SECOND EDITION

HYDRODYNAMICS AND WATER QUALITY

Modeling Rivers, Lakes, and Estuaries

ZHEN-GANG JI

with website

WILEY

Hydrodynamics and
Water Quality

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Modeling Rivers, Lakes, and Estuaries

Zhen-Gang Ji

Second Edition

WILEY

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In memory of Dr. John M. Hamrick for his important contributions to the modeling of surface waters.

Contents

Preface to the Second Edition

The first edition of this book was successful and well received by the environmental and water resources community. It is extremely gratifying to see that both the English edition and the Chinese edition have become an essential reference for practicing engineers, scientists, and water resource managers, as well as an excellent text for advanced undergraduate and graduate students in engineering and environmental sciences.

As mentioned by Singh (2009) while reviewing the first edition: “On the whole, the topics are well organized, the prose is easy to read and understand, the style is lucid, and there is a wealth of information reflecting the knowledge and experience of the author. The book will also be useful to practicing water and environmental engineers.” The same strategy and style have been continued and strengthened in the second edition.

Multidisciplinary modeling has increased dramatically in the past decade, so is the need for an intergraded coverage of these disciplines. The increase in computer power, involving the use of parallel computing, has made it possible to run comprehensive hydrodynamic and water quality models time and cost effectively. The objective of this book is to present an integrated coverage of hydrodynamics, sediment processes, toxic fate and transport, and water quality and eutrophication in surface waters, including rivers, lakes, estuaries, coastal waters, and wetlands.

This book is about processes and modeling these processes. It is not about models. Detailed discussions on models are referred to their manuals and reports and are minimized in this book. The theories, processes, and modeling of these processes presented in this book are generally applicable to numerical models, not just a particular model. This book illustrates the principles, basic processes, mathematical descriptions, and practical applications associated with surface waters. Instead of trying to give detailed coverage of every aspect of surface water processes and their mathematical descriptions, this book focuses on solving practical problems in surface waters.

In the 8 years since the first edition was published, I have received numerous comments from readers on the book and suggestions on how it could be improved. I have also built up a large amount of new materials based on my own experience in research and teaching. With the aid of all this information, I have made the changes and additions in the second edition. All chapters have been revised and updated with works published in the recent years. Compared with the first edition, the second edition has contents increased by more than 40%, including more than 120 new/updated figures and nearly 450 new references. More specifically, the second edition adds the following:

1) A new chapter on wetlands. This chapter focuses on shallow water processes in wetlands and the simulation of these processes with surface water models.
2) A new chapter on risk analysis. This chapter is devoted to two essential and interrelated topics: extreme value theory and environmental risk analysis.
3) A new section on the impact of wind waves on sediment transport.
4) A new section on the mathematical representation and multi-year modeling of submerged aquatic vegetation.
5) A new section on the long-term variation and simulation of pollutants in a lake.
6) A new section on the water quality modeling of a shallow estuary.
7) A new appendix on the EFDC_Explorer, which is a Windows-based graphic user interface (GUI) for pre and postprocessing of the Environmental Fluid Dynamics Code (EFDC).
8) A new website for the book (www.wiley.com/go/ji/hydrodymanics_water_quality). It includes sample applications that are discussed extensively in this book, including their source codes, executable codes, input files, output files, and some results in animations. These applications illustrate the modeling of a channel, a river, an estuary, and a lake, respectively. The website also contains model manuals, reports, technical notes, and utility programs.

I would like to thank all those who showed a steady, extraordinary interest in this book. They gave me the motivation, courage, and opportunity to undertake the challenge of a new edition. The book has also benefited from my teaching at the Catholic University of America and inputs from my students. Jianping Li and his team translated the first edition into Chinese and gave insightful comments on how to improve the book. Working with the Wiley staff was once again a pleasure. I thank, in particular, my editors, Bob Esposito and Vishnu Narayanan.

September 2016 *Zhen-Gang Ji*
Fairfax, Virginia

Reference

Singh, V.P. (2009) Review of hydrodynamics and water quality: modeling rivers, lakes, and estuaries by Zhen-Gang Ji: Wiley Interscience, John Wiley & Sons, Inc., 111 Rivers Street, Hoboken, NJ 07030; 2008; 676 pp. ISBN: 978-0-470-13543-3. *Journal of Hydrologic Engineering*, **14** (8), 892–893.

Foreword to the First Edition

The management of surface water resources is essential for human and ecosystem health and social and economic growth and development. Water resources professionals use a wide range of technical management tools firmly based on the physical, biological, mathematical, and social sciences. This work addresses the fundamental physical and biological processes in surface water systems that provide the basis for both deeper understanding and management decision making. The complexity of the natural surface water environment combined with the ever-increasing capabilities of computers to simulate the temporal evolution of systems represented by differential equations has made hydrodynamic and water quality models essential tools for both science and management. Although the present work discusses modeling and presents case studies involving model applications, the author has appropriately chosen to emphasize processes and their commonality and differences between different surface waterbody types.

This book is organized as follows: An introductory chapter precedes four chapters on fundamental hydrodynamic and water quality processes, followed by two chapters that discuss modeling in the context of regulatory programs and model credibility and performance. The book concludes with three chapters on rivers, lakes, and coastal waterbodies. The overarching emphasis of the presentation is the interaction of hydrodynamic and water quality or physical and biogeochemical processes. Chapter 2 presents the fundamentals of surface water hydrodynamics in the context of the three-dimensional (3D), Reynolds-averaged, hydrostatic, or primitive equations of motions, as well as related dimensionally reduced formulations including the shallow-water and St Venant equations. The understanding of and ability to predict surface water hydrodynamics is important in its own right, addressing topics including riverine floods, water supply reservoir operations, coastal surges, and estuarine salinity intrusion. It readily follows that the physical transport and fate of dissolved and suspended materials is governed by hydrodynamic advection and turbulent diffusion. The term "water quality" is used in two general contexts in this book as well as in current professional practice. The most general context includes the presence and behavior of dissolved and suspended materials in amounts undesirable for human and ecosystem health, as well as agricultural and industrial use. The more limited historical context, often referred to as "conventional water quality," addresses pathogenic organisms and dissolved oxygen dynamics including eutrophication and aquatic carbon, nitrogen, and phosphorous cycles.

