Wu-Seng Lung

Water Quality Modeling That Works

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ISBN 978-3-030-90482-1 ISBN 978-3-030-90483-8 (eBook)
https://doi.org/10.1007/978-3-030-90483-8

This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

To Kathy

Preface

My motivation for writing this book is grounded in memories of my first professional work experiences, at Hydroscience, where I began working in 1975. It was at Hydroscience where I had the privilege of meeting and working with Dr. Donald J. O'Connor on estuarine water quality modeling, and where I quickly learned from our weekly meetings that I was simply yet another just out of school individual running a model, and not actually doing any modeling. Dr. O'Connor's approach involved gaining important physical insights into the receiving water system by examining the field data gradually developed a model for the water system in his thoughts. Such a practice really intrigued me and fundamentally changed the way I approach water quality modeling. While working under Dr. Robert V. Thomann on Lake Ontario eutrophication modeling, he always stressed the importance of configuring the model with the correct values of coefficients supported by data. How to interpret the modeling results is equally or perhaps even more important. Dr. Dominic M. Di Toro has reminded me that model performance can only be judged from how well they reproduce observations and how parameters are fit to the field data to estimate the necessary coefficients. When all is said and done, modeling without data is a waste of time. This enriching experience at Hydroscience and the Manhattan (all three were faculty at Manhattan College in New York City) doctrine has stayed with me throughout my professional career.

In 1987, Dr. Thomann predicted that water quality modeling would benefit from a significant increase in spatial and temporal resolutions in the years to come. He cautioned, however, that obtaining accurate results would continue to hinge on the mastering of underlying modeling skills by the modeler. Thus, almost four decades later—with technological advances such as machine learning—when we ask whether the role of skilful modelers can be replaced by, in essence, computing on "autopilot," the answer is unequivocally negative. Today, many want to configure and run MIKE 21, for example, without data support and do not care about the results correct or not, and even worse, they often times manipulate the computations to get the results they want. In addition, they just learn to use the interface to run the model and do not care what is behind it. I have seen this practice occur in many places and hope to deliver a strong message to reverse this trend.

Water quality modeling and photography are, in certain ways, a similar exercise. The frameworks used—water quality models and camera systems—are parallel devices. The rapid advancement of digital technology and many accessories have produced more and more sophisticated camera systems these days, just like many highly sophisticated water quality modeling frameworks do. However, these modern marvels cannot replace the human thoughts behind the camera that set the lighting and composition, an art based on the skills of the photographer. Along these same lines, water quality modelers have field data, a form of science, something much more reliable than art. The use of field data to enhance the skills for the modeling analysis is the key of this book.

A data analysis plays several significant roles in a water quality modeling study. It enables the modeler to better understand the existing water quality conditions with available data, independently quantifies key kinetics rates to configure the model, provides checkpoints in the model calibration, and identifies any potential data gaps. However, the step of performing data analysis is often ignored, leaving the modeler a significant amount of guesswork on model configuration in assigning key parameters and coefficients. This book presents techniques to independently quantify model coefficients with strong data support such as mass transport coefficients, kinetic coefficients in BOD/DO, and eutrophication modeling of various water systems.

A new set of technical issues on BOD/DO modeling also challenges the modelers these days. A refined concept of the BOD based on long-term BOD data to quantify the BOD/DO kinetics of CBOD and nitrification for the modeling analysis is presented. Laboratory tests to obtain spatially variable deoxygenation rates in the receiving water are demonstrated. The persistent eutrophication problem is still with us today. To assist modelers, a large number of eutrophication modeling studies of rivers, lakes, reservoirs, and estuaries are presented in this book. Each displays different features of complex interactions in the system: switching from DO endpoint to chlorophyll *a* endpoint, from nutrient limitation to flow limitation for algal growth, and seasonal limiting nutrient between nitrogen and phosphorus, turbidity maximum mediated eutrophication, and algal-related diurnal DO variations. Understanding these physical insights is much more meaningful than simply running models without data support.

Over the past three decades, the mixing zone determination has become a popular subject in implementing water quality standards and has created a greater push for a modeling analysis to support water quality management. This book presents the mixing zone modeling analysis supported by field data with applications to whole effluent toxicity (WET), metals, temperature, color, and estrogens. Once again, field data are crucial to support this modeling work. Acidification and eutrophication are the two extremes in a wide spectrum of water quality condition in ambient systems. Acidification has been closely associated with energy production, resulting in the water–energy nexus (e.g., pH and sulfate modeling of acid mine drainage). Interestingly, the pH-mediated sediment phosphorus release that led to the 1983 blue-green algal blooms in the Potomac Estuary was the key to that successful investigation. This book also presents a succinct version of carbonate equilibrium leading into pH modeling using an engineering approach with a number of case studies.

Modeling the fate and transport of endocrine disrupting chemicals (EDCs) and pharmaceutical and personal care products (PPCPs) in water systems is becoming an urgent matter given the sharp increase in the number and widespread use of these so-called emerging chemicals. First, key processes and their kinetics of modeling the fate and transport of metals in watersheds and receiving waters are presented. The focus is also on estrogens, an EDC most commonly found in domestic wastewaters but generally ignored by regulatory agencies to date. Modeling estrogens in the South River Watershed in Virginia is presented on this topic. Instantaneous sorption equilibrium is visited for pharmaceuticals. Significant concentration differences predicted for the dissolved triclosan due to the slow sorption kinetics are predicted for the Patuxent Estuary.

Finally, the model is well calibrated and verified with field data. The modeler proceeds to produce model predictions under future conditions for water quality management. Can the modeler claim a victory and go home? No, not by a long shot! A key question the modeler can expect to face from decision makers is: How do you know your model prediction results are correct? No model verified under existing conditions can fully operate as a framework free of uncertainty. Open boundary conditions are difficult to assign for tidal systems (i.e., an estuary) under future conditions when interior load reductions influence the boundary conditions. Is the sediment system in equilibrium with the external loads? Reality check applications such as model post-audit are presented to illustrate the difficulties a modeler can potentially face.

