial t} = \frac{W_{SS}}{V} - \omega_{SS} \frac{[SS]}{D_w} - \frac{Q_{out} \cdot [SS]}{V}$$
loading settling outflow
(6-59)

$$\frac{\partial [PHYT]}{\partial t} = K_{ag}[PHYT] - K_{ar}[PHYT] - K_{ad}[PHYT] - \omega_a \frac{[PHYT]}{D_w}$$
(6-60)
growth respiration death settling

Dissolved Oxygen (DO):

$$\frac{\partial DO}{\partial t} = k_2 (DO_s - DO) - k_{BOD} \Theta_{BOD}^{T-20} BOD - \frac{64}{14} k_{NI} \Theta_{NI}^{T-20} \left(\frac{DO}{K_{NIT} + DO}\right) [NH_3] \cdot f(pH)$$

reaeration oxidation nitrification

$$-\frac{SOD}{D_{w}}\Theta_{SOD}^{T-20} + \frac{138*32}{106*12}K_{ag} [PHYT] - \frac{138*32}{106*12}K_{ar} [PHYT] - \frac{32}{12}k_{SOM}\Theta_{SOM}^{T-20}[SOM]$$
sediment demand growth respiration SOM decay
(6-61)

Carbonaceous Biochemical Oxygen Demand (BOD):

$$\frac{\partial BOD}{\partial t} = \frac{W_{BOD}}{V} - k_{BOD} \Theta_{BOD}^{(T-20)} BOD + \frac{32}{12} K_{ad} [PHYT] - \frac{Q_{out} \cdot BOD}{V}$$

loading oxidation death outflow (6-62)

$$-\frac{5}{4}\frac{32}{14}k_{DN}\Theta_{DN}^{(T-20)}\left(\frac{K_{NO3}}{K_{NO3}+DO}\right)[NO_{3}^{-}]-v_{s}(1-c_{BOD})\cdot\frac{BOD}{D_{w}}$$

denitrification settling

Organic Nitrogen (ON):

$$\frac{\partial [ON]}{\partial t} = \frac{W_{ON}}{V} + \frac{16*14}{106*12} K_{ar} f_{ON} [PHYT] - k_{ON} \Theta_{ON}^{T-20} \left(\frac{[PHYT]}{K_{mPc} + [PHYT]}\right) [ON]$$

loading respiration mineralization (6-63)

$$-v_{s}(1-c_{ON})\frac{[ON]}{D_{w}} - \frac{Q_{out} \cdot [ON]}{V}$$

settling outflow

Nitrate Nitrogen (NO_3^-) :

$$\frac{\partial [NO_3^-]}{\partial t} = \frac{W_{NO3}}{V} + k_{NI} \Theta_{NI}^{T-20} \left(\frac{DO}{K_{NIT} + DO}\right) [NH_3] \cdot f(pH) - \frac{Q_{out} \cdot [NO_3^-]}{V}$$

loading nitrification outflow (6-64)

$$-\frac{16*14}{106*12}K_{ag}(1-P_{NH3})[PHYT] - k_{DN}\Theta_{DN}^{T-20}\left(\frac{K_{NO3}}{K_{NO3}+DO}\right)[NO_{3}^{-}]$$
growth
denitrification

$$\frac{\partial [NH_{3}]}{\partial t} = \frac{W_{NH3}}{V} + \frac{16*14}{106*12} K_{ar} (1 - f_{ON}) [PHYT] + k_{ON} \Theta_{ON}^{T-20} \left(\frac{[PHYT]}{K_{mPc} + [PHYT]}\right) [ON]$$

$$loading respiration mineralization$$

$$-\frac{16*14}{106*12} K_{ag} P_{NH3} [PHYT] - k_{NI} \Theta_{NI}^{T-20} \left(\frac{DO}{K_{NIT} + DO}\right) [NH_{3}] \cdot f(pH)$$

$$growth nitrification$$

$$+\frac{16*14}{106*12} k_{SOM} \Theta_{SOM}^{T-20} [SOM] - \frac{P_{N} \{\Theta_{SS} [SS]\}}{D_{w}} [NH_{3}] - \frac{Q_{out} \cdot [NH_{3}]}{V}$$

$$release adsorption outflow (6-65)$$

$$\frac{\partial [OP]}{\partial t} = \frac{W_{OP}}{V} + \frac{31}{106*12} K_{ar} f_{OP} [PHYT] - \frac{Q_{out} \cdot [OP]}{V}$$

loading respiration outflow (6-66)

$$-k_{OP} \Theta_{OP}^{T-20} \left(\frac{[PHYT]}{K_{mPc} + [PHYT]} \right) [OP] - v_s (1 - c_{OP}) \frac{[OP]}{D_w}$$

mineralization settling

Inorganic Phosphorus(PO₄):

$$\frac{\partial [PO_4]}{\partial t} = \frac{W_{PO4}}{V} + \frac{31}{106*12} K_{ar} (1 - f_{OP}) [PHYT] + k_{OP} \Theta_{OP}^{T-20} \left(\frac{[PHYT]}{K_{mPc} + [PHYT]}\right) [OP] - \frac{Q_{out} \cdot [PO_4]}{V}$$

$$loading respiration mineralization outflow$$

$$-\frac{31}{106*12} K_{ag} [PHYT] - \frac{P_p \{\omega_{SS} [SS] + \omega_{Fe} [Fe]\}}{D_w} [PO_4] + \frac{31}{106*12} k_{SOM} \Theta_{SOM}^{T-20} [SOM]$$

$$growth adsorption release$$
(6-67)

Total Iron (*Fe*):

$$\frac{\partial [Fe]}{\partial t} = \frac{W_{Fe}}{V} + \frac{S_{Fe}}{D_w} \Theta_{Fe}^{(T-20)} - \omega_{Fe} \frac{[Fe]}{D_w} - \frac{Q_{out} \cdot [Fe]}{V}$$
loading release settling outflow
$$(6-68)$$

Total Inorganic Carbon (CT):

$$\frac{dCT}{dt} = K_e \{ [CO_2(aq)]_s - [H_2CO_3^*] \} - K_{ag} [PHYT] + K_{ar} [PHYT]$$

$$+ k_{BOD} \Theta_{BOD}^{(T-20)} \cdot BOD + \frac{5}{4} \frac{12}{14} k_{DN} \Theta_{DN}^{(T-20)} \left(\frac{K_{NO3}}{K_{NO3} + DO} \right) NO_3^-] + k_{SOM} \Theta_{SOM}^{T-20} [SOM]$$

$$(6-69)$$

$$[H^{+}] = \frac{-(K_{1}A_{c} - K_{1} \cdot CT) + \sqrt{(K_{1}A_{c} - K_{1} \cdot CT)^{2} - 4A_{c}(K_{1}K_{2}A_{c} - 2K_{1}K_{2} \cdot CT)}}{2A_{c}}$$
(6-70)

$$pH = -\log_{10}[H^+] \tag{6-71}$$

6.5.3 Model calibration and evaluation

Model calibration and evaluation are important steps for model development. Field observations for a single period of time are used for what is called "model calibration", which is the process of adjusting the model parameters to best describe observed water quality for a particular data set. Model evaluation is the process of assessing the degree of reliability of the calibrated model using one or more independent data sets. The calibrated model parameters are held constant and the independent initial and boundary conditions used to simulate new conditions. These new simulations are compared with the independent evaluation data collected within the model domain to assess the degree of model reliability to make certain types of simulations. The overall reliability of the model to predict future conditions increases in proportion to the amount of historical data that the model is able to describe successfully.

(1) Model calibration

As mentioned above, data from September 14 to 24, 1998 were used for model calibration. Model forcing functions include Photosynthetically Active Radiation (*PAR*) and water temperature which are indicated in Figure 6-12. Pollutant loading and outflow can be neglected in the model calibration because the inflow and outflow were very small, and there was little rainfall during the period. Most of the model initial conditions were determined from the monitoring data. Some model initial conditions, such as sediment oxygen demand (*SOD*) are difficult to measure and must therefore be determined either by reasonable assumptions or directly by calibration (as model parameters).

It is worth noting that model calibration results can often be *ill-posed* (Beck, 1987; Martin, 1999). An *ill-posed* calibration occurs when more than one combination of parameter selections produces effectively the same model simulation over a limited range. In addition, observed data may be limited and uncertain, and the parameter estimates sensitive to errors in the observations. The number of possible combinations of uncertain parameters that can yield similar simulations increases nonlinearly as the number of uncertain model parameters increases. An *ill-posed* or non-unique calibration is a frequent problem in complex model calibration (Beck, 1987). In order to avoid *ill-posed* or uncertain calibrations, it is necessary to reduce the number of calibrated parameters. In this study, we take three steps to calibrate the model: 1) trial and error with process analyses, 2) random search for important parameters based the results from step 1), and 3) trial and error with process analyses again. During the first stage of model

calibration, we first analyze the relationships between processes and state variable variations, then use trial and error method to estimate the range of important parameters. For example, DO and pH have obvious diurnal variations. These variations result mainly from algal photosynthesis and respiration. Other processes such as BOD decay, sediment oxygen demand (SOD), sediment organic matter decay, atmospheric exchange may affect DO concentration, but these processes have little effect on its diurnal variations. Therefore when we calibrate the diurnal variations of DO and pH, algal growth rate, respiration rate and death rate, and algal settling rate are the focus, while other parameters are determined a priori from preliminary analyses and literature values. Similarly the ranges of other important parameters will be calibrated based on process analyses. After the first step, algal growth rate constant, algal respiration rate constant, nutrient halfsaturation constants for algal growth, adsorption coefficient for orthosphosphate and ammonia, and settling rates for phytoplankton, organic matter, suspended sediment, and total iron are found important to calibrate the model. These important parameters are calibrated by using random search method, while other parameters are selected and fixed based on the first step. Because the magnitudes for different state variables are very different, the goodness of fit is judged by the relative error (Thomann, 1982):

$$RE = \frac{\sum_{i}^{N} (O_i - S_i)}{\sum_{i}^{N} O_i} \times 100\%$$
(6-72)

Random search results for some parameters are shown in Figure 6-13 and Figure 6-14. Figure 6-13 indicates that the half-saturation constants for phosphorus and nitrogen should be less than 0.08 mg/L and 0.4 mg/L respectively, while the half-saturation constant for carbon is not important for the calibration. From Figure 6-14, phytoplankton settling rate should be around 0.15-0.30 m/day. The histogram of relative errors of *DO*

and pH are shown in Figure 615, which indicates that the relative errors of DO and pH are less than 40% and 14% respectively.