The remaining three process-oriented chapters address three broad water quality categories: sediment transport, toxic contaminants, and eutrophication. Sediment transport, which is also important in water supply and navigation, has important water quality implications related to water clarity, habitat suitability, and its ability to transport adsorbed materials. The chapter on toxic contaminants provides an overview of the transport and fate of heavy metals and hydrophobic organic compounds, both of which adsorb to inorganic and organic sediments. The final process chapter presents the traditional water quality or water column eutrophication process formulations, as well as the associated remineralization or diagenesis of settled organic material. The presentation of process formulations in these four chapters is complemented by the inclusion of illustrative results from actual studies.

Many scientific and engineering studies of surface water systems are in response to regulatory requirements directed at protecting human and aquatic ecosystem health. In the United States, the major regulatory programs include the National Point Discharge Elimination System (NPDES), total maximum daily load (TMDL), and Superfund Remedial Investigation/Feasibility Study (RI/FS). Chapter 6 provides an overview of the role of hydrodynamic and water quality modeling in TMDL development, which leads to the following chapter on model performance evaluation.

The use of models for decision making requires the establishment of the model's scientific credibility using accepted quantitative methods, which are outlined in Chapter 7. The book concludes by focusing on specific aspects of three major groups of surface water systems: streams and rivers, lakes and reservoirs, and estuaries and coastal regions. Many of the example case studies are based on the author's professional experience. These case studies, as well as those integrated into earlier chapters, provide excellent guidance in the organization and execution of hydrodynamic and water quality studies.

In *Hydrodynamics and Water Quality*, Dr Ji has produced a work that should be an essential reference for practicing engineers, scientists, and water resource managers, as well as a text for advanced undergraduates and graduate students in engineering and environmental sciences. The author has brought extensive professional experience and insight to the field, and it has been my pleasure to have worked and collaborated with him over the past decade.

Tetra Tech, Inc. *John M. Hamrick*
Fairfax, VA

Preface to the First Edition

The objective of this book is to present an integrated coverage of hydrodynamics, sediment processes, toxic fate and transport, and water quality and eutrophication in surface waters, including rivers, lakes, estuaries, and coastal waters. The book is intended to serve as a reference book for graduate students and practicing professionals with interest in surface water processes and modeling. Mathematical modeling of surface waters has made great progress in past decades and has become a powerful tool for environmental and water resources management. There are growing needs for integrated, scientifically sound approaches that identify surface water problems and simulate these waterbodies numerically.

This book illustrates principles, basic processes, mathematical descriptions, and practical applications associated with surface waters. Instead of trying to give detailed coverage of every aspect of hydrodynamics, sediment transport, toxics, and eutrophication processes, this book focuses on solving practical problems in rivers, lakes, estuaries, and coastal waters. After Chapter 1 (Introduction), each of the next five chapters (2–6) is devoted to one basic and important topic: hydrodynamics, sediment transport, pathogens and toxics, water quality and eutrophication, and external sources and total daily maximum load (TMDL), respectively. Chapter 7 provides general discussions on mathematical modeling and statistical analysis. Based on the theories and processes presented in Chapters 2–7, rivers, lakes, and estuaries and coastal waters are discussed in Chapters 8, 9, and 10, respectively. Each chapter (after Chapter 1) is organized as follows: it begins with an introduction of basic concepts, proceeds to discussions of physical, chemical, and/or biological processes and their mathematical representations, and concludes with case studies. Organizing the book in this application-oriented approach allows readers to easily locate information that is needed for their studies and to focus on the relevant chapters/sections.

Most of the theories and technical approaches presented in the book have been implemented in mathematical models and applied to solve practical problems. Throughout the book, case studies are presented to demonstrate (1) how the basic theories and technical approaches are implemented into models, and (2) how these models are applied to solving practical environmental/water resources problems. These examples and cases studies are based on either simplified analytical solutions or my professional practice.

A memorable quote from the James Bond movie *From Russia with Love* is that "training is useful, but there is no substitute for experience," which is directly applicable to the modeling of rivers, lakes, and estuaries. Experience is a key element of modeling and is also one of the primary reasons why modeling is often called an "art." The case studies described in detail throughout the book exemplify this premise. A slightly modified version of this quote also perfectly describes the relationship between modeling and field sampling: *modeling is useful, but there is no substitute for field sampling*. Law ordains that a person is innocent until proven guilty. A numerical model (and its results), in my opinion, is guilty until proven innocent by data. This highlights the importance of calibrating models against measured data.

This book is about processes and modeling these processes. It is not about models. Detailed discussions on models are referred to their manuals and reports and are minimized in this book. The theories, processes, and modeling of these processes presented in this book are generally applicable to numerical models, not just a particular model. It is my intention to make the book unique in three ways:

1. This book will cover state-of-the-art hydrodynamics, sediment transport, toxics fate and transport, and water quality in surface waters in one comprehensive text. In the past 10 years, environmental engineering, water resources engineering, and computer engineering have changed dramatically, especially with respect to progress in mathematical models and computer technology. Comprehensive mathematical models are now routinely used in solving practical engineering problems. This book provides essential and updated information.

2. Instead of trying to cover every detail of hydrodynamics, sediment transport, toxics, and water quality, this book will focus on how to solve practical problems in surface waters. Basic theories and technical approaches are presented, so that mathematical models can be understood and applied to simulate processes in surface waters. From the book, readers will not only understand basic principles but also learn how to use the models/tools to solve their problems in professional practice. Information is presented only on a need-to-know basis. For example, tides, salinity, and open boundary conditions are not discussed until Chapter 10, where estuaries and coastal waters are covered, since these topics are more likely to be relevant in the modeling of estuaries rather than of rivers or lakes.
3. A modeling package on a CD, including electronic files of numerical models, case studies, and model results, is attached to the book. Relevant user manuals and technical reports are also available. This becomes helpful when a reader plans to use the models and tools described in the book to solve practical problems in surface waters. The input files of the case studies described in the book can also serve as templates for new studies.