Instead of discussing the running of models without data support, this book emphasizes the physical insights and field data support required to successfully perform water quality modeling. The goal is to reduce the degree of art in the exercise and significantly increase science and engineering in the modeling analysis. Environmental engineers and scientists engaged in quantifying the water quality impacts of pollutants to specific water systems will find this book valuable in their day-to-day practices. This book reinforces the critical importance of properly understanding the physical attributes of water systems. This is also what sets this book apart from the volumes currently available in the water quality modeling field—nearly all other books in the field are categorized as textbooks and, unlike this book, offer few practical examples or exercises to follow. Therefore, this book targets the advanced modelers with the urge and desire to master their skills.

In closing, I would like to thank my Ph.D. Advisor, Prof. Raymond P. Canale at the University of Michigan, who introduced me to this new (at that time) and exciting (still at this time) field filled with unforgettable experiences. My training at Michigan was invaluable. I would also like to thank him for introducing me to Hydroscience upon the completion of my Ph.D. I have also been fortunate to participate in several international studies sponsored by NATO, Universitas 21, and University of Virginia's Global Study Program. The Metro Council of Minneapolis and St. Paul provided funding and volumes of data to work on the upper Mississippi River and Lake Pepin. Funding for the Patuxent Estuary modeling work was provided by the State of Maryland and the Smithsonian Environmental Research Center. Many other sponsors have contributed to the work presented in this book. I am also indebted to my long-time

colleague and friend, Dr. Jan-Tai Kuo of National Taiwan University (NTU) on many river and reservoir modeling studies in Taiwan. Preparation of this manuscript could not be completed without the assistance of my former Ph.D. students. Dr. Sen Bai at Tetra Tech provided many excellent suggestions as to the content of the book and assisted with fecal coliform modeling. Dr. Alex Nice of AECOM provided immeasurable assistance on the Patuxent Estuary eutrophication and metals modeling work. Dr. Dong Liu foresaw the importance of non-instantaneous equilibrium of pharmaceuticals in water systems. Dr. Xiaomin Zhao's (now at Paradigm Environmental) work on tracking estrogens in watersheds laid the groundwork for future studies. I was also fortunate to work with Dr. Chien-Hung Chen (now at Stantec in Taiwan) on the Danshui River BOD/DO study as his Ph.D. thesis Advisor at NTU. The assistance of Dr. Shih-Kai Ciou (with Sinotech Engineering Consultants in Taiwan) on providing the data and model results of the Feitsui Reservoir in Taiwan is really appreciated. Dr. Wai Thoe of Hong Kong Environmental Protection Department provided material on *E. coli* modeling of Hong Kong beaches. I am also grateful to my Technical Editor, Monica Wedo, for improving this manuscript; her work is really appreciated.

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Abbreviations

μg/L	Micrograms per Liter
μmho/cm	Micromhos per Centimeter
1Q10	1-day 10-year Low Flow
7Q10	7-day 10-year Low Flow
ACSA	Augusta County Service Authority
ADMI	American Dye Manufacturing Manufacturers Institute
AFO	Animal Feeding Operations
AHOD	Areal Hypolimnetic Oxygen Deficit
AIZ	Allocated Impact Zone
AOC	Assimilable Organic Carbon
ATE	Acute Toxicity Endpoint
BOD	Biochemical Oxygen Demand
BOD_5	5-day Biochemical Oxygen Demand
BPA	Biphenyl A
CAFO	Concentrated Animal Feeding Operations
$CBOD_5$	5-day Carbonaceous Biochemical Demand
$CBOD_u$	Ultimate Carbonaceous Biochemical Demand
CCC	Criterion Continuous Concentration
CCMS	Committee on the Challenge of Modern Society
cfs	Cubic Feet per Second
CFU	Colony Forming Unit
CMC	Criterion Maximum Concentration
cms	Cubic Meters per Second
COD	Chemical Oxygen Demand
COVID-19	Coronavirus
CPCB	Central Pollution Control Board
CRE	Caloosahatchee River Estuary
CSO	Combined Sewer Overflow
CTE	Chronic Toxicity Endpoint
CWA	Clean Water Act
DIN	Dissolved Inorganic Nitrogen

DIP	Dissolved Inorganic Phosphorus
DJB	Delhi Jal Board (Delhi Water Board)
DMA	Dimethylarsenate
DO	Dissolved Oxygen
DOC	Dissolved Organic Carbon
DOM	Dissolved Organic Matter
E. coli	*Escherichia coli*
E1	Estrone
E2	Estradiol
E2α	17α-estradiol
E2β	17β-estradiol
EDC	Endocrine Disrupting Chemical
EE2	17α-ethinylestradiol
ENR	Enrofloxacin
EPA	Environmental Protection Agency
HEPP	Hydroelectric Power Plant
ICPRB	Interstate Council of the Potomac River Basin
lbs/day	Pounds per Day
MCL	Maximum Contaminant Level
MDNF	Momentum-Dominated Near Field
MFL	Minimum Flow Limit
mg/L	Milligrams per Liter
mgd	Million Gallons per Day
MMA	Methylarsonate
MOU	Memorandum of Understanding
MPCA	Minnesota Pollution Control Agency
MPN	Most Probable Number
MRLC	Multi-Resolution Land Characteristics Consortium
MWCOG	Metropolitan Washington Council of Governments
NATO	North Atlantic Treaty Organization
NBOD	Nitrogenous Biochemical Oxygen Demand
ng/L	Nanograms per Liter
NM	New Mexico
NOAA	National Oceanic and Atmospheric Administration
NOEC	No Observable Effect Concentration
NP	Neptunium
NPDES	National Pollutant Discharge Elimination System
Ortho-P	Orthophosphate
PEM	Potomac Estuary Model
POC	Particulate Organic Carbon
POM	Particulate Organic Matter
PON	Particulate Organic Nitrogen
POP	Particulate Organic Phosphorus
PPCP	Pharmaceutical and Personal Care Product
PPO_4	Particulate Phosphate