Based on the results of random search, we use trial and error method again to find a set of parameters that can make the model output fit well the observed data. The final calibration results are shown in Figure 616. The calibrated parameters are listed in Table 6-5. The final calibration results indicate that the relative errors for *DO*, *pH*, *PO*₄, and *NH*₃ are 6.73%, 2.91%, 4.96%, 31.88% respectively.

(2) Model evaluation

After the previous step, the calibrated model is then used to predict water quality for additional data set. This process is called model evaluation. The evaluation data set is chosen from October 25 to November 6 as mentioned above. Forcing function data for model evaluation are shown in Figure 611. The evaluation parameters are listed in Table 6-5, and eveluation results are shown in Figure 6-17. The relative errors for *DO*, *pH*, *PO*₄ and *NH*₃ are 6.46%, 1.59%, 7.87% and 27.77% respectively.

(3) Discussion

Model calibration and evaluation data are selected after the second and third fertilization. Ammonia and orthophopshate are both declining nearly monotonically during the analysis period because of sediment adsorption and settling.

During the calibration period, ammonia declines more quickly than the evaluation period. We believe that this results from different cation exchange capacity (CEC) in the two analysis periods. Soil minerals can exibit two types of charge, constant and variable or pH-dependent charge (Sparks, 1995). In most soils there is a combination of constant and variable charge. The variable charge component in soils changes with pH due to protonation and deprotonation of functional groups on inorganic soil minerals such as kaolinite, amorphorus materials, metal oxides, oxyhydroxides, and hydroxides, and layer silicates coated with metal oxides and soil organic matter. High pH soils have high CEC. From the monitoring data, pH in the calibration period (8.2-9.4) is much higher than that in the evaluation period (around 7.2), so soils in the calibration period have higher CEC and high capacity to adsorb ammonium. This also indicates the importance to include pH as a state variable in developing biogeochemical model.

Simulated results of phytoplankton biomass in both analysis periods have similar trends with measured fluorescence. But in the calibration period, measured fluorescence increases much faster than simulated results. This may result from the assumption of constant maximum growth rate and respiration rate. During algal bloom, it may be wrong to assume that algal maximum growth rates are constant, resulting in large uncertainties in the prediction model for algal bloom. In the evaluation period, we need to adjust the algal growth rate, respiration rate, and algal settling rate in order to fit the trend of the observed fluoroscence. This implies that the dominant algal species changes during the evaluation period compared with the calibration period.

During both analysis periods, simulated results of nitrate have small changes compared with high background concentrations. In our model, there are four processes that affect nitrate variations, including algal uptake, algal respiration, nitrification, and denitrification. From our mechanism analyses, algal growth prefers ammonium, and ammonium concentration is high in the pond, so nitrate plays an unimportant role in algal growth. Denitrification will occur under low DO concentrations, but DO is oversaturated during the analysis periods, so denitrification has little effect on nitrate variations. Nitrification depends on ammonia concentration. This process could not change nitrate concentration significantly because the ammonia concentration is much smaller than the nitrate background concentrations. The residual nitrate changes may be due to measurement errors, or some other unidentified sources. Ideally model evaluation should be carried out with the same model parameterization as for calibration. However, from the above analysis and observed data, we can not use the same parameters due to significant changes between the two analysis periods. Model parameters for the model calibration and evaluation are listed in Table 6-5.

We observe a phase lag between the simulated results and the observed data of DO and pH in the model evaluation period. The forcing function data PAR and monitoring results of DO, pH are shown in Figure 6-18. We see the phase lag does exist in the original data. A phase lag in the evaluation data but not in the calibration data requires additional investigation.

6.5.4 Sensitivity analysis

Sensitivity analysis is a test of a model in which the value of a single parameter is changed (while all others remain constant), and the impact of this change on the dependent variable is observed. This analysis can identify sensitive parameters that have significant effects on the dependent variable.

In this model, there are 15 state variables and many biogeochemical processes and parameters. As mentioned in the model calibration, different processes induce different effects on the state varibales. For example, our sensitivity analysis results show that, of the parameters in the model, algal growth rate constant, algal respiration rate constant, algal death rate, and algal settling rate are sensitive parameters for the simulation results of DO and pH, while these parameters have no significant effect on orthophosphate and ammonia because of the very high background concentrations of these nutrients. Atmospheric exchange coefficient of DO can cause the mean DO to change, but it has little effect on the obvious diurnal variation of DO and other state variables. The sediment-nutrient adsorption coefficients are sensitive for the magnitudes of orthophosphate and ammonia, but their effects on DO and pH are not significant. From the processes in our model, nutrient concentration will affect DO and pH by algal uptake and growth, and this effect depends on nutrient half-saturation constants. Based on random research results in Figure 6-13, because of high background of nutrient concentration, the relative errors of DO and pH will be less that 40% and 14% relatively for different combinations of nutrient half-saturation constants. Detailed model parameter sensitivity classifications for different state variables are shown in Table 6-6.

No.	State variables	Symbols	Units
1	Suspended Solids	SS	mg/L
2	Phytoplankton Biomass	PHYT	mg C/L
3	Dissolved Oxygen	DO	mg/L
4	Carbonaceous Biochemical Oxygen Demand	CBOD	mg/L
5	Sediment Oxygen Demand	SOD	g/m ² -day
6	Organic Nitrogen	ON	mg N/L
7	Ammonia Nitrogen	NH ₃	mg N/L
8	Nitrate Nitrogen	NO3 ⁻	mg N/L
9	Organic Phosphorus	OP	mg P/L
10	Ortho-Phosphorus	PO_4	mg P/L
11	Total Iron	Fe	mg/L
12	Carbon Dioxide	$H_2CO_3^*$	mol/L
13	Bicarbonate	HCO_3^-	mol/L
14	Carbonate	CO_3^{2-}	mol/L
15	Sediment Organic Matter	SOM	mg C/L

 Table 6-1
 Summary of State Variables

Particle		Particle densities (g/cm ³)			
Diameter	Diameter (mm)		2.00	2.50	2.70
Fine	0.300	300.00	400.00	710.00	800.00
sand	0.050	94.00	120.00	180.00	200.00
	0.050	94.00	120.00	180.00	200.00
	0.020	15.00	19.00	28.00	32.00
Silt	0.010	3.80	4.70	7.10	8.00
	0.005	0.94	1.20	1.80	2.00
	0.002	0.15	0.19	0.28	0.32
Clay	0.002	0.15	0.19	0.28	0.32
	0.001	0.04	0.05	0.07	0.08

Table 6-2Stoke's Settling Velocities (m/day) at 20° C

Species	$H_f^{ heta}$
$CO_2(g)$	-393.51
$CO_2(aq)$	-413.80
$H_2CO_3^*$	-699.65
HCO3 ⁻	-691.99
CO_{3}^{2-}	-677.14
H_2O	-285.83
OH	-229.99
$H^{\!+}$	0

 Table 6-3 Standard Formation Enthalpies (KJ mol⁻¹)