June 15, 2007
Fairfax, Virginia

Acknowledgments for the First Edition

Many people have contributed to this book over the years that it has taken to write. My former and present colleagues provided great support and encouragement in my professional career and while I was drafting the manuscript, including Robert LaBelle, James Kendall, and Walter Johnson of Minerals Management Service; James Pagenkopf and Leslie Shoemaker of Tetra Tech; Alan Blumberg of HydroQual; and George Mellor of Princeton University. Professor Cesar Mendoza, my former advisor at Columbia University, helped me in revising the manuscript. Professor Ji-Ping Chao of National Marine Environmental Forecast Center, China, guided me through my early years of scientific research.

I would like to thank the colleagues and friends who took time from their work to review the chapters of this book. Their comments and advice added to the usefulness of the book. I would like to acknowledge their thoughtful reviews of the manuscript and discussions over the years with them. I am most grateful to Yi Chao (Jet Propulsion Laboratory), Sayedul Choudhury (George Mason University), Tal Ezer (Old Dominion University), Weixing Guo (Schlumberger Water Services), Earl Hayter (US Environmental Protection Agency), Michio Kumagai (Lake Biwa Environmental Research Institute, Japan), Chunyan Li (Louisiana State University), Cesar Mendoza (University of Missouri-Rolla), Leo Oey (Princeton University), Kyeong Park (University of South Alabama), Jian Shen (Virginia Institute of Marine Science), Andy Stoddard (Dynamic Solutions), Dong-Ping Wang (State University of New York at Stony Brook), Tim Wool (US Environmental Protection Agency), Yan Xue (National Oceanic and Atmospheric Administration), Zhaoqing Yang (Battelle Marine Sciences Laboratory), Kirk Ziegler (Quantitative Environmental Analysis), and Rui Zou (Tetra Tech).

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My gratitude also goes to Mac Sisson (Virginia Institute of Marine Science) and Sharon Zuber (College of William and Mary) who carefully edited the entire manuscript. Wei Xue provided assistance in drawing some of the graphics. I would also like to thank Bob Esposito (John Wiley & Sons, Inc.) for his help in publishing this book and Kenneth McCombs (Elsevier) for initiating and encouraging me to start this long journey of book writing.

Last, but not least, I would like to express my deepest gratitude to my wife (Yan) and our two daughters (Emily and Tiffany). Their encouragement and support, as well as their tolerance of my long hours, made this book a reality. Also, I would like to thank the grandparents who helped us in raising our daughters and encouraged me to do my best in my career.

Abbreviations

ADCP	acoustic Doppler current profiler
AOCR	dissolved oxygen/carbon ratio
Bbbl	billion barrels
bbl	barrels
BC	boundary condition
BOEM	Bureau of Ocean Energy Management
BRI	Blackstone River Initiative
BS	boundary segment
CBOD	carbonaceous biochemical oxygen demand
CDOG	Clarkson Deepwater Oil & Gas
CDF	cumulative distribution function
CERP	Comprehensive Everglades Restoration Program
cfs	cubic feet per second
Chl *a*	chlorophyll *a*
cms	cubic meters per second
C.L.	confidence limit
COD	chemical oxygen demand
CSOD	carbonaceous sediment oxygen demand
CWA	Federal Clean Water Act
1D, 2D, 3D	one-, two-, three-dimensional
DA	drainage area
DIN	dissolved inorganic nitrogen
DDT	dichlorodiphenyltrichloroethane
DIP	dissolved inorganic phosphorus
DM	dissolved matter
DMR	discharge monitoring reports
DO	dissolved oxygen
DOC	dissolved organic carbon
DON	dissolved organic nitrogen
DOP	dissolved organic phosphorus
DWH	Deepwater Horizon oil spill
ECMWF	European Center for Medium Range Weather Forecasting
E. coli	*Escherichia coli*
ECOM	Estuarine, Coastal, and Ocean Model
EFDC	Environmental Fluid Dynamics Code
EIS	environmental impact statement
EOF	empirical orthogonal function
EPA	US Environmental Protection Agency
ERA	environmental resource area
ET	evapotranspiration
EVT	extreme value theory
FDEP	Florida Department of Environmental Protection
Fcb	fecal coliform bacteria
FFT	fast Fourier transform
FPIP	fraction of predated phosphorous produced as inorganic phosphorus
GEV	generalized extreme value
GLS	grouped land segment
GOM	Gulf of Mexico
GPD	generalized Pareto distribution
GUI	graphic user interface
GPC	Game and Parks Commission
HSPF	Hydrologic Simulation Program-FORTRAN
iid	independently and identically distributed
IPCC	Intergovernmental Panel on Climate Change
IRL	Indian River Lagoon
LA	local allocations
LHS	left-hand side
LOEM	Lake Okeechobee Environmental Model
LNG	liquefied natural gas
LPOC	labile particulate organic carbon
LPON	labile particulate organic nitrogen
LPOP	labile particulate organic phosphorus
LS	land segment
MAE	mean absolute error
Mbbl	thousand barrels
ME	mean error
ML	maximum likelihood
MMbbl	million barrels
MOS	margin of safety
MPN	most probable number
MRRE	mean relative RMS error
MSL	mean sea level
N	nitrogen
NBOD	nitrogenous biochemical oxygen demand
NDEQ	Nebraska Department of Environmental Quality
NH_4	ammonia nitrogen
Nit	nitrification rate