RMZ	Regulatory Mixing Zone
SFWMD	South Florida Water Management District
SOD	Sediment Oxygen Demand
TCMP	2-chloro-6-(trichloromethyl) pyridine
TCS	Triclosan
TIC	Total Inorganic Carbon
TKN	Total Kjeldahl Nitrogen
TMDL	Total Maximum Daily Load
TP	Total Phosphorus
TRC	Total Residue Chlorine
TSS	Total Suspended Solids
TU_a	Acute Toxicity Unit
TU_c	Chronic Toxicity Unit
TWBC	Tidal Basin and Washington Ship Channel
UPRC	Upper Potomac River Commission
USGS	United States Geological Survey
UV	Ultraviolet
UVa	University of Virginia
VDEQ	Virginia Department of Environmental Quality
VEC	Valued Ecosystem Component
VIMS	Virginia Institute of Marine Science
VPDES	Virginia Pollutant Discharge Elimination System
WET	Whole Effluent Toxicity
WLA	Wasteload Allocation
WQBEL	Water Quality-Based Effluent Limit
WWTP	Wastewater Treatment Plant
ZID	Zone of Initial Dilution

Chapter 1
Challenges in Modeling for Water Quality Management

In his paper entitled: System Analysis in Water Quality Management—a 25 Year Retrospect, Thomann (1987) predicted a significant increase in spatial and temporal resolutions of water quality models in the years to come. A decade later, he confirmed his prediction in another landmark paper entitled: The Future Golden Age of Predictive Models for Surface Water Quality and Ecosystem Management (Thomann 1998). He indicated that the remaining challenges lie in how to obtain the correct model results supported by data for use in water quality management. Given field data, what is the number one challenge in water quality modeling? The answer: what if the model results do not reproduce the field data.

Water quality modelers must rely on science and data, the two fundamental pillars to support the modeling analysis, by increasing the objectiveness of our modeling work. Accordingly, water quality modeling would let the data speak while letting the science to guide. The design and focus of this book is on performing water quality modeling with these two goals in mind. Our emphasis is not on models, regardless of whether they are simple or complex. Rather, we focus on modeling analyses with strong scientific and data support. It is noted that modeling cannot generate data; rather, modeling is used to interpret data and to generate predictions with such data that have been used to properly calibrate and verify the model. Without strong data support, these modeling frameworks will not otherwise provide a meaningful analysis. Can sophisticated models (or modeling frameworks) replace the role of a skillful modeler by, in essence, putting them on "auto-pilot"? The answer is unequivocally negative. Spatial resolution is not the key for a successful modeling analysis for water quality management. Instead, modeling skills with strong data support are crucial to obtaining defensible results for water quality management. As such, readers of this book should not expect to see merely a parade of modeling frameworks. Instead, readers should expect, and enjoy, an active discussion about the salient features of the modeling analysis, albeit a simple task of deriving a single, key model coefficient value.

W.-S. Lung, *Water Quality Modeling That Works*,
https://doi.org/10.1007/978-3-030-90483-8_1

1.1 The Potomac Estuary Algal Bloom

This chapter begins with an interesting, classic example of using a water quality model to solve a mystery of a eutrophication issue, which demonstrates the essence of modeling, not just running models, for water quality management. The progression of water quality problems in the Potomac Estuary (Fig. 1.1) started in the late 1960s when extensive algal blooms developed in addition to a depressed dissolved oxygen (DO) condition in the Washington, DC vicinity (Thomann 1987). Following a series of significant reductions in biochemical oxygen demand (BOD) and ammonia loads in the 1970s, the low DO problem was eliminated.

When it comes to nutrient reductions to mitigate algal blooms in the Potomac Estuary, the debate has always been between nitrogen and phosphorus (i.e., which one is the limiting nutrient). It was first argued that nitrogen was the limiting nutrient