Symbol	Symbol's magning	Valua	Source
Symbol	Eraction of dissolved BOD	0.5	Ambrose et al (1993a)
CBOD	Fraction of dissolved organic nitrogen	1.0	Ambrose et al. (1993a)
C_{ON}	Fraction of dissolved organic phosphorus	0.5	$ \begin{array}{c} \text{Ambrose et al. (1993a)} \\ \text{Ambrose et al. (1993a)} \end{array} $
D	Depth of effective benthic sediment laver	$0.2 \sim 0.7 \mathrm{m}$	Ambrose et al. (1993a)
	Vertical diffusion coefficient	$0.35 \text{ m}^2/\text{s}$	Calculated
E_{SOD}	Diffusive exchange coefficient of SOD	0.55 1175	Sulculated
fon	Fraction of dead algae recycled to dissolved <i>ON</i>	0.25~0.5	Ambrose et al. (1993a)
for	Fraction of dead algae recycled to dissolved <i>OP</i>	0.5	Ambrose et al. (1993a)
K_{ad}	Algal death rate		
K_{CO2}	CO_2 atmospheric exchange rate		
K_{O2}	Reaeration coefficient	0~100 /day	Chen and Orlob (1975)
k_{BOD}	<i>BOD</i> decay rate at 20°C	0.1~0.3 /day	Chen and Orlob (1975)
k_{DN}	Denitrification rate at 20°C	0.1 /day	Di Toro et al. (1980)
k_{NI}	Nitrification rate at 20°C	0.05~0.15 /day	Bowie et al. (1985)
k _{NIT}	Half-saturation constant for nitrification	$2.0 \text{ mg} O_2/L$	Bowie et al. (1985)
K_{NO3}	Half-saturation constant for denitrification	$0.1 \text{ mg} O_2/L$	Ambrose et al. (1993a)
k_{ON}	Organic N mineralization rate at 20°C	0.02~0.2 /day	Bowie et al. (1985)
k _{OP}	Organic P mineralization rate 20°C	0.1~0.4 /day	Bowie et al. (1985)
<i>k</i> _{MN}	See equation (6-19)	25 µg N/L	Ambrose et al. (1993a)
k _{mPc}	See equation (6-20), (6-21), (6-24), (6-25)	1.0 mg C/L	Ambrose et al. (1993a)
ksom	Sediment organic matter decay rate	0.06 /day	Cole et al. (1995)
k_{C}	Half-saturation constant for carbon	$0.5 \sim 0.6 \text{ mg/L}$	Chen and Orlob (1975)
k_N	Half-saturation constant for nitrogen	0.3 ~0.4 mg/L	Chen and Orlob (1975)
k _P	Half-saturation constant for phosphorus	0.03~0.05 mg/L	Chen and Orlob (1975)
I_s	Light intensity for algal maximum growth	200~350 Ly/day	Bowie et al. (1985)
P_p	Adsorption coefficient for phosphorus		
$\dot{P_N}$	Adsorption coefficient for ammonia		
S_{Fe}	Release rate of iron	0.3~0.5 SOD	Cole et al. (1995)
v_s	Organic matter setting rate	0.46~1.5 m/day	Cole et al. (1995)
$\omega_{\!$	Phytoplankton settling rate	0.05~0.5 m/day	Chen and Orlob (1975)
ω_{e}	Iron settling rate	0.5~2.0 m/day	Cole et al. (1995)
Q_{DD}	Temperature factor for BOD	1.047	Ambrose et al. (1993a)
Q_{N}	Temperature factor for denitrification	1.045	Di Toro et al. (1980)
Q_{re}	Temperature factor for iron release	1.08	Ambrose et al. (1993a)
\boldsymbol{Q}_{NI}	Temperature factor for nitrification	1.08	Ambrose et al. (1993a)
\mathcal{O}_N	Temperature factor for organic N mineralization	1.08	Ambrose et al. (1993a)
\mathcal{Q}_{P}	Temperature factor for organic P mineralization	1.08	Ambrose et al. (1993a)
Q_{OD}	Temperature factor for SOD	1.08	Ambrose et al. (1993a)
Q_{OM}	Temperature factor for SOM	1.08	Cole et al. (1995)

 Table 6-4 Summary of Other Model Parameters

Symbol	Symbol's meaning	Calibration	Evaluation
CROD	Fraction of dissolved <i>BOD</i>	0.5	0.5
CON	Fraction of dissolved organic nitrogen	0.5	0.5
COP	Fraction of dissolved organic phosphorus	0.5	0.5
D_m	Depth of effective benthic sediment layer	0.2 m	0.2 m
Eson	Diffusive exchange coefficient of SOD	0.02	0.02
fon	Fraction of dead algae recycled to dissolved ON	0.5	0.5
for	Fraction of dead algae recycled to dissolved OP	0.5	0.5
$K_{a\sigma Max}$	Maximum algal growth rate	2.10 /day	2.70 /day
K _{arMax}	Maximum algal respiration rate	0.52 /day	0.47 /day
K_{ad}	Algal death rate	0.05 /day	0.05 /day
K_{CO2}	CO_2 atmospheric exchange rate	0.40 /day	0.40 /day
K_{O2}	Reaeration coefficient	0.20 /day	0.20 /day
k_{BOD}	<i>BOD</i> decay rate at 20°C	0.15 /day	0.15 /day
k_{DN}	Denitrification rate at 20°C	0.1 /day	0.1 /day
k_{NI}	Nitrification rate at 20°C	0.1 /day	0.1 /day
k_{NIT}	Half-saturation constant for nitrification	$2.0 \text{ mg } O_2/L$	$2.0 \text{ mg } O_2/\text{L}$
K_{NO3}	Half-saturation constant for denitrification	0.1 mg <i>O</i> ₂ /L	0.1 mg O_2/L
k_{ON}	Organic N mineralization rate at 20°C	0.4 /day	0.05 /day
k_{OP}	Organic P mineralization rate 20°C	0.1 /day	0.1 /day
k_{MN}	See equation (6-19)	25 μg <i>N</i> /L	25 μg <i>N</i> /L
k_{mPc}	See equation (6-20), (6-21), (6-24), (6-25)	1.0 mg <i>C</i> /L	1.0 mg C/L
k _{SOM}	Sediment organic matter decay rate	0.05 /day	0.05 /day
k_C	Half-saturation constant for carbon	0.70 mg/L	0.70 mg/L
k_N	Half-saturation constant for nitrogen	0.20 mg/L	0.20 mg/L
k_P	Half-saturation constant for phosphorus	0.075 mg/L	0.075 mg/L
I_s	Light intensity for algal maximum growth	300 Ly/day	300 Ly/day
P_p	Adsorption coefficient for phosphorus	0.05	0.05
P_N	Adsorption coefficient for ammonia	0.55	0.05
S_{Fe}	Release rate of iron	0.1 <i>SOD</i>	0.1 <i>SOD</i>
v_s	Organic matter setting rate	0.14 m/day	0.14 m/day
ω_{t}	Phytoplankton settling rate	0.24 m/day	0.12 m/day
ω_{Fe}	Iron settling rate	0.09 m/day	0.09 m/day
ω_{ss}	Sediment settling rate	0.10 m/day	0.10 m/day
Θ	Temperature factor for algal growth	1.047	1.047
Θ_{BOD}	Temperature factor for <i>BOD</i>	1.047	1.047
Θ_{DN}	Temperature factor for denitrification	1.045	1.045
Θ_{Fe}	Temperature factor for iron release	1.08	1.08
Θ_{NI}	Temperature factor for nitrification	1.08	1.08
Θ_{DN}	Temperature factor for organic N mineralization	1.08	1.08
Θ_{DP}	Temperature factor for organic P mineralization	1.08	1.08
Θ_{SOD}	Temperature factor for SOD	1.08	1.08
Θ_{SOM}	Temperature factor for SOM	1.08	1.08

 Table 6-5 Model Parameterization Results in the Pond

Note: Bolded values indicate parameter changes between model calibration and model evaluation.

No.	State variables	Sensitive parameters
1	Suspended Solids	[1] Sediment settling rate
2	Phytoplankton Biomass	[1] Algal growth rate, respiration rate, death rate,
		and settling rate
3	Dissolved Oxygen	[1] The same as phytoplankton biomass
		[2] O ₂ atmospheric exchange rate
4	Biochemical Oxygen Demand	[1] Organic matter settling rate
		[2] Decay rate
5	Sediment Oxygen Demand	[1] Diffusive coefficient
6	Organic Nitrogen	[1] Organic matter settling rate
		[2] Mineralization rate
7	Ammonia Nitrogen	[1] Sediment adsorption coefficient
8	Nitrate Nitrogen	-
9	Organic Phosphorus	[1] Organic matter settling rate
10	Ortho-Phosphorus	[1] Sediment adsorption coefficient
11	Total Iron	[1] Iron release rate
		[2] Iron settling rate
12	Carbon Dioxide	-
13	Bicarbonate	[1] The same as phytoplankton biomass at high
		pH, but no sensitive parameters at low pH
14	Carbonate	-
15	рН	[1] The same as phytoplankton biomass
		[2] CO ₂ atmospheric exchange coefficient
16	Sediment Organic Matter	[1] Phytoplankton settling rate
		[2] Decay rate

Table 6-6 Sensitive Parameters for Different State Variables in the Pond

Note:

[1] - critical parameters; [2] - important parameters



Figure 6-1 State Variable Interactions



Figure 6-2 Water Density at Different Temperatures



Figure 6-3 pH Factor for Nitrification



Figure 6-4 Carbonate Species vs. pH



Figure 6-5 Light Factor for Algal Growth



Figure 6-6 Total Solar Radiation and Photoperiod



Figure 6-7 Henry Constant K_H for CO₂ Dissolution



Figure 6-8 Equilibrium Constant K1 for H2CO3 Dissolution



Figure 6-9 Equilibrium Constant K₂ for HCO₃⁻ Dissolution



Figure 6-10 Deployment of Main Equipment at the Pond Experiment


Figure 6-11 DO and pH Monitoring Results of the Pond



Figure 6-12 Measured PAR and Temperature of the Pond



Figure 6-13 Random Search Results for Nutrient Half-Saturation Constants



Figure 6-14 Random Search Result of Phytoplankton Settling Rate



Figure 6-15 Histogram of Relative Error of DO and pH





Figure 6-16 Model Calibration Results of the Pond



Note: The pond was fertilized with 14 L liquid fertilizer (11-37-0) on September 13.

Figure 6-16 Model Calibration Results of the Pond (con't)



Figure 6-16 Model Calibration Results of the Pond (con't)



Figure 6-16 Model Calibration Results of the Pond (con't)



Figure 6-16 Model Calibration Results of the Pond (con't)





Figure 6-17 Model Evaluation Results of the Pond



Note: The pond was fertilized with 14 L liquid fertilizer (11-37-0) on October 24.

Figure 6-17 Model Evaluation Results of the Pond (con't)



Figure 6-17 Model Evaluation Results of the Pond (con't)



Figure 6-17 Model Evaluation Results of the Pond (con't)



Figure 6-18 Monitoring Results of DO, pH and PAR of the Pond

CHAPTER 7

APPLICATION OF LAKE WATER QUALITY MODEL TO LAKE LANIER

Our ultimate study objective is Lake Lanier. After the biogeochemical model structure was tested with the pond data in Chapter 6, we now apply this model to study Lake Lanier ecosystem behavior. In this chapter, we first calibrate the biogeochemical model with observed vertical profile of DO and pH, and observed surface concentration of chlorophyll *a*, and then use the calibrated model to explore some unknows such as benthic sediment effects on pelagic water quality. Finally, scenario analyses with different nutrient inputs are studied for future lake behavior and lake management.