NO_3	nitrate nitrogen
NOAA	National Oceanic and Atmospheric Administration
NPDES	National Pollutant Discharge Elimination System
OBC	open boundary conditions
OCS	Outer Continental Shelf
ON	organic nitrogen
OP	organic phosphorus
OSCAR	oil spill contingency and response
OSRA	oil spill risk analysis
P	phosphorus
PAH	polycyclic aromatic hydrocarbons
PBAPS	Peach Bottom Atomic Power Station
PC	personal computer; principal component
PCB	polychlorinated biphenyls
PCS	Permit Compliance System
PDF	probability density function
pH	power of hydrogen
PM	particulate matter
PO_4p	particulate phosphate
PO_4d	dissolved phosphate
PO_4t	total phosphorus
POM	Princeton Ocean Model
PON	particulate organic nitrogen
POT	peaks-over-threshold
PP	probability–probability
ppb	parts per billion
ppt	parts per thousand
PROFS	Princeton Regional Ocean Forecast System
QQ	quantile–quantile
RAE	relative absolute error
RHS	right-hand side
RMS	root-mean-square
RMSE	RMS error
ROMS	Regional Ocean Modeling System
RPD	rooted plant shoot detritus
RPE	rooted plant epiphyte
RPOC	refractory particulate organic carbon
RPON	refractory particulate organic nitrogen
RPOP	refractory particulate organic phosphorus
RPR	rooted plant root
RPS	rooted plant shoot
RRE	relative RMS error
SA	available silica; surface area
SAV	submerged aquatic vegetation
SFWMD	South Florida Water Management District
SG	specific gravity
SLE	St. Lucie Estuary
SMB	Sverdrup, Munk, and Bretschneider
SRP	soluble reactive phosphorus
SSC	suspended sediment concentration
SU	particulate biogenic silica
SWAN	Simulation WAve Nearshore
T	transpiration
TAM	total active metal
TDS	total dissolved solids
TKN	total Kjeldahl nitrogen
TMDL	total maximum daily load
TOC	total organic chemicals
TP	total phosphorus
TS	transpiration stream
TSS	total suspended solids
UBWPAD	Upper Blackstone Water Pollution Abatement District
USACE	US Army Corps of Engineers
USGS	US Geological Survey
WLA	waste load allocations

About the Companion Website

This book is accompanied by a companion website

www.wiley.com/go/ji/hydrodynamics_water_quality

The website includes sample applications that are discussed extensively in this book, including their source codes, executable codes, input files, output files, and some results in animations. These applications illustrate the modeling of a channel, a river, an estuary, and a lake, respectively. The website also contains model manuals, reports, technical notes, and utility programs.

1 Introduction

This chapter introduces surface water systems and the modeling of these systems. The contents of this book are also summarized here.

1.1 Overview

Surface water systems are waters naturally open to the atmosphere, such as rivers, lakes, reservoirs, estuaries, and coastal waters. The most common uses of surface waters include the following:

1. Aquatic life support
2. Water supply
3. Recreation such as swimming, fishing, and boating
4. Fisheries
5. Transportation.

People rely on surface waters for recreation, water supply, and fish production (e.g., Fig. 1.1). Surface waters are also critical for the survival of many species. Tens of thousands of birds, mammals, fishes, and other wildlife depend on surface waters as habitats to live, feed, and reproduce.

Rivers are naturally flowing waterbodies. They are a watershed's self-formed gutter system and usually empty into an ocean, lake, or another river. An example is the Illinois River watershed, located in Oklahoma and Arkansas (Fig. 1.2). The watershed acts as a collector of all kinds of water (and pollution) discharges. Lakes (and reservoirs) often act as receiving basins downstream from the surrounding watershed. Lakes modify these inflows from the watershed, serving both as filters and buffers. They retain water, sediment, toxics, and nutrients in response to in-lake hydrodynamic, chemical, and biological processes and dampen the extremes of discharges. Estuaries may also act as filters for the sediment and nutrients discharged from rivers and surface runoff.

Surface waters are at once resilient and fragile. They are constantly changing as a result of both natural and human forces. The ecosystem of surface waters is an interactive system that includes hydrodynamic characteristics (e.g., water depth and flow velocity), chemical characteristics (e.g., solids, dissolved oxygen (DO), and nutrients), and characteristics associated with the biological community of the water column and benthos. Large amounts of nutrients and contaminants enter into a variety of surface waters. Under siege from all directions, the ecosystems often face assault in the form of increasing populations, inadequately planned land use, and pollutants from farms, homes, and factories. Although every surface water system is unique, many face similar environmental problems: eutrophication, pathogen contamination, toxic chemicals, loss of habitat, and decline in fish and wildlife. These problems, in turn, can cause declines in water quality, living resources, and overall ecosystem health.

Table 1.1 is a water budget showing the distribution of water over the earth (Lvovich, 1971). Rivers and lakes, though critical to civilization, contain a very small fraction of the total water budget. The water cycle (also known as the hydrologic cycle) represents the movement and endless recycling of water between the atmosphere, the land surface, and the ground. No matter what water quality problems that an ecosystem is associated with, its water cycle is often a key factor affecting the problems. From raging streams to the slow movement of water through the ground, as illustrated in Fig. 1.3, water is in constant motion. The water cycle begins with water evaporation from the earth's water surface, soil, and plants. The vast majority of evaporation occurs from the oceans. Once in the air, the water vapor is transported by winds and may later condense into clouds. A portion of the water vapor falls to the ground as precipitation in the form of rain or snow.

As precipitation returns water to the land surface, a portion of it seeps into the ground and becomes groundwater. The remaining portion, which does not infiltrate the soil but flows over the surface of the ground to a stream, is called surface runoff. The water flowing through the ground can also return to the surface to supply water to rivers and lakes. All land that eventually drains to a common river or lake is considered to be in the same watershed. By a network of streams that flows into larger and larger streams, the water that is not

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Figure 1.1 A farmer pumps water out of the Nile River, Egypt, for irrigation. *Source:* Photograph by Zhen-Gang Ji.