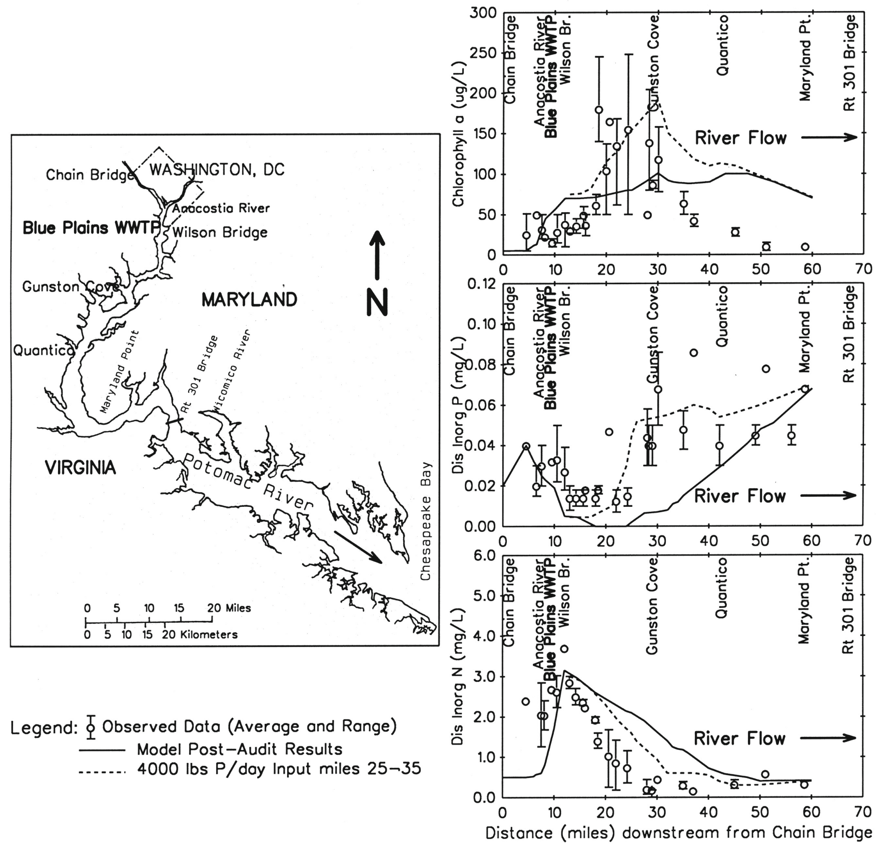

Fig. 1.1 The Potomac River estuary and 1983 blue algal bloom data

and that nitrogen should be controlled. However, algal blooms in the form of the blue-green algae, *Microcystis aeruginosa*, can fix nitrogen from the atmosphere, defeating the purpose of controlling nitrogen. Conversely, concern was also expressed over the release of phosphorus from the sediment. Eventually, the phosphorus removal strategy was founded on the notion that with sufficient reduction of phosphorus, it could be made the limiting nutrient (Thomann 1987). Since it was considered cheaper to remove phosphorus than nitrogen, the phosphorus removal program was instituted. Such action led to significant reductions in point source phosphorus input to the Potomac Estuary from 24,000 lbs/day in the late 1970s to less than 2000 lbs/day by early 1980s at a cost of US$1B for phosphorus removal at municipal wastewater treatment plants (WWTPs).

By early 1980s, the total wastewater flows from nine major WWTPs to the Potomac Estuary amounted to 446 million gallons per day (mgd) with the Blue Plains WWTP (see the location of this facility in Fig. 1.1) as the single largest discharger at 310 mgd. Following a major algal bloom in the Potomac in 1977, an intensive effort was then undertaken to update the modeling framework for eutrophication, resulting in the Potomac Eutrophication Model (PEM) (Thomann and Fitzpatrick 1982). This model, including sediment–water interactions, was calibrated and verified using 7 years of data and was then used to analyze nutrient control alternatives (Thomann 1987). In the meantime, the phosphorus concentrations in the Potomac Estuary continued to decrease and algal blooms disappeared.

With the phosphorus reductions almost fully in place, another major bloom occurred in the summer of 1983 in the form of *M. aeruginosa* with chlorophyll *a* measured at about 300 μg/L in the main channel and 800 μg/L in the embayments. A collective effort between government agencies, the Metropolitan Washington Council of Governments (MWCOG), the state environmental agencies (Maryland, Virginia, and Washington DC), and Interstate Council of the Potomac River Basin (ICPRB) was initiated to investigate. Understandably, a number of questions were asked:

1. What was the cause of the bloom?
2. The Blue Plains WWTP effluent total phosphorus (TP) concentration was around 0.4 mg/L in 1983. Would the situation be relieved when the Blue Plains WWTP effluent TP levels reached the target of 0.2 mg/L?
3. What are the most likely mechanisms responsible for the bloom?
4. Would the PEM be able to reproduce the bloom?

The investigation panel put these questions to the PEM. When the PEM was applied with the summer 1983 meteorological and hydrological data, it tracked the onset of the bloom up to about 100 μg/L by the end of July, but then failed to reproduce the further intensification of the bloom (see the comparison of model results and data in the top right plot of Fig. 1.1).

The model results did not match the field data—a challenge to the modelers. An immediate responsive action is to increase the algal growth rate with the hope to grow more algae, right? However, the second plot of Fig. 1.1 gives us the answer. The model could not grow more algae because it ran out of food, i.e. dissolved inorganic phosphorus (DIP) around the area approximately 20 miles downstream from the Chain Bridge (see the middle right plot of Fig. 1.1). Lacking DIP was the principal reason for the failure of the PEM to capture the full bloom. Interestingly, PEM results over-predicted the dissolved inorganic nitrogen (DIN) in the Potomac Estuary (see the bottom right plot of Fig. 1.1).

The under-predicting DIP and over-predicting DIN suggested that if the PEM had extra phosphorus, the bloom would go higher, which would take up more nitrogen, resulting in lower calculated DIN and a better match with the DIN data. Next, using the PEM as a tool, the investigation panel asked the PEM for an additional amount of phosphorus to sustain the bloom. Model sensitivity analyses responded that there were additional phosphorus sources of about 4000–8000 lbs/day needed to overcome the shortage of phosphorus. The dashed lines in Fig. 1.1 shows the effect of including this source: matching the chlorophyll *a*, DIP, and DIN data much better. The PEM partially explains the observed data but had not provided all the answers to the above questions. What this modeling analysis shows is that changing model coefficient values must have justifications. The interplay between model results and data led the investigation panel to seek additional phosphorus sources for the summer 1983 algal bloom.

1.2 Searching for Additional Phosphorus Sources

A possible phosphorus source could be diffusive release of DIP from the sediment to the water column. A phosphorus release at levels of about 40–80 mg P/m^2/day was necessary to produce 4000 lbs/day of the phosphorus to sustain the bloom (Thomann et al. 1985). It is known that such releases can occur in substantial amounts under anaerobic conditions. However, as noted, the DO in the Potomac was generally above 3–4 mg/L. Excessive oxygen was being produced by the bloom via photosynthesis, therefore there was no shortage of DO in the water column, nor in the sediment. In response, Di Toro and Fitzpatrick (1984) proposed a hypothesis for an aerobic sediment release of this order for the Potomac Estuary.