7.1 Model Inputs and Forcing Functions

Model inputs and forcing functions include nutrient loadings (point sources, nonpoint sources, and atmospheric deposition), vertical temperature profile, solar radiation at different depth, and hydrologic conditions. Nutrient loadings and vertical temperature profile have been discussed in Chapter 3 and Chapter 5 respectively. Solar radiation has been discussed in Section 6.4 of Chapter 6. The following will discuss hydrologic conditions by using a water budget model.

A lake water budget is the physical analysis of the lake based on the conservation of mass. Water input to the lake may be from rainfall (*P*), streamflow into the lake (*Q*), surface runoff (Q_r), and subsurface runoff (Q_s). Outflow from the lake could be evaporation (*E*), outflow from the lake (Q_{out}), and subsurface seepage losses (Q_d). Thus,

$$\frac{dV}{dt} = (P + Q + Q_r + Q_s) - (E + Q_{out} + Q_d)$$
(7-1)

where V is the water volume in the lake.

Rainfall can be measured using rain gages or channel stage measurements with rating curves. Streamflow and overland runoff into and out of the lake can be measured using weirs. The time rate of change of storage can be measured using a stage recorder for the water surface elevation along with the necessary topographic data of the site. Subsurface runoff in to (Q_s) and out of (Q_d) the lake are the most difficult elements of the water balance to measure. These can sometimes be estimated using elevation measurements of observation wells placed around the perimeter of the lake. However, this requires a number of measurements and an assumption of homogeneity of subsurface runoff characteristics in the area allocated to each observation well. To use Equation (7-1), it is necessary to specify a time increment dt for which each of the elements are measured. In the absence of observation well data, we neglect the effects of Q_s and Q_d for simplification, and assign total inflow (Q_{in}) equals $Q+Q_r$, then equation (7-1) becomes:

$$\frac{dV}{dt} = P + Q_{in} - Q_{out} - E \tag{7-2}$$

In Lake Lanier, outflows are mainly the discharges over the spillway and the discharges though the turbines, which can be obtained from reservoir releases.

From equation (7-2), if the right side terms are known at different times, the storage of the lake can be calculated dynamically, and then the water level and surface area can be estimated based on the storage-water level and water level-surface area relationships (shown in Figure 7-1).

In equation (7-2), rainfall (*P*), inflow (Q_{in}) and outflow (Q_{out}) can be obtained from the website of American Army Corps of Engineers (ACE) at Buford Dam:

http://water.sam.usace.army.mil/acfframe.htm.

Evaporation E could be estimated based on wind speed, water temperatue, air temperature, humidity or vapor pressure deficit, and radiation rates as in Penman Equations (1948, 1958), but these meteorogical data are not in hand. Therefore the mean

annual lake evaporation contour from the Environmental Data Service is used, and we uniformly distribute the annual lake evaporation into each day.

Rainfall data from 1996 is shown in Figure 7-2. Inflow and outflow data are indicated in Figure 7-3. Annual evaporation of Lake Lanier is $42 \sim 44$ inches/yr from the mean annual lake evaporation contour of the United States.

The modeling results are shown in Figure 7-4. Figure 7-4(a) indicates that the simulated water level fits the observed water level quite well when evaporation is considered, which means the estimation of lake evaporation is acceptable. The model result for the case where lake evaporation is not considered, is presented in Figure 7-4(b).

The simulated dynamic water volume will be used for pollutant dilution in the water quality model. In fact, the modeling result is useful in application. As we know, rainfall (P) can be measured by using rain gages, lake water level is easy to measure, and outflow (Q_{out}) can be easily obtained from reservoir releases. The most difficult part in Equation (7-2) is the lake inflow (Q_{in}) . After equation (7-2) is calibrated, we can use the calibrated equation to estimate inflow (Q_{in}) based on known parameters.

7.2 Model Calibration

The 1996/97 monitoring data in Lake Lanier (Upper Chattahoochee River Basin Group's Study) is chosen for model calibration. The data has complete vertical distributions for DO, pH, temperature, and specific conductance, although other variables have no complete vertical distributions, such that the model is only calibrated for the vertical profiles of DO and pH.

Lake Lanier water temperature, dissolved oxygen, and pH have uniform spatial distributions and variable vertical distributions. So we are trying to study these characteristics by developing a vertical distribution model. Because of the limitation of 1-D vertical distribution model (it can not reflect spatial variations of nutrients, such as the

difference between nearshore and deep lake), our model calibration focuses on the central lake, which on average represents approximately the whole lake behavior. Although submerged flow from Chattahoochee exists, vertical mixing will dominate after long distance transport to the central portion of the lake. Therefore nutrient inputs from the watershed are distributed uniformly with depth in this model calibration and application.

During the calibration to Lake Lanier, most of the rates and constants are fixed based on the calibration and evaluation results in the pond discussed in Chapter 6. The mass diffusion coefficient D_z is determined by thermal modeling of Lake Lanier in Chapter 5. Algal respiration rate constant, algal half-saturation constants of nutrients, settling rate of different species, atmospheric exchange rates of O_2 and CO_2 , and the parameters related to benthic sediment effects (iron release rate, diffusive exchange rate for *SOD*) are calibrated specifically for Lake Lanier by random search and trial and error. Table 7-1 shows the calibrated model parameters in Lake Lanier. Calibration results for *DO* and *pH* are shown in Figure 7-5. The standard deviations of simulated *DO* and *pH* are shown in Figure 7-6. Both simulated and observed concentrations of chlorophyll *a* are high in late spring 1996, the reason being that spring rainfall increased nutrient loading, and water temperature in late spring was high enough for algal growth.

In this model, vertical variations are mainly affected by three physical processes: diffusion, settling and mixing. In the hypolimnion, mixing is a dominant process, while the effect of mass diffusion is relatively small. Thus the calibration curves of DO and pH are almost straight lines in the hypolimnion. These straight lines fit the winter data well, but have biases over the summer data. Does groundwater flux affect the hypolimnetic profile of DO and pH? If so, this effect should appear in the temperature profile, but from the measured temperature profile, no groundwater flux effect is apparent. Perhaps the bias results from the assumption of constant falling velocity of organic matter. Near the bottom of the lake, a high density of negatively charged particles creates an electrostatic resistance to gravity, so the falling velocity of organic matter is slowing towards the bottom of the lake. This slowing increases the accumulation of organic matter towards the bottom of the lake, and decreases dissolved oxygen concentration when organic matter decays.

In 1996, water pH in Lake Lanier was in the range of $6 \sim 8$. This range is similar to the pH range of the pond evaluation data. So calibrated results indicate the adsorption coefficient for ammonia is similar for these two data sets. Calibrated algal half-saturation constants for nitrogen and phosphorus are much smaller than calibrated results in the pond. This suggests that perhaps different algal species are present in the pond and Lake Lanier, or model structure needs to change in different ecosystems.

Calibration result shows that the atmospheric exchange between O_2 and CO_2 are different. O_2 atmospheric exchange only occurs in the epilimnion, while CO_2 atmospheric exchange occurs in the epilimnion as well as in the hypolimnion. The exchange rate of CO_2 in the hypolimnion is about a half of the epilimnion. This result implies the necessity of double checks on both O_2 and CO_2 for lake water quality modeling.

7.3 Benthic Sediment Effect Analysis

Lake benthic sediment is an important sink or source for overlying fresh water, it has great influence on lake ecosystems. The rate and character of mineralization of aquatic matter in bottom sediments depend on the composition of substances reaching the bottom, and on the character and depth of the water body. Physico-chemical conditions of the sediment and overlying water have a significant influence on the mineralization of organic matter in sediments (Parker and Rasmussen, 2001). The wind and the surface area of a shallow lake will determine the actual size of resuspension and the dynamics of the interface. The frequent stirring of the sediment may even cause a remarkable lack of zoobenthos (Lastein 1976). However, in relatively deep lakes, water movements will cause mixing of only a few mm of surface sediments. If their effect were more intensive, the subtle time-depth changes in stratigraphy of fossils in cores would not exist (Stockner & Lund 1970).

The exchange across the interface is regulated by a variety of mechanisms. Among the most important are: mineral-water equilibrium, sorption processes, notably ion exchange, redox interactions depending on oxygen supply, and the activities of organisms. The exchange rates depend on the local diffusion coefficient as well as on the environmental control of inorganic and organic (enzymatic) reactions (Mortimer 1971). The process of release of dissolved substances takes place by actual dissolution of particles, as well as by metabolic activity of organisms. The latter is responsible for the decomposition of organic matter and its mineralization, a process of release of its inorganic components and their return back into circulation. Products of bacterial reactions can bring about further changes in sediment chemistry. Wood (1975) suggested that of several mechanisms responsible for the movement of material across the sediment -water interface, ordinary diffusion is probably the least important, while turbulent exchange, release of gases from microbial activity, and the movement of certain biota are of considerable importance. While this may be so in shallow water deposits, it would appear that molecular diffusion would be of considerable importance in deep waters, where the other mechanisms will be of low intensity (Berner 1976).