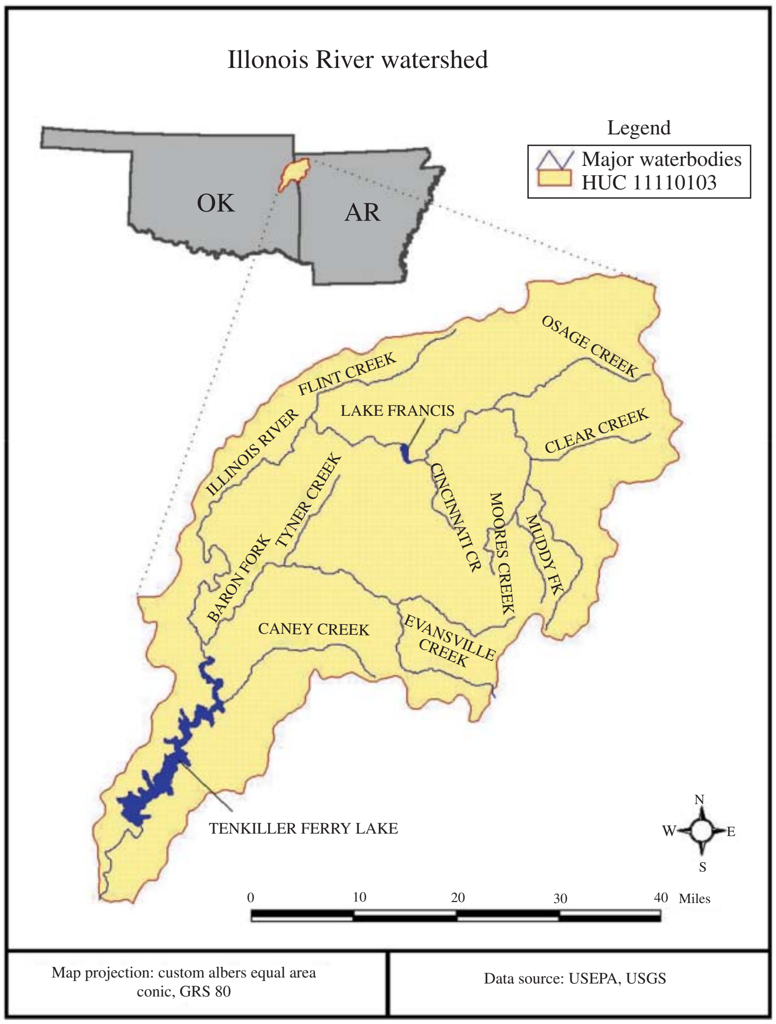

Figure 1.2 Illinois River watershed, Lake Tenkiller drainage basin, the lake, and its main tributaries.

Table 1.1 Distribution of water on earth.

Region	Volume (10^3 km^3)	Percentage (%) of total
Oceans	1,350,000	94.12
Groundwater	60,000	4.18
Ice	24,000	1.67
Lakes	230	0.016
Soil moisture	82	0.006
Atmosphere	14	0.001
Rivers	1	–

Source: Based on Lvovich (1971).

evaporated back into the atmosphere eventually reaches the oceans. Therefore, land use activities in a watershed can affect the water quality of surface waters, such as rivers, lakes, and estuaries, as contaminants are carried by runoff and groundwater to these surface waters. To accurately estimate pollution loadings to a surface water system, the water cycle of the watershed must be considered accordingly.

1.2 Understanding Surface Waters

Surface water systems, such as rivers, lakes, and estuaries, are often closely linked to each other (Fig. 1.4). What happened in a river could potentially affect an estuary/ocean that is far away from the river. Hydrodynamic, sediment, and water quality processes in these systems are complex and need sophisticated tools to represent them. Three important tools used in supporting water quality management are (1) observation, (2) theoretical analysis, and (3) numerical modeling. Although each tool has advantages, each has also certain disadvantages. The appropriate way to apply these tools is to better understand and make use of them according to their properties (Ji, 2004). Also, in the end, the professional judgment of the engineers and the managers inevitably comes into play.

In terms of helping decision makers identify the scope of the environmental problems, reliable measured data are invaluable. Observation is the only way to know the real characteristics of the ecosystem and to provide the basis for theoretical analysis and numerical modeling. Only after certain observations are made can theoretical analysis and numerical modeling help understand the hydrodynamic and water quality processes and produce reliable results for supporting decision making. These processes, in many cases, cannot be described well in mathematical models before they are measured in real waterbodies.

But measured data alone are rarely sufficient to make informed decisions on water quality management plans, especially when it comes to large and complex waterbodies. Because of budget, time, and technical constraints,

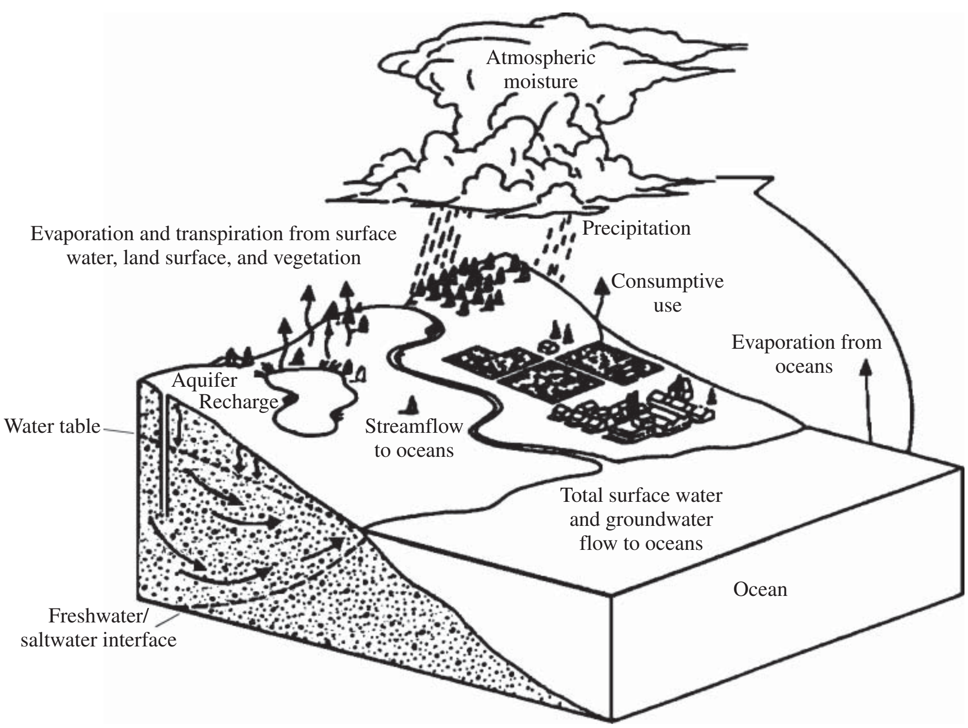

Figure 1.3 Water's natural cycle. *Source:* EHC (1998). Reproduced from Coastal Challenges: A Guide to Coastal and Marine Issues with permission from the National Safety Council's Environmental Health Center, February 1998.