The mechanism proposed for the Potomac Estuary event during the summer of 1983 is related to the high pH that occurred during August and September. The sorption of phosphorus is highly pH dependent. If the pH rises in the overlying water, this effect will diffuse through the sediment–water interface and reduce the sorption of DIP to the iron oxides/hydroxides. Although the sorbents are still present, their ability to sorb is reduced due to the high pH and therefore, the phosphorus flux should increase. If the sorption potential of the oxides/hydroxides is completely eliminated, then high pH aerobic DIP flux should be essentially equal to the anaerobic DIP flux. In both of these cases, the sorption barrier has been removed by dissolution in the anaerobic case, or the sorption capacity has been eliminated by the high pH in the aerobic case. The result of either of these mechanisms is a large increase in the DIP flux to the overlying water. It should be noted that this mechanism should not affect the flux of ammonia to the overlying water since its sorption to the oxides/hydroxides is orders of magnitude less than for phosphorus. Thus, the sorption hypothesis predicts that only phosphorus flux will be increased by high pH events.

1.3 pH Rise During the Bloom

Examination of the DIP and TP data in the Potomac Estuary shows that it was not until the August and September surveys that the increase in DIP and TP between milepoints 20 and 40 was readily evident. Coincidently, that corresponded to the time in which pH first rose above 9.0, as shown in Fig. 1.2. Note that during July

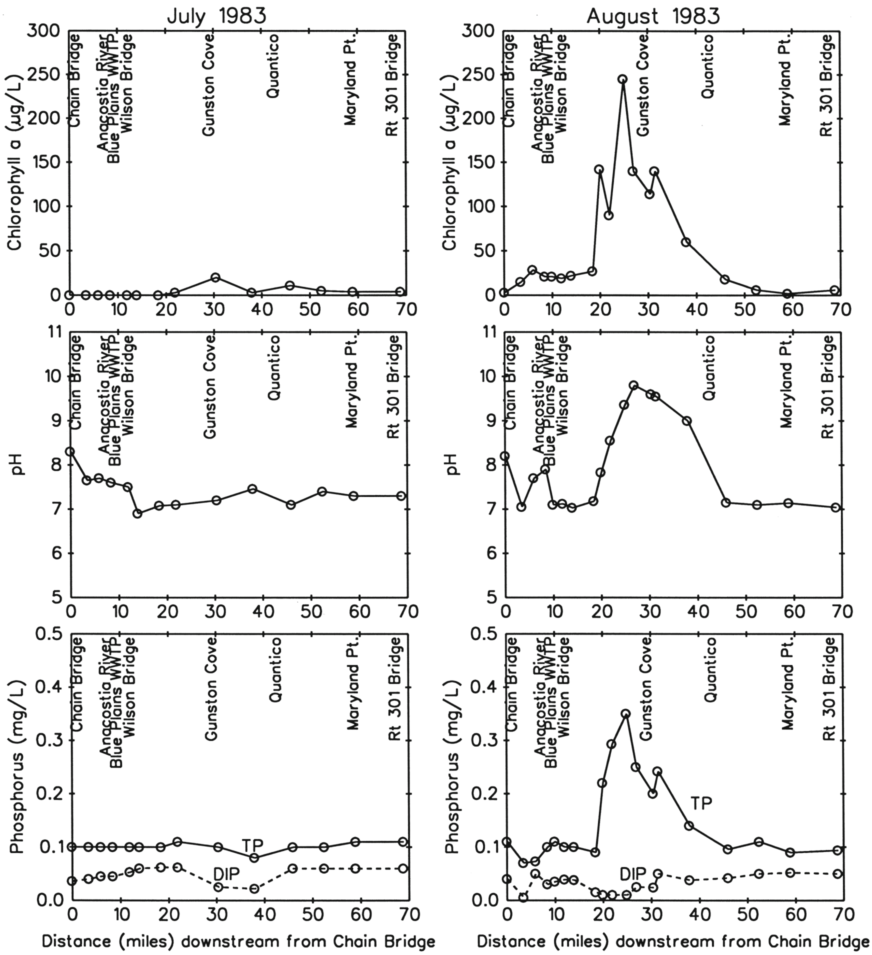

Fig. 1.2 Chlorophyll *a*, pH, and phosphorus levels in summer 1983

the pH was generally below 7.5 between milepoints 25 and 40, while during August and September the pH rose to above 9.0 and was as high as 10.0 in this region. The TP shows a relatively flat profile for July followed by a sharp rise in TP between milepoints 20 and 40.

The preceding hypothesis by Di Toro and Fitzpatrick (1984) supported by the high pH in the Potomac Estuary in August 1983, may have resulted in a subsequent high aerobic phosphorus release from the sediment. By reproducing the environmental conditions (i.e. high pH in the aerobic overlying water) for the sediment from the Potomac Estuary, Seitzinger (1983, 1984, 1985) was able to measure an aerobic release flux of phosphorus matching the range of 4000–8000 lbs/day, thereby confirming the aerobic release from the sediment under high pH conditions.

1.4 Impact of Nitrification in Wastewater

Since the pH levels recorded in 1983 were among the highest ever measured in the Potomac Estuary, the next question then to be asked is "Why was the pH unusually high in 1983?" What was different between that year and previous years? The high pH in 1983 leads one to examine the alkalinity of the estuary since alkalinity is the acid-neutralizing capacity of a system. Because the photosynthetic reaction removes CO_2 from the water with a potential increase in pH, the resulting actual pH change will depend on the initial alkalinity (Stumm and Morgan 1996). The most readily identifiable difference in the structure of the estuary system between 1983 and earlier years is that by 1983 nitrification facilities were on line at the Blue Plains WWTP, the major point source input (Thomann et al. 1985). Nitrification reduces the alkalinity of the effluent and therefore alkalinity changes may be a result of treatment practices.