Some of the most intense, post-depositional chemical changes observed in aquatic sediments occur within a short distance of the sediment-water interface (Berner, 1980). In fact, geochemical reactions such as organic matter decay are commonly strongest in the upper few millimeters of sediments, which results in pronounced near-surface chemical gradients of the species involved in such reactions (Reimers et al., 1984; Archer et al.,

1989). A particularly striking and geochemically important example of this type phenomenon is the development of extremely sharp gradients in dissolved O_2 , H_2S , and H^+ as a consequence of sulfide oxidation in the vicinity of the sediment-water interface (J φ rgensen et al., 1983; J φ rgensen and Revsbech, 1983).

Some of the most important reactions directly resulting from the bacterial decomposition of organic matter are the removal of dissolved oxygen, reduction of nitrate, iron, manganese, sulphate and other elements and compounds, and production of CO_2 , CH_4 , NH^{4+} , PO_4^{3-} , and HS^- . The intensity will depend on the content of organic matter and oxygen availability. Products of bacterial reactions can bring about further changes in sediment chemistry.

Redox potential E_h is also an important factor that influence sediment benthic reactions. Sediments with lowest E_h have the greatest oxygen uptake (Mortimer, 1941, 1942). Hallberg (1973) suggested that a sediment having a redox potential value lower than zero should not necessarily be considered as being anoxic. The level of E_h is strongly correlated with the oxygen concentration in the interstitial and overlying water. The change in E_h is reflected in chemical reductions, and it is well known that at <350 mv, NO_3^- is reduced to NH_4^+ (Edwards, 1958), at <+300 mv Fe(III) is reduced to Fe(II) (Mortimer, 1941), with maximum solubility of Fe at +80 to -100 mv (Serruya, 1971), at <+100 mv of sulphur takes place (Baas-Becking et al., 1960), and that strongly reduced sediments have E_h of 0 to -250 mv.

The exchange rate between ground water and lake water may be another important factor which affects release of dissolved substances. Horizontal variations in hydrostatic pressure of groundwater may cause vertical percolation of pore water through sediments. The flow direction of this seepage may be upward or downward, depending on local conditions. The flow rate is proportional to the pressure gradient in the direction of flow and perviousness of the soil (Darcy's law). Because the concentrations of dissovled substances are usually higher than those in the overlying water, an upward flow of groundwater tends to enhance the internal loading, but the actual flux across the interface is controlled by the intricate interaction between advection, diffusion, and reactions in the boundary layer. Fillos (1976) designed a laboratory experiment to test the effect of groundwater flux through the sediments. The experiment results showed that the release of phosphorus due to ground water flux is about four times of no ground water inflow during anaerobic conditions (Fillos, 1976).

In our geochemical model, three benthic sediment components are considered: sediment oxygen demand, sediment organic matter, and iron release from benthic sediment. Benthic sediment affects dissolved oxygen in the water column by two different ways. One is that oxygen diffuses into the bottom sediments and is then consumed. The other is essentially the rate at which reduced organic substances in sediment are conveyed into the water column, and are then oxidized (Bowie, 1985). Cole (1995) assumed iron release rate from bottom sediments is proportional to sediment oxygen demand:

$$S_{Fe} = c_{Fe} \cdot SOD \tag{7-3}$$

where:

 S_{Fe} – iron release rate from bottom sediment (g/m²-day)

 c_{Fe} – coefficient. c_{Fe} is 0.1 by model calibration in Lake Lanier (Table 7-1).

SOD – sediment oxygen demand (g/m²-day)

Calibrated results of *SOD*, *SOM* and iron release rate are shown in Figure 7-7. From Equation (6-17) in Chapter 6, *SOD* is related to the difference between bottom *DO* concentration in the water column and sediment *DO* concentration. During the transition period, the water column has a high *DO* concentration at the bottom, while *DO* concentration at the bottom is very low during the stratification period. This explains the *SOD* variation in Figure 7-7. From Equation (6-18) in Chapter 6, *SOM* is influenced by

three factors: phytoplankon settling, particulate *BOD* settling, and *SOM* decay. The increase of *SOM* in Figure 7-7 indicates the source is greater than the sink, which can be seen from nutrient loading analysis in Chapter 3. Total iron, orthophosphate, and dissolved inorganic carbon results are shown in Figures 7-8 through 7-10 respectively. Orthophosphate concentration in the water column is low because of adsorption by suspended sediments and iron. The concentration of dissolved inorganic carbon is relatively high around the lake bottom in winter, which is similar to the measured profile in winter 1999 (Figure 3-23).

7.4 Model Uncertainty Analysis

Uncertainty is a state or condition of incomplete or unreliable knowledge wich is omnipresent in model studies. It is clearly important as an indication of the values of the information in a model term for which the uncertainty is associated. Models without considerations of uncertainty are deficient, and use of these models results in an evaluation of management strategies with unknown risks (Reckhow, 1983).

Uncertainty is often discussed and analyzed in conjunction with the concepts of probability and risk. For example, decision making under uncertainty refers to the situation in which the appropriate governing probability law is unknown so that even probabilities may at best be estimated (Reckhow, 1983). Techniques of uncertainty analysis mainly include sensitivity analysis, first-order analysis, Monte Carlo simulation, and Kalman filtering. Of these four methods, sensitivity analysis is somewhat different from the other three methods in that it is not intended to be used to aggregate error terms and determine total estimation error in a particular variable. Rather, it is used to assess the impact of uncertainty in one model term on the estimation of another model term. Sensitivity analysis can identify sensitive parameters that have significant effect on the dependent variable. This identification is very useful. In application of calibration and evaluation, we can focus on sensitive parameters.

Given the incomplete description of natural systems and the inherent uncertainties in the model structure and input data, it is desirable to have model output in the form of a probability or frequency distribution rather than a deterministic value. Several procedures have been proposed to quantify uncertainties in water quality modeling studies. Whitehead and Young(1979), Spear and Hornberger (1983), and Qaisi (1985) applied Monte Carlo simulation to water quality modeling. Burges and Lattenmaier (1975), Gardner et al.(1981), Scavia et al.(1981), and Warwick(1997) investigated the difference of first-order error analysis and Monte Carlo method in river and reservoir water quality management. Bowles and Grenny(1978) applied the Kalman Filter technique for river water quality simulation.

Uncertainty analysis mainly includes uncertainty about model structure, uncertainty about model parameters, and uncertainty associated with input and predictions of future behavior of the system (Beck, 1987).

(1) Uncertainty about model structure

Our model focuses on hypolimnetic DO and pH, and the effect of benthic sediment at different seasons, while the food web is not fully included. In this point, the uncertainty of the model structure is obvious, although the model structure was tested by the aquaculture pond data.

(2) Uncertainty about model parameters

In this application, some parameters are drawn from calibration and evaluation results of the pond, other parameters are determined by using random search and trial and error method. Because of the large number of model parameters, it is difficult to find the globally optimized parameters. This kind of uncertainty is from the difficulty of mathematical treatment on non-linear systems. The random search results for algal halfsaturation constant of phophorus and organic matter settling rate are shown in Figure 7-11 and 7-12 respectively. Figure 7-11 indicates the half-saturation constant of phosphorus could be around 0.003 mg/L. Figure 7-12 indicates the settling rate should be around 0.10 m/day. Figure 7-13 shows the random search results with different combinations of algal half-saturation constants and settling velocities. Standard deviation of DO is in the range of $1.56 \sim 1.62$ mg/L, and standard deviation of pH is in the range of $0.52 \sim 0.54$ units. These results indicate that the simulated DO and pH are relatively stable with different parameter combinations.

Sensitivity analysis results (Table 7-2) indicate that the diffusive exchange rate for *SOD* (E_{SOD}) is a sensitive parameter which affects both *DO* and *pH* simulation results, followed by O_2 atmospheric exchange rate (K_{O2}). The CO_2 atmospheric exchange rate (K_{CO2}) is a slightly sensitive parameter for *pH* modeling, while algal respiration rate (K_{arMax}) and iron release rate (S_{Fe}) are not sensitive for *DO* and *pH* simulations.

(3) Uncertainty about input

As noted above, the input to a lake is difficult to quantify, using uncertain input to calibrate and evaluate a complex model must result in uncertainty in the output. Uncertainty analysis about input will be discussed in the following scenario analysis.

(4) Other uncertainties

There exist some other uncertainties, such as uncertainty due to natural variability, inadequate sampling or experimental design, measurement error, etc. We do not address on these uncertainties here, although they may have great impacts on model calibration.

7.5 Scenario Analysis

Scenarios are images of the future, or alternative futures. They are neither predictions nor forecasts. Rather, each scenario is one alternative image of how the future might unfold. A set of scenarios assists in the understanding of possible future developments of complex systems. Some systems, those that are well understood and for which complete information is available, can be modeled with some certainty, as is frequently the case in the physical sciences, and their future states predicted. However, many ecosystems are not well understood, and information on the relevant variables is so incomplete that they can be appreciated only through intuition and are best communicated by images. Prediction is not usually feasible in such cases.

Scenarios help in the assessment of future developments in complex systems that are either inherently unpredictable, or that have high scientific uncertainties. In this study, scenario analyses are made with different inputs. It is worth noting that when we do scenario analyses with different loadings, we consider two different conditions. One is that the inputs for different nutrient species are increased or decreased at the same time, because these nutrient species are highly correlated in Lake Lanier watershed based on the discussion in Chapter 3. The other is that only phosphorus loading is changed while other nutrient loadings are maintained at the nominal level. The simulated results of the two conditions are shown in Figure 7-14 and 7-15 respectively. It can be seen from Figure 7-14 that the simulated maximum concentration of orthophosphate has a small increase when pollutant loading increases, which indicates a large amount of orthophophate is adsorbed by suspended sediment or iron. This suggests that phosphorus is an important limiting factor for algal growth in many southeastern lakes. If we increase all nutrient loadings by two or three times at the same time, the maximum concentration of chlorophyll *a* in the water column will be 8.47 μ g/L or 11.42 μ g/L respectively. While if we only double or triple phosphorus loading alone, the maximum concentration of chlorophyll *a* in the water column will be 9.32 μ g/L or 13.53 μ g/L respectively.