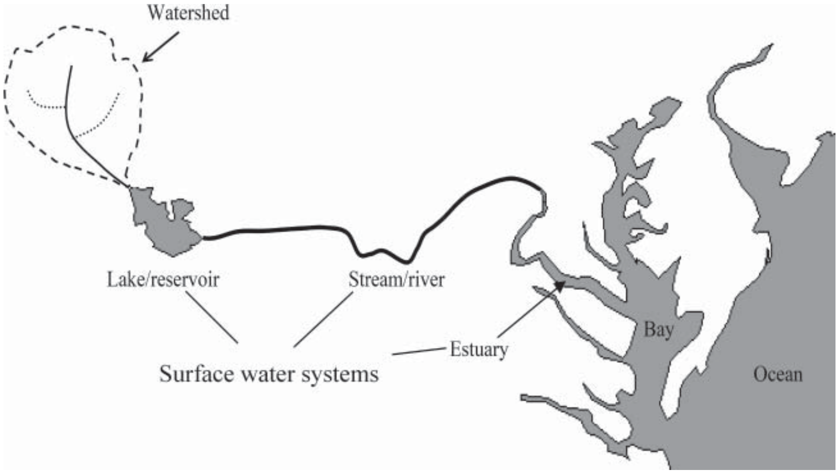

Figure 1.4 Relationship between different surface water systems. *Source:* Based on Kalin and Hantush (2003).

field measurements are often limited to certain small areas (or fixed locations) and within certain periods. Measured data can go only so far in pointing the direction toward sound water quality policies and practices. Further, data errors can result in ambiguous interpretation and misunderstanding of the real physical, chemical, and/or biological processes. In these cases, theoretical analysis and numerical modeling become important. Through calibration and verification, numerical models are capable of realistically representing the hydrodynamic, sediment, toxic, and water quality conditions of the waterbody. The models can then be used as tools to support decision making.

The key parameters used to represent the hydrodynamic and water quality conditions of surface waters include (1) water temperature, (2) salinity, (3) velocity, (4) sediment, (5) pathogens, (6) toxics, (7) DO, (8) algae, and (9) nutrients.

Water temperature is an important parameter representing the conditions of a waterbody. It also affects when animals and plants feed, reproduce, and migrate. Periodic power plant discharges can cause sudden changes in temperature and be disruptive to a local ecosystem. If the water temperature rises too high, the DO level deceases, directly threatening aquatic life and contributing to eutrophication. In estuaries and coastal waters, salinity is a key parameter representing the environmental conditions. Water velocity plays a key role in transporting and mixing water quality variables.

Sediment enters surface waters from many sources and can alter the habitat of benthic organisms once they settle. Sediments can cause siltation in harbors and navigation channels. Sediments cloud the water, making it difficult for plants, such as underwater grasses, to receive sufficient sunlight to survive. Sediments are also important carriers of pollutants. Sediment transport can move the pollutants far away from their sources.

Pathogens, toxic metals, and organic chemicals are often derived from wastewater, farms, and feedlots. They can be transported to beaches and recreational waters, causing direct human exposure and disease. Pathogens may also accumulate in aquatic biota, such as oysters, clams, and mussels, causing disease when consumed by humans.

DO is one of the most important parameters of water quality and is used to measure the amount of oxygen available for biochemical activity in water. Adequate DO concentrations are a requirement for most aquatic animals. The natural balance of DO can be disrupted by excessive wastewater loads of nutrients. Nutrients can come from wastewater treatment plants, fertilizers, and atmospheric deposition. Nutrients are essential for plants and animals, but excessive nutrient loading can cause algae overproduction, disrupting the natural balance. When algae die and decay, they deplete the DO in water.

Water quality management needs information to identify and evaluate various alternatives for achieving economic and water quality goals. Economic goals are often to achieve cost effectiveness, whereas water quality goals are usually set to meet certain water quality standards. The effectiveness of management alternatives may be measured in terms of how well they accomplish these goals. To determine this effectiveness often requires an assessment of the current state of the waterbody and how it has changed over time. Information is needed about the likely response of the waterbody to the management alternatives, such as decreasing nutrient loads from specific sources or increasing water inflows to the ecosystem, which may require a significant amount of infrastructure investment. It is paramount to be able to predict the consequences and effectiveness of the alternatives as accurately as possible, thus incorporating this information into decision making.

Assessing the water quality of a surface water system requires expertise from many disciplines. Although the various processes may be described independently, they interact in complex ways. Multiple disciplines (hydrodynamics, sediment transport, pathogens and toxics, eutrophication, etc.) interact with each other to address water quality objectives. The result is not simply the assemblage of multiple disciplines working independently on a problem. Physical, chemical, and biological processes also vary over a broad spectrum, both in time and space. Spatial variations largely depend on the topography of the waterbody and external loadings. Temporal variations may have long-term (yearly), seasonal (monthly), diurnal (hourly), and short-term (minutes) time scales.

Often, water quality is defined in terms of concentrations of the various dissolved and suspended substances in the water, for example, temperature, salinity, DO, nutrients, phytoplankton, bacteria, and heavy metals. The distribution of these substances has to be calculated by the water quality model. Based on the principle of conservation of mass, the concentration change can be represented simply in a one-dimensional (1D) form (Ji, 2000a):

$$\frac{\partial C}{\partial t} = -U\frac{\partial C}{\partial x} + \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) + S + R + Q \qquad (1.1)$$

where C = substance concentration, t = time, x = distance, U = advection velocity in the x-direction, D = mixing and dispersion coefficient, S = sources and sinks due to settling and resuspension, R = reactivity of chemical and biological processes, and Q = external loadings to the aquatic system from point and nonpoint sources. It would be an oversimplification to say that this book is all about Eq. (1.1), but it is safe to say that this equation includes the major elements of hydrodynamics, sediment, toxics, and eutrophication. Many discussions in this book can be related to this equation directly or indirectly.