Figure 1.3 shows the longitudinal profiles of alkalinity levels for several years from 1969 to 1983. These latter data for 1982–83 show that since the late 1970s there has

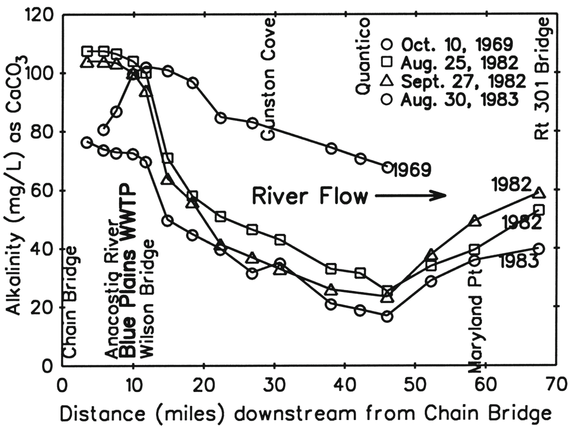

Fig. 1.3 Historical alkalinity trend in the Potomac River estuary

been a significant change in the alkalinity of the waters of the estuary. During the summer months of 1983, the alkalinity of the water entering the estuary from the upper watershed ranged from 80 to 110 mg/L as $CaCO_3$. The alkalinity coming from wastewater treatment plant discharges might be expected to increase the alkalinity of the upper estuary usually by about 20 mg/L above the alkalinity from the upper basin. With the installation of nitrification at the Blue Plains WWTP, the alkalinity mass has been significantly reduced (see Tables 1.1 and 1.2). The nitrification process consumes alkalinity in the water column as presented in the carbonate equilibrium (see Chap. 5 acidification modeling). Such treatment generally uses about 7.14 mg/L alkalinity per mg/L ammonia nitrogen oxidized (Thomann et al. 1985). These data suggest that the buffering capacity of the estuary has been reduced and that this may be related to the operation of the nitrification process.

Table 1.1 Alkalinity mass in the upper Potomac estuary (Thomann et al. 1985)

Sampling date	River flow (cfs)	Estimated wastewater alkalinity (lb/day)	Alkalinity mass in upper 30 miles (lbs)
10/10/1969	2100	369,000	49,380,000
8/22/1977	1600	323,000	45,170,000
8/25/1982	4200	250,000	37,968,000
9/27/1982	1800	250,000	29,430,000
7/5/1983	6140	140,000	37,224,000
8/30/1983	1900	140,000	24,820,000

Table 1.2 Monthly average alkalinity (mg/L) as $CaCO_3$ in blue plains WWTP effluent (Thomann et al. 1985)

Month	1975	1978	1980	1981	1983	1984
Jan		91	105	131	33	29
Feb		101	123	103	37	33
Mar		102	115	87	26	36
Apr		116	100	84	30	33
May	93	112	105	95	27	39
Jun	128	113	117	76	26	54
Jul	107	99	112	88	35	51
Aug	124	99	110	61	47	44
Sep	101	120	116	85	51	70
Oct	111	143	120	98	60	76
Nov	123	148	120	108	43	
Dec	120	118	110	113	31	
Avg	113	114	113	94	37	47

Prior to the 1980s, most of the nitrogen discharged was in ammonia form. Ammonia was oxidized bacterially to nitrates, potentially creating about 250,000 lbs/day of acid. However, the utilization of nitrates by algal cells resulted in the production of alkalinity about equal to that of acid produced by the bacterial oxidization of ammonia, and thus no change in either alkalinity, pH, or the buffering capacity took place. Beginning in the early 1980s, most of the wastewater ammonia was nitrified at the WWTPs and thus a potential acidic load to the estuary was removed. Therefore, one would have anticipated that alkalinity in the upper estuary in 1982 and 1983 would have increased due to increased alkalinity by the production of alkalinity when the algal cells assimilated the nitrates in the estuary. This increase did not occur. In fact, there was a net further reduction in the buffering capacity in the estuary. Why?

The additional reduction in alkalinity may be related to the low pH and low alkalinity in the wastewater effluents, especially at the Blue Plains WWTP. There could have been some iron discharged from the Blue Plains WWTP, which further decreased that alkalinity when the iron in the wastewater discharge mixed with receiving waters and precipitated into the sediment.

It has been well established that bicarbonate content determines whether natural waters are well or poorly buffered (Ruttner 1963). Carbonate-carbonic acid mixtures have a remarkable and important characteristics of preventing major fluctuations in pH when reacting with other acid-salt combinations. The pH of water is determined by the reaction between CO_2 and carbonate, more specifically, by the H^+ ions arising from the dissociation of H_2CO_3 and OH^- ions arising from the hydrolysis of bicarbonate. In well-buffered water the change in pH due to the addition of either an acid or base is very small in proportion to the amount of acid or base added.

1.5 Environmental Conditions to Kick-Off the Bloom

Thomann et al. (1985) pointed out the following observations related to the summer 1983 algal bloom in the Potomac River:

1. River flows were 30–80% of normal
2. Percent sunshine ranged from 70 to 80%, generally higher than in previous years
3. Wind speed averaged about 6.5 miles per hour, significantly lower than in previous years
4. Two-dimensional estuarine mass transport.

With the low flows, adequate nutrients, and ideal environmental conditions, an initial algal bloom began in July and early August of 1983. This initial algal bloom reduced the amount of carbon dioxide and bicarbonate, thereby further increasing the pH. The lack of buffering capacity allowed the pH to increase significantly in the upper estuary from milepoint 20 to 40 in the reach where the initial bloom was observed. Once the enhanced bloom began, the pH increased to over 9.5. At this pH level, the release of both nitrogen and phosphorus from the sediments was significantly enhanced, thus self-perpetuating the blooms. In previous years when blooms occurred, the pH did not increase over 8.0. However, in 1983, the pH increased from about 7.0 near Woodrow Wilson Bridge (MP 12) to over 9.5 between MP 25–30 (Fig. 1.2). These are the areas where the highest concentrations of phosphorus were measured in late August 1983.