The scenario analysis with inputs is useful for watershed management. For example, if water quality standards for Lake Lanier are known, the permitted maximum pollutant

loading can be calculated by this kind of analysis, and then use the results to guide land development in the watershed.

7.6 Conclusions and Discussion

In this study, the complete processes of model development are presented: identification of mechanisms \rightarrow model parameter identification \rightarrow model structure testing \rightarrow model calibration and evaluation \rightarrow sensitivity analysis and uncertainty analysis. The fitted model results in the pond and Lake Lanier indicate that the model structure is rational and the parameter values determined by random search and trial and error methods are reasonable.

Sensitivity analysis in the pond shows that algal growth rate, respiration rate and settling rate are the most sensitive parameters which affect the simulation result of *DO* as well as *pH*. However, when the modified model was applied in Lake Lanier (low phytoplankton productivity), these parameters are not sensitive. The pond is highly eutrophied, chlorophyll *a* concentration exceeds 100 μ g/L in most time of the monitoring period, which is much higher than other surface waters. For instance, chlorophyll *a* concentration in Lake Lanier is usually less than 4 μ g/L. When the model (modified to provide a vertical profile) was applied in Lake Lanier, phytoplankton growth, respiration and settling are not important processes. This implies that the sensitivity of phytoplankton growth and respiration mechanisms in this model depends on the phytoplankton productivity of the studied ecosystem.

Model calibration results in Lake Lanier show that the atmospheric exchange of O_2 and CO_2 are different. O_2 atmospheric exchange only occurs within the epilimnion, while CO_2 atmospheric exchange occurs within the epilimnion as well as the hypolimnion. The exchange rate of CO_2 at the hypolimnion is about a half of the epilimnion. This result implies the necessity of calibrate both O_2 and CO_2 for lake water quality modeling.

The phenomenon that the diffusive exchange rate (E_{SOD}) for the potential SOD in Lake Lanier is a sensitive parameter indicates that benchic sediments have significant impacts on lake water quality. SOD is high during the transition period and low during stratification period. Iron release rate has similar variations with SOD.

Scenario analysis with different inputs into Lake Lanier indicates that the simulated maximum concentration of orthophosphate results in a small increase when pollutant loading increases, which indicates a large amount of orthophosphate is adsorbed by suspended sediment or iron. This suggests that phosphorus is an important limiting factor for algal growth in many southeastern lakes.

If we increase all nutrient loadings by two or three times at the same time, the mximum concentration of chlorophyll *a* in the water column is 8.47 μ g/L or 11.42 μ g/L respectively. While if we only double or triple phosphorus loading individually, the maximum concentration of chlorophyll *a* in the water column will be 9.32 μ g/L or 13.53 μ g/L respectively. This difference is caused by different sediment-phosphorus adsorptions.

It is worth noting that the vertical DO profile in the growing season in 1996 is different from that in 1999. Figure 3-21 in Chapter 3 indicates that the concentration of dissoved oxygen is highest at the thermocline, but this is not the case from 1996/97 data. Positive heterograde profiles of DO could be due to a) phytoplankton photosynthetically settling from photic zone, b) light penetration to metalimnion where there is slow mixing so that any oxygen produced stays around and builds up, and c) input of oxygen-rich river water that is denser than surface water. If the third explanation is the case, we should see the similar profile in 1996/97, which is contradictory to the monitoring data in the lake.

Symbol	Symbol's meaning	Pond Calibration	Lake Calibration
CROD	Fraction of dissolved <i>BOD</i>	0.5	0.5
CON	Fraction of dissolved organic nitrogen	0.5	0.5
COR	Fraction of dissolved organic phosphorus	0.5	0.5
00P D	Depth of effective benthic sediment laver	0.5 0.2 m	0.2 m
E_{sop}	Diffusive exchange coefficient of SOD	0.02	0.58
f_{ON}	Fraction of dead algae recycled to dissolved <i>ON</i>	0.5	0.50
for	Fraction of dead algae recycled to dissolved <i>OP</i>	0.5	0.5
JOP KagMax	Maximum algal growth rate	2.10 /day	2.10 /day
KarMar	Maximum algal respiration rate	0.52 /day	0.15 /day
Kad	Algal death rate	0.05 /day	0.05 /day
Kcoz	CO_2 atmospheric exchange rate	0.40 /day	0.30 /day
Koz	Reaeration coefficient	0.20 /day	0.15 /dav
k_{ROD}	<i>BOD</i> decay rate at 20°C	0.15 /day	0.10 /day
k_{DN}	Denitrification rate at 20°C	0.1 /day	0.10 /day
k_{NI}	Nitrification rate at 20°C	0.1 /day	0.10 /day
k_{NIT}	Half-saturation constant for nitrification	$2.0 \text{ mg} O_2/\text{L}$	2.0 mg \dot{O}_2/L
K_{NO3}	Half-saturation constant for denitrification	$0.1 \text{ mg } O_2/\text{L}$	$0.1 \text{ mg } O_2/L$
k _{ON}	Organic N mineralization rate at 20°C	0.4 /day	0.05 /day
k _{OP}	Organic P mineralization rate 20°C	0.1 /day	0.1 /day
$k_{M\!N}$	See equation (6-19)	25 μg <i>N</i> /L	25 μg <i>N</i> /L
k_{mPc}	See equation (6-20), (6-21), (6-24), (6-25)	1.0 mg <i>C</i> /L	1.0 mg <i>C</i> /L
k _{SOM}	Sediment organic matter decay rate	0.05 /day	0.02 /day
k_C	Half-saturation constant for carbon	0.70 mg/L	0.70 mg/L
k_N	Half-saturation constant for nitrogen	0.20 mg/L	0.035 mg/L
k_P	Half-saturation constant for phosphorus	0.075 mg/L	0.003 mg/L
I_s	Light intensity for algal maximum growth	300 Ly/day	300 Ly/day
P_p	Adsorption coefficient for phosphorus	0.05	0.05
P_N	Adsorption coefficient for ammonia	0.55	0.05
S_{Fe}	Release rate of iron	0.1 SOD	0.1 <i>SOD</i>
v_s	Organic matter setting rate	0.14 m/day	0.10 m/day
ω_{t}	Phytoplankton settling rate	0.24 m/day	0.12 m/day
ω_{Fe}	Iron settling rate	0.09 m/day	0.09 m/day
ω_{ss}	Sediment settling rate	0.10 m/day	0.10 m/day
Θ	Temperature factor for algal growth	1.047	1.047
Θ_{BOD}	Temperature factor for BOD	1.047	1.047
Θ_{DN}	Temperature factor for denitrification	1.045	1.045
Θ_{Fe}	Temperature factor for iron release	1.08	1.08
Θ_{NI}	Temperature factor for nitrification	1.08	1.08
Θ_{DN}	Temperature factor for organic N mineralization	1.08	1.08
Θ_{DP}	Temperature factor for organic P mineralization	1.08	1.08
Θ_{OD}	Temperature factor for SOD	1.08	1.08
Θ_{SOM}	Temperature factor for SOM	1.08	1.08

 Table 7-1 Model Parameterization Results in Lake Lanier

Note: Bolded values indicate parameter changes between pond calibration and lake calibration.

ESOD	Standard Deviation of DO	Standard Deviation of <i>pH</i>
0.28	1.9323	0.5358
0.38	1.6977	0.5355
0.48	1.5846	0.5351
0.58 (nominal)	1.5606	0.5349
0.68	1.5959	0.5347
<i>K</i> ₀₂	Standard Deviation of DO	Standard Deviation of <i>pH</i>
0.05	1.9327	0.5354
0.15 (nominal)	1.5606	0.5349
0.25	1.6732	0.5348
0.35	1.7490	0.5348
0.45	1.7985	0.5347
K _{CO2}	Standard Deviation of DO	Standard Deviation of <i>pH</i>
0.20	1.5606	0.5352
0.30 (nominal)	1.5606	0.5349
0.40	1.5606	0.5413
0.50	1.5606	0.5450
0.60	1.5606	0.5494
K arMax	Standard Deviation of DO	Standard Deviation of <i>pH</i>
0.15 (nominal)	1.5606	0.5349
0.20	1.5653	0.5350
0.30	1.5705	0.5390
0.40	1.5703	0.5391
0.50	1.5688	0.5390
S _{Fe}	Standard Deviation of DO	Standard Deviation of pH
0.1*SOD (nominal)	1.5606	0.5349
0.2*SOD	1.5617	0.5350
0.3*SOD	1.5624	0.5350
0.4*SOD	1.5630	0.5351

SOD – sediment oxygen demand E_{SOD} – sediment diffusive exchange rate of SOD K_{O2} – O_2 atmospheric exchange rate

 $K_{CO2} - CO_2$ atmospheric exchange rate K_{arMax} – algal respiration rate S_{Fe} – iron release rate from sediment





Figure 7-1 Storage, Surface Area vs. Elevation



Figure 7-2 Rainfall in 1996



Figure 7-3 Inflow and Outflow in 1996







Figure 7-5 Model Calibration Results of Lake Lanier


Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-5 Model Calibration Results of Lake Lanier (Con't)



Figure 7-6 Calibration Result of Surface Chlorophyll *a* of Lake Lanier



Figure 7-7 Calibrated SOD, SOM and Iron Release Rate



Figure 7-8 Total Iron Simulation Result



Figure 7-9 Orthophosphate Simulation Result



Figure 7-10 Dissolved Inorganic Carbon Simulation Result



Figure 7-11 Random Search Result of algal half-saturation constant of phosphorus



Figure 7-12 Random Search Result of Organic Matter Settling Rate



Figure 7-13 Histograms of Standard Deviations of DO and pH



Figure 7-14 Scenario Analysis with Different Inputs







Figure 7-14 Scenario Analysis with Different Inputs (Con't)



Figure 7-14 Scenario Analysis with Different Inputs (Con't)



Figure 7-15 Scenario Analysis with Different Phosphorus Inputs

CHAPTER 8

SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

8.1 Summary

Lake Lanier is a 38,500 acre impoundment created by Buford Dam in north Georgia. It is the most important impoundment in the Atlanta metropolitan area. The reservoir is used for water supply, hydropower generation, flood control and recreation. Buford Dam, which impounds Lake Lanier, is located about 50 miles northeast of Atlanta. Average inflow to the lake is 2074 cubic feet per second. Of this flow, about 70% is contributed by the Chattahoochee River and the Chestatee River. The Lake Lanier watershed covers 1040 mi² which includes land in Forsyth, Habersham, Hall, Lumpkin, White, Dawson, Gwinnett and Union Counties.