The changes in the concentration C in Eq. (1.1) are determined by the following:

1. The hydrodynamic processes control the water depth (D), the advection (represented by the U term), and mixing (represented by the D term), which will be described in Chapter 2.
2. The size and properties of sediment (or particular organic matter) affect the settling and resuspension (represented by the S term), which will be illustrated in Chapter 3.
3. The chemical and biological reactions of pathogens, toxics, and/or nutrients are represented by the R term, which will be presented in Chapters 4 and 5.
4. External loadings from point and nonpoint sources are included by the Q term, which will be elaborated in Chapter 6.

The applications of Eq. (1.1) (and its more complicated versions) to rivers, lakes, estuaries, and wetlands are presented in Chapters 8–11, respectively.

1.3 Modeling of Surface Waters

"Modeling is a little like art in the words of Pablo Picasso. It is never completely realistic; it is never the truth. But it contains enough of the truth, hopefully, and enough realism to gain understanding about environment systems" (Schnoor, 1996). The two primary reasons to conduct modeling are (1) to better understand physical, chemical, and biological processes and (2) to develop models capable of realistically representing surface waters, so that the models can be used to support water quality management and decision making.

The modeling of surface waters is complex and evolving. Presently, the success of a modeling study, especially sophisticated 3D and time-dependent modeling studies, still depends heavily on the experience of the modeler. There is no complete agreement among the professionals regarding the "best" approach to modeling rivers, lakes, estuaries, coastal waters, and wetlands.

Water quality management requires the understanding of the key processes affecting environmental problems in order to evaluate management alternatives. Examples of such environmental problems include the following:

1. Thermal pollution due to power plant discharges
2. Sedimentation in harbors causing siltation and high dredging costs
3. Eutrophication due to excessive nutrient loadings
4. Low DO conditions caused by wastewater discharges
5. Accumulation of toxic materials in the sediment bed.

Water quality management increasingly depends on accurate modeling. This dependence is further amplified by the adoption of the watershed-based approach to pollution control. Models enable decision makers to select better, more scientifically defensible choices among alternatives for water quality management. In many cases, the models are used to evaluate which alternative will be most effective in solving a long-term water quality problem. Management decisions require the consideration of existing conditions as well as the projection of anticipated future changes of the water system. In these applications, the models not only need to represent the existing conditions but also have to be predictive and give conditions that do not yet exist. Models are also used to provide a basis for economic analysis, so that decision makers can use the model results to evaluate the environmental significance of a project, as well as the cost–benefit ratio.

Three key factors have contributed to the great progress in the modeling of surface waters:

1. Better understanding and mathematical descriptions of physical, chemical, and biological processes in rivers, lakes, estuaries, coastal waters, and wetlands;
2. Availability of fast and efficient numerical schemes;
3. Progress in computer technology.

The powerful, yet affordable computers in combination with fast numerical algorithms have enabled the development of sophisticated 3D hydrodynamic and water quality models. These advanced models contain very few simplifying approximations to the governing equations. Personal computers (PCs) have evolved rapidly to become the standard platform for most engineering applications (except for very large-scale problems). The PCs represent the most widely used computer platform today. Models developed on a PC can be transformed to other PCs without much difficulty. The relatively low prices of PCs also make modeling more cost effective. Because of the rapid advances in computer technology, PCs are now widely used in surface water modeling studies. As a matter of fact, all case studies presented in this book were conducted on PCs.

Models play a critical role in advancing the state of the art of hydrodynamics, sediment transport, and water quality, and of water resources management. Because of their requirements for precise and accurate data, models also ultimately contribute to the design of field data collection and serve to identify data gaps in characterizing waterbodies. Models are used to analyze the impact of different management alternatives and to select the ones that result in the least adverse impact to the environment.

Models are often used to improve the scientific basis for theory development, to make and test predictions, and to clarify cause–effect relationships between pollutant loadings and the receiving waterbody. Reliable predictions stand out as a salient requirement for models, because decisions can have costly social and economic consequences on businesses, municipalities, and even entire states. Models are often used to evaluate and test potentially expensive water quality management alternatives prior to their implementation. The cost of a hydrodynamic and water quality modeling study is usually a small fraction of the implementation cost. Models can simulate changes in an ecosystem due to changes in internal and/or external conditions, such as water elevation variations or increased external pollutants. These simulations predict positive or negative changes within the ecosystem due to the management actions, such as improved sewage treatment or reduced agricultural runoff. These simulations are obviously far more cost effective than testing expensive management actions on a trial-and-error basis, thus making models a useful tool for water quality management. Since huge financial investment is at stake, accurate model results are imperative to support the costly implementation.

In the past decades, hydrodynamic and water quality models have evolved from simplified 1D, steady-state models, such as the legendary QUAL2E model (Brown and Barnwell, 1987), to complex 3D, time-dependent models of hydrodynamics, sediment, toxics, and eutrophication. Three-dimensional modeling has matured from a research subject to a practical engineering tool. Over this same period, computational requirements for realistic 3D modeling have changed from supercomputers, to high-end workstations, and then to PCs.

These advanced 3D and time-dependent models, which can also be readily applied to 1D and 2D problem settings, provide a powerful computational tool for sediment transport, water quality, eutrophication, and toxic chemical fate and transport modeling studies. Their hydrodynamic submodel provides (1) flow field, (2) water depth, (3) temperature and salinity, (4) mixing, and (5) bottom shear stress.

Flow field, water depth, and mixing are used to determine mass transport of solids, toxics and other constituents. Bottom stress is used to estimate the exchange between the water column and sediment bed as a result of sediment deposition and resuspension. Since the mid-1980s, these models (e.g., Blumberg and Mellor, 1987; Hamrick, 1992; Sheng, 1986) have successfully transformed from academic research to practical tools for managing surface water systems.

Numerous models have been developed in the past decades. Many of them are actually based on similar theories and numerical schemes, even though the input and output formats of these models may look very different. For example, the Estuarine, Coastal, and Ocean Model (ECOM) (HydroQual, 1991a, 1995a) and the Environmental Fluid Dynamics Code (EFDC) (Hamrick, 1992) both have hydrodynamic theories similar to the Princeton Ocean Model (POM) (Blumberg and Mellor, 1987). The POM, ECOM, EFDC, and CH3D (Sheng, 1986) models all use the sigma coordinate in the vertical and a curvilinear grid in the horizontal. The CE-QUAL-ICM model (Cerco and Cole, 1994; Cerco, 2015), the WASP model (Wool et al., 2002), and the EFDC model have eutrophication theories similar to that of the RCA model (HydroQual, 2004). The Chesapeake Bay sediment flux model (Di Toro and Fitzpatrick, 1993) and its modified versions have almost become the "standard" sediment diagenesis model in eutrophication modeling.