The investigation team also summarized the impact of the two-dimensional mass transport in the Potomac Estuary on the initiation of the algal bloom as follows (Thomann et al. 1985). Increased spring runoff into the estuary followed by a rapid decline in flow in mid-July of 1983 resulted in increased stratification in the water column and strength of the lower estuary circulation. Sediment release point at the end of the salinity intrusion acts as a source for the stimulation of phytoplankton in this area. The phosphorus source is further enhanced by anoxic conditions in the lower reaches. Both nitrogen and phosphorus sources at the end of the salt-water intrusion are also enhanced by particulate associated nutrients being recycled in a manner similar to the "turbidity maximum" phenomena. Settling rates of particulates, including phytoplankton, are impeded (or may even be reversed) by vertical velocities in the salinity intrusion area and hence may remain in the water column (i.e., not settled into the sediment). The ability to calculate these phenomena via a one-dimensional model with longitudinal dispersion in the PEM may be inadequate, as it does not capture this complex downstream hydrodynamic circulation.

1.6 Model Enhancement

While results from the PEM with the support of water quality data had led to the discovery of the additional phosphorus loads needed to sustain the algal bloom, the missing mechanism of aerobic phosphorus release under high pH conditions would need to be included in the model for future use. The following mechanisms are therefore required to refine the PEM:

1. Aerobic phosphorus release under high pH levels
2. pH-alkalinity equilibrium in the water column to model pH, alkalinity, and acidity
3. Two-layer mass transport.

While much discussion has focused on the first two items, the unique two-dimensional estuarine mass transport must be factored in as well. Particulate matter discharged to the estuary (and the nutrient associated with the particles) settles from the upper layer to the lower layer in the water column. It is then transported upstream to a convergence region where vertical transport of the solids occurs; a "turbidity maximum" occurs in the area near the limit of salinity intrusion. This phenomenon has been studied in some detail with respect to the suspended solids in estuaries (Thomann et al. 1985). Lung and O'Connor (1984) and O'Connor and Lung (1981) gave a comprehensive analysis on turbidity maximum for a number of estuaries in the U.S. (see Sect. 4.5). The Patuxent Estuary model by Lung and Nice (2007) is another example of this two-dimensional mass transport affecting nutrient remaining in suspension near the location of the turbidity maximum. It is clear that the location of turbidity maximum is where the chlorophyll *a* peak occurs in the Potomac Estuary (between MP 20–30). The original PEM was a one-dimensional segmentation with lateral (vertically mixed) side segments for embayments, and therefore incapable of mimicking the two-dimensional mass transport; the original PEM must be upgraded to account for this phenomenon.

1.7 Summary and Conclusions

The initial effort of reproducing the 1983 bloom failed with the PEM. However, a closer look at the model results helped to identify missing phosphorus source(s) in the Potomac Estuary. Further, the modeling analysis was able to quantify the amount of missing phosphorus loads needed to substantiate the bloom in the summer of 1983. Once again, the importance of water quality data could not be underestimated. The interplay of modeling results and data eventually led to solving this mystery; neither modeling nor data alone was the silver bullet to the investigation.

The 1983 Potomac Estuary algal bloom investigation turned out to be an interesting scientific probe. The investigative panel consisted of leading scientists on phytoplankton and algal bloom, with specific expertise on blue-green algae and the Potomac Estuary. Their systematic efforts led by Thomann identified the cause of the bloom. Continued probing with the aid of the PEM provided answers to additional questions on the bloom.

Note that the sophistication of the PEM in the 1980s is no match with today's water quality modeling frameworks. The spatial discretization of the PEM was limited due to computation power at that time. None of these matter in this case, however. The failure of the original PEM to capture the bloom intensification in August and September is a clear example where mechanisms not included in a model formulation become apparently significant after some level of treatment (phosphorus removal and nitrification in this case) had been installed (Thomann and Mueller 1987). Some of the highly used modern models do have these features.

The inability of PEM to capture the bloom intensification in 1983 does not suggest that eutrophication modeling is of little value. On the contrary, the PEM provided one of the more important bases to zero in on the hidden mechanism and missing source of phosphorus. The key to this successful investigation proved to be the high caliber investigative panel members, who relied as much on water quality data as the supporting modeling analysis. Water quality modeling is not just pushing buttons. Physical insights into the system uncovered by the investigation team were the most important asset. The serendipitous outcome of this example is turning the water quality model that does not work into water quality modeling that works. In addition, water quality modeling must be supported by two pillars: research (science) and monitoring (data), which are the center of discussions in this book.

1.8 Setting the Stage for This Book

It is the author's strong conviction that responding to the challenges in modeling for water quality management is not about using the most sophisticated models. Rather, the modeler's skill and data support are of the utmost importance for overcoming any challenges. Therefore, this book will not discuss water quality modeling frameworks, either proprietary or freely distributed codes. Instead, this book promotes the approach of emphasizing modeling analysis with strong support of field data. Running models without data support, with very few exceptions, is totally meaningless and a waste of time. In addition, we repeatedly demonstrate physical insights into the modeled system and its key mechanisms throughout this book. We do not run models simply because we want to. We do modeling for a very practical mission; to provide answers to decision makers for developing water quality management strategies. This book is designed to help modelers with the necessary skills to fulfill this mission and to address the challenge: What if the model results do not reproduce the data?

Data analysis is a first task that many water quality modelers often neglect to perform prior to the modeling analysis. The significance of performing a thorough data analysis is two-fold: it not only provides significant insight into the interaction of the water quality constituents, but also enables a water quality modeler to conceptualize the formulation of this proposed "model." This is significant because a water quality model of a given system is developed progressively, within the modeler's mind. The data analysis portion, contained in the second chapter of the book, sends a strong message to the reader: data analysis is critical to the success of water quality modeling.