The principal type of problem to which a lake environment is subject is the degradation of water quality through the excessive accumulation of nutrient material deriving from both agricultural and municipal development within the lake's catchment. Such a problem is usually referred to as (cultural) eutrophication. For a Southeastern lake (or reservoir) such as Lake Lanier, the region's warm climate, highly erodible and deeply weathered soils, and growing waste loads, present a great challenge for water management.

The increased availability of nutrients in the lake, particularly phosphorus (P), nitrogen (N) and carbon (C) compounds, creates conditions ripe for the explosive transient growth of micro-organism (phytoplankton) populations which occupy a position at the *base* of the lake's ecosystem. As a result the lake ecosystem not only becomes

temporarily unbalanced during certain periods of the annual cycle, but will also change gradually - from year to year - in terms of species abundance and diversity. Although the large growth of phytoplankton can be unsightly, they can also be linked with taste and odor problems, fish kills and a loss of regional income from tourism around the lake. They can also markedly increase the costs of treating the lake's water if it is used for drinking water supply. Therefore, it is very important to develop a robust model (or models) for the lake water quality management.

General speaking, this dissertation covers several areas of interest in characterizing water quality in Lake Lanier: the watershed and its capacity to generate pollutant loads including short-term and long-term estimations; the principal tributaries, which link the watershed to the lake; horizontal and vertical variations of water quality within the lake; limnochemical variations, including interactions with phytoplankton biomass; sediment-fresh water interactions; lake stratification and mixing; and interactions between the underlying groundwater and surface water. Specifically, the following studies have been conducted in this dissertation:

(1) GIS mapping for Lake Lanier watershed

GIS was used to delineate the watershed boundary, topography, landuse/landcover, soil type, lake shoreline, and to locate different kinds of point sources. This information can be useful for lake water quality management. For example, locations of point sources can identify their receiving water bodies, which is important to estimate water pollutant loading.

(2) Analysis of water quality characteristics and identification of water quality issues

Analysis of water quality characteristics is mainly based on five data sets: i) Holder (1966/67, monthly); ii) EPA's National Eutrophication Survey (1973); iii) EPA's Clean Lake Study (1991, monthly); iv) Upper Chattahoochee River Basin Group's Study (monthly and biweekly, 1996/97); v) Our supplementary sampling data in August 1999 and December 1999. The data sets are summarized and used to characterize water quality variability: a) at various locations within the lake; b) with depth below the surface; c) by season of the year; d) over the past thirty years of record. The analysis focuses on the physical, chemical and biological parameters related to nutrient cycling in Southeastern lakes or reservoirs, including temperature, dissolved oxygen, pH, Secchi depth, total suspended sediment and turbidity, specific conductance and alkalinity, chlorophyll *a* and biomass, and nutrients.

Based on the analysis of water quality characteristics and the intensive survey of stakeholders, decision-makers and scientists residing in the watershed, water quality issues are identified in this study.

The water quality characteristics and water quality issues are important considerations for the selection of water quality modeling state variables.

(3) Water quality characterization by using factor analysis and cluster analysis

In this dissertation, factor analysis and cluster analysis are used to i) classify correlated tributary water quality parameters into parameter categories that have similar temporal characteristics, ii) group tributaries and regions within the lake into spatial categories that have similar water quality parameter characteristics, and iii) provide longterm water quality monitoring strategies.

(4) Evaluation of nutrient loading into Lake Lanier

Nutrient loading includes external loading and internal loading. External nutrient loading includes tributary inflows (which includes storm runoff), lake inputs from municipal wastewater treatment plants and industry facilities, atmospheric deposition, and perhaps groundwater. Internal nutrient loading includes nutrient settling into and release from the bottom sediment.

The regression model of discharge-sediment-nutrient is used to quantify sediments and nutrient loads from tributary inflows. This model is derived from previous 20 years' data, and can be used to estimate daily nutrient loading as well as annual nutrient loading. Daily nutrient loading is the input for the developed biogeochemical model.

A sediment-water interaction model is developed to estimate internal nutrient loading (settling and release). The model can be used for annual internal loading analysis or long-term internal loading analysis.

(5) Vertical temperature distribution modeling

The model can avoid complicated heat balance in the air-water interface which was used by almost every existing model. In this model, the measured water surface temperature is regressed using a sinusoidal curve and is directly regarded as the upper boundary of the model, the measured thermocline variation is utilized to control the dynamics of thermocline depth, which is very important to quantitatively determine the depths of epilimnion and hypolimnion. The case study of Lake Lanier temperature modeling indicates that the model is adequate.

The modeling result of water temperature is one of the forcing functions for the developed biogeochemical model.

(6) Hydrologic modeling

This model is relatively simple and is mainly derived from water budget. The modeling results of daily inflow, outflow, and water volume provide hydrological condition for the developed biogeochemical model.

(7) Biogeochemical modeling

The developed biogeochemical model is a comprehensive vertical distribution model. In contrast to most other models of impounded water bodies, the model couples an account of the conventional relationships among C, N, P (as nutrients, primarily) and chlorophyll-a, with both the carbonate-pH subsystem and the Fe-sediment subsystem.

8.2 Conclusions

(1) Water quality characteristics of Lake Lanier

- (a) Lake Lanier water temperature, pH, and dissolved oxygen concentration distribution are basically uniform horizontally, but highly variable in the vertical direction. No clear long-term changes are apparent.
- (b) TSS, turbidity, and secchi disc depth have an obvious spatial distribution, with higher TSS and turbidity near tributaries and lower values downstream. Secchi disc depth has the reverse distribution. No clear long-term changes are apparent, other than small changes in the seasonal distribution.
- (c) The concentration of chlorophyll *a* and biomass have variable spatial distribution, higher in the upper portions of the lake and lower in the lower lake. This distribution has not changed markedly during the past thirty years of study.
- (d) During the growing season (or stratification period), the highest DO concentration and pH occur at around the thermocline due to photosynthetic activity of phytoplankton settling from the photic zone.
- (e) Lake Lanier can be classified as a *mesotrophic lake* based on the trophic concept.

(2) Water quality issues

- (a) Eutrophication (or green water or nutrients in the survey): Loading of nutrients (primarily phosphorus) to Lake Lanier was identified as a primary water quality concern. Increases in nutrient loading will cause an increase in aquatic plants, a decrease in water clarity, and a decrease in dissolved oxygen in certain areas of the lake.
- (b) Dissolved oxygen: Another water quality concern is the depression of dissolved oxygen in the lake due to temperature stratification that isolates bottom waters of the lake from atmospheric sources of oxygen.

- (c) Bacteria: Pathogenic bacteria were identified as a water quality concern due to high recreational use of the lake. Elevated concentrations of bacteria have been observed in many lake tributaries, although the surface waters of the lake itself have remained in compliance with water quality standards.
- (d) Aquatic toxicity: Toxicity of the reclaimed water discharges in the direct vicinity of wastewater outfalls was identified as a concern by the public due to constituents such as ammonia, chlorine, metals, and organic toxicants.
- (e) Sedimentation (or brown water in the survey): Accelerated sedimentation of Lake Lanier due to loading of eroded soils was identified as potential concern.
- (f) Temperature/stratification: The effect of reclaimed water discharges on thermal stratification of Lake Lanier also is a concern, in that it could introduce nutrient laden bottom waters of the lake to the lake surface, where they could trigger additional algal growth.

(3) Factor analysis and cluster analysis on Lake Lanier water quality

- (a) Factor analysis of the comprehensive data set (from 1996/97) indicates that variability in all but the total nitrogen, nitrite/nitrate nitrogen, and alkalinity in the lakes' tributaries are dominated by non-point source, storm runoff. It is probable that increases in these organic forms of nutrients, sediments, and metals are likely caused by overland flow and soil erosion associated with storm runoff. Oxidized forms of nitrogen appear to be dominated by point sources which result from wastewater treatment plants and industrial facilities. Alkalinity is neither dominated by point sources or non-point sources because it has both natural and anthropogenic sources.
- (b) Cluster analysis of the same data set (tributaries) indicates that the tributaries to Lake Lanier can be divided into five homogeneous groups: 1) Small Upper Basin Streams (including the East Fork of the Little River, Flat Creek North, Wahoo

Creek, Balus Creek, and the West Fork of the Little River); 2) Large Upper BasinStreams (including the Chestatee and Chattahoochee Rivers); 3) Limestone Creek;4) Six Mile Creek; 5) Flat Creek South. This result is very useful for guiding monitoring design in water quality for the purpose of management.

(c) Cluster analysis on the same data set (17 lake stations) indicates that variability of the lake is such that the lake can be treated as a set of four, homogeneous subvolumes, a result with obvious implications for development of the models and in practice, strategies for monitoring changes in water quality for the purpose of management.

(4) Nutrient loading (including external and internal loading) analysis

- (a) Nutrient loading is important in characterizing the disturbances entering the lake from its surrounding watershed. Knowledge of the variation in loadings of sediment and nutrients in the principal tributary flows (the Chattahoochee River and Chestatee River) is especially crucial to exploration of the future response of the lake. It appears that the regression relationships between discharge, sediment and nutrients may be able to simulate patterns of loading adequately.
- (b) Macroscopic assessment (by nutrient budget) of the movement of nutrients through the lake indicates some unknown sources and/or sinks, above and beyond what can be accounted for by conventional assumptions about settling to the bottom sediment and subsequent release therefrom. Among a number of candidate mechanisms for these sources/sinks is the movement of water across the interface between surface water and groundwater.
- (c) Long-term loading analysis based on the regression relationships indicates that sediment loading correlates well with available observed data of the lake, while nutrient loadings do not. These results could be explained by the fact that sediments are dominated by physical process in the lake, while nutrients appear to

be dominated by biogeochemical processes. The latter indicates the importance of correctly characterizing the biogeochemical mechanisms in the lake.

(5) Vertical temperature modeling

- (a) In this model, there is only one parameter (heat dispersion coefficient D_z) which needs to be calibrated. This will greatly decrease model calibration difficulty and increase modeling reliability. Our calibration result by using Monte Carlo simulation method shows that D_z at stratification period is about 0.35 m²/day in Lake Lanier.
- (b) Modeling results in Lake Lanier indicate the model is efficient and the modeling approach is reasonable. However, the model is not intended to be used for prediction.

(6) Hydrologic modeling

(a) The hydrologic modeling results indicates that the simulated water level fits the observed water level quite well if lake evaporation (average evaporation is assumed) is considered. Otherwise modeling results will not fit the observed data.

(7) Biogeochemical modeling

- (a) In the aquaculture pond, with its high primary productivity, successful matching of the observed diurnal oscillations in both DO and pH with this model is most sensitive to algal growth rate, respiration rate and settling rate. In Lake Lanier, however, with its much lower primary productivity, the modeling results indicate this is not be the case.
- (b) The model calibration result for Lake Lanier shows that the atmospheric exchange between O_2 and CO_2 are different. O_2 atmospheric exchange only occurs within epilimnion, while CO_2 atmospheric exchange occurs within epilimnion as well as hypolimnion. The exchange rate of CO_2 at hypolimnion is about a half of

epilimnion. This result implies the necessity of double check on both O_2 and CO_2 for lake water quality modeling.

- (c) Model calibration for the pond suggests that algal growth rate may change with time during algal bloom, which indicates that it is difficult to predict algal bloom.
- (d) Model calibration and evaluation results for the pond indicate that algal growth rate, respiration rate, and algal settling rate for the two analysis periods need to be different to fit the measured trends of fluorescence. This suggests that the dominant algal species may change during the two analysis periods.
- (e) Sediment adsorption with ammonia is related to pH. High pH has high adsorption capacity, which supports the theory of pH-dependent charges of soils.
- (f) Sensitivity analysis result in Lake Lanier shows that the diffusive exchange rate (E_{SOD}) for SOD is a sensitive parameter, which indicates that benthic sediment has great effect on lake water quality. SOD is high during transition period and low during stratification period. Iron release rate has similar variation with SOD.
- (g) Scenario analysis with different inputs into Lake Lanier indicates that the simulated maximum concentration of orthophosphate has a small increase when pollutant loading increases, which indicates a large amount of orthophosphate is adsorbed by suspended sediment or iron. This suggests that phosphorus is an important limiting factor for algal growth in many southeastern lakes.
- (h) If we increase all nutrient loadings by two or three times at the same time in Lake Lanier, the maximum concentration of chlorophyll *a* in the water column will be 8.47 μ g/L or 11.42 μ g/L respectively. While if we only double or triple phosphorus loading individually, the maximum concentration of chlorophyll *a* in the water column will be 9.32 μ g/L or 13.53 μ g/L respectively.

8.3 Recommendations

(1) Recommendations for lake management alternatives

(a) Point source control

• Investigation shows that some point sources do not meet the pollutant discharge standard, indicating stricter enforcement of permit limits is warranted.

(b) Non-point source control

- Reduction of contamination potential from septic tanks involves: on-site inspections and control actions following complaints, monitoring installation of new septic systems, routine inspection of critical areas, increasing community awareness of symptoms and responsible agency for reporting septic tank problems, and increased citizen awareness of proper septic tank maintenance.
- Reduction of contamination potential from cattle includes: proper storage and disposal of manure collected from dairy confinement facilities, avoid spreading manure onto saturated soils (often present during winter), prevent direct defecation of cattle into streams by fencing them out, review the design criteria for diary oxidation ponds which discharge to streams.
- Reduction of fecal coliform from both cattle and poultry operations includes: locating confinement areas where they will not flood during storms, improving manure storage facilities to reduce leakage, using riparian buffer strips along waste application sites, preventing the spread of manure under conditions conducive to runoff (saturated soils, surface channeling, wet weather).
- Reduce soil erosion and sedimentation by planting vegetation at critical areas.

(c) Nutrient inflow control from tributaries

• During dry season, nutrient inflow from tributaries is an important source to the lake. This kind of nutrient loading can be reduced by reasonable regional
development planning and optimization management, especially optimization control of trans-regional pollution.

(d) Internal nutrient loading control

- Monitor iron concentration in the lake sediment. Oxidized iron forms a ligand exchange with phosphate and removes it from the biologically available fractions. A decrease in the loading of oxidized iron may result in more frequent algal blooms due to increased phosphate availability.
- Study sulphate concentration in the lake sediment, if it is high, analyze the reason and control it. Under anoxic condition, sulfate will be reduced to sulfide which can strongly combined with Fe (III) or Fe (II), and may thereby release phophate from iron-phosphorus bonding.
- Study nutrient exchange between lake water and ground water to determine the exchange rate and direction, and then provide effective mitigation measures.

(e) Wetland protection

• Functions of wetlands are the physical, chemical, and biological processes occurring in and make up the ecosystem. Processes inlude the movement of water through the wetland into streams or the lake; the decay of organic matter; the release of nitrogen, sulfur, and carbon into the atmosphere; the removal of nutrients, sediment and organic matter from water moving into the wetland; and the growth and development of all the organisms that require wetland for life.

(2) Recommendations for water quality monitoring design

 The cornerstone of lake water quality management is monitoring data. Unfortunately, lake water quality monitoring is expensive, time consuming, labor intensive and spatially extensive. A well-designed water quality monitoring plan must preserve scarce resources by minimizing the number of monitoring stations and the types of variables monitored, while at the same time maintaining the quality of the collected information.

- Based on cluster analysis on tributary data, a monitoring station should be situated on the largest tributary in the first group (Wahoo Creek) to track the behavior of those streams. Notwithstanding the fact that the Chestatee and Chattahoochee Rivers have much in common, they should both be monitored because they are the largest tributaries to Lake Lanier. Although the remaining three tributaries (Limestone Creek, Six Mile Creek, and Flat Creek South) are small, they behave differently from the other tributaries and require monitoring. In all, water quality monitoring in six tributaries to Lake Lanier is recommended.
- Because the bulk of nutrient inputs appear to be from stormwater, stage-dependent sampling is recommended. Water quality sampling should be concomitant with discharge measurements over a wide range of discharges (e.g., at 10% exceedence frequency intervals). Additional sampling for nitrates should focus on those tributaries where wastewater treatment and land application facilities are located. Sampling should be performed during average and below average flow conditions to avoid the influence of stormwater dilution.
- Cluster analysis of water quality data from 17 lake stations was used to determine whether various parts of Lake Lanier could be grouped into homogeneous zones. Based on the analysis here, we recommend the use of four zones: 1) the lowest part of the lake near the dam (Stations 1-5); 2) the central part of the lake (Stations 6-10); 3) the upper part of the lake (Stations 12-17) nearest the influent tributaries; and 4) the embayment near Flat Creek South (Station 11). In all, water quality monitoring at four lake stations is recommended. These observations should be collected at one to two meter intervals from the water surface to the maximum depth of the lake at the station on a monthly basis.

(3) Recommendations for future studies

- Nutrient loading is always very difficult to quantify. Although the regression relationships derived from previous 20 years' data appear to be able to simulate patterns of loading adequately in this study, these relationships are not able to predict loadings related to future changes, especially land use development. Therefore it is recommended to use GIS models to simulate nutrient loadings, and then calibrate the important parameters in the GIS model based on comparison of the results from the two approaches.
- Sediment-water interaction is an another difficult problem to overcome. In our sediment-water interaction model, the important coefficients of sediment settling rate and release rate are basically drawn from previous study in a different lake. Field measurement to determine the two coefficients is recommended.
- Our macroscopic assessment from the nutrient budget indicates that the exchange between lake water and groundwater has great effect on lake water quality. Further study about this issue including groundwater monitoring design is recommended.
- Lake Lanier nutrient concentrations have longitudinal, lateral and vertical variations, and Lake Lanier shoreline is very complex. A fully three dimensional hydrodynamic model incorporating the proposed biogeochemical mechanisms is recommended.

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