The first two water quality endpoints addressed in this book are DO and chlorophyll *a*. The impairment of DO is caused by BOD, a conventional pollutant. Given the many new twists presented by BOD in modern day stream modeling, this topic deserves renewed attention and re-focus, particularly as it relates to polluted streams by highly intense discharges one after another along the streams. Despite the long history of controlling problems arising out of DO, which are connected intimately with primary productivity and sediment effects, problems arising from DO still tend to be considerably more complex than generally believed by Thomann (1987). Next is the water quality issue of nutrient/eutrophication, which is not only tied to the DO endpoint, but also leads to the chlorophyll *a* endpoint. The problems related to nutrient/eutrophication are the most difficult models with which we have encountered due to complexity of the plant biology, the non-linear interactions between nutrients and aquatic plants, and the interactions of the sediment (Thomann 1987). The case studies presented in the following sections represent a unique and interesting modeling analysis to resolve eutrophication problems.

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Chapter 2
Data Analysis

A data analysis serves many roles in supporting water quality modeling. At a minimum, it can be a simple task of examining available data to get a preliminary understanding of the water system. Next, a data analysis prior to selecting and configuring modeling framework(s) is a necessary step in modeling for water quality management. A complete understanding of the system to be modeled is essential to setting up the model with the available data. Furthermore, some key processes can be independently quantified (i.e. assigning model coefficient values) prior to model configuration. Third, a data analysis also compiles necessary information for model calibration and verification. At the fullest extent, the modeler could gain additional physical insights into the system via an interplay between model results and data. Many model input elements ranging from environmental conditions, hydrological conditions, mass transport coefficients, to kinetics parameters can be independently derived from a data analysis prior to model configuration. This chapter presents a wide spectrum of data analyses ranging from a simple review of existing data to derivation of model coefficients associated with physical, chemical, and biochemical processes. A properly performed data analysis could also identify data gaps needed for fine tuning the model. Through these examples, the importance of this often neglected task will be demonstrated.

2.1 Data Screening—Lake Peipsi and Vrhovo Reservoir

Under the North Atlantic Treaty Organization (NATO) Committee on the Challenges of Modern Society (CCMS), an ecological system modeling study of coastal lagoons was launched in 1998. The University of Virginia (UVa) participated to provide water quality expertise to the program. Waters from the Baltic States provided some interesting sites for application of water quality modeling to assist the management of these water bodies. Lake Peipsi, the largest trans-boundary lake in Europe, lying on the border between Estonia and Russia in northeast Estonia (see Fig. 2.1) was

W.-S. Lung, *Water Quality Modeling That Works*,
https://doi.org/10.1007/978-3-030-90483-8_2

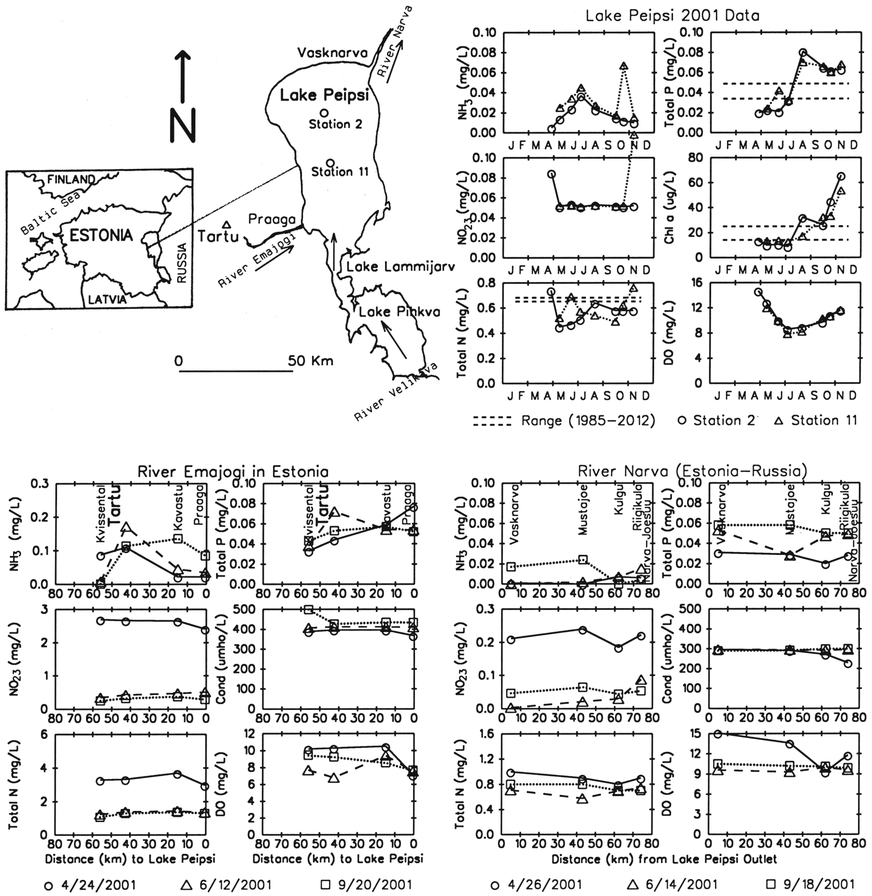

Fig. 2.1 Water quality of Lake Peipsi, River Emajogi, and River Narva

one of the water systems selected for a preliminary water quality screening. As the fifth largest lake in Europe, it has a surface area of 3555 km^2 with a mean depth of 8.3 m. With a volume of 25 km^3 and an annual average flow of 265 m^3/s (cms), the lake has a residence time about 3 years. This flow comes from watersheds of River Emajogi (30%) in Estonia and River Velikaya (70%) in Russia. River Velikava flows into Lakes Pihkva and Lammijarv, which in turn discharge into Lake Peipsi. The lake has been widely studied for eutrophication concerns (Kangur et al. 2003; Noges et al. 2004; Kangur and Mols 2008; Buhvestova et al. 2011; Blank et al. 2017). The 2001 water quality data of Lake Peipsi, River Emajogi (major inflow), and River Narva (lake outflow) were made available by Ministry of the Environment for the review. Figure 2.1 presents data of key water quality constituents for Lake Peipsi, River Emajogi (the feeding stream), and River Narva (the outflow waterway), respectively, from surveys in April, June, and September of 2001.