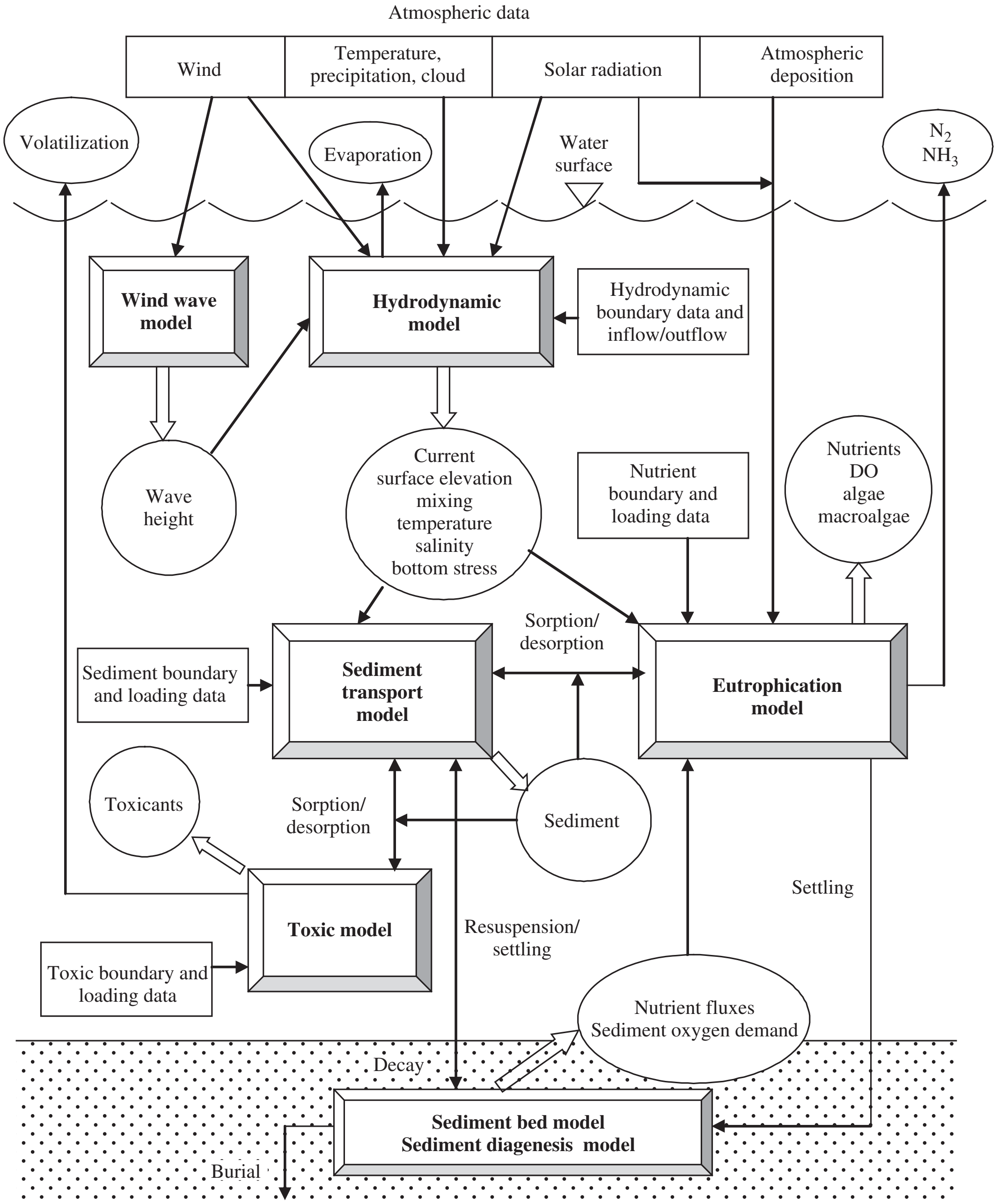

Figure 1.5 Major components (submodels) of the EFDC model.

These advanced models often include several coupled submodels for different physical, chemical, biological processes in surface waters, such as (1) hydrodynamic model, (2) wind wave model, (3) sediment model, (4) toxic model, (5) eutrophication model, (6) sediment diagenesis model, and (7) submerged aquatic vegetation (SAV) model.

As an example, Fig. 1.5 illustrates the major components of the EFDC model. In addition to computational modules, these advanced models tend to evolve into complex software systems, comprising many tools and sources of information. They may contain components for grid generation, data analysis, preprocessing, post-processing, statistical analysis, graphics, and other utilities. Examples of these modeling packages include EFDC, ECOM, MIKE 3 (DHI, 2001), and TRIM (Casulli and Cheng, 1992).

Even though the basic theories of the aforementioned models (and other models) might have been universally agreed upon, choosing the “best” model for a particular application is the subject of considerable controversy. It is beyond the scope of this book to get into the subtleties of this controversy. This book does not review models and does not recommend the so-called best model for surface water modeling. There are dedicated reports covering particular aspects of model review and model selection (e.g., Tetra Tech, 2001; Imhoff et al., 2004; HydroGeoLogic, 1999).

Note that models are rarely either right or wrong: they lead the modelers either to proper conclusions or to improper conclusions. Therefore, how to use and interpret model results is as important as the model results themselves. In this light, models are similar to other tools in engineering: they can either be productively used or abused. The experience of the modeler plays a vital role in a successful modeling application. This is a primary reason why modeling is also called an "art."

1.4 About This Book

This book is about processes, their modeling, and how to use models to support decision making. Instead of addressing models, this book is focused on theories, mathematical representations, and numerical modeling of processes in surface waters. Through case studies, the modeling of rivers, lakes, estuaries, coastal waters, and wetlands is illustrated.

Chapters 2–5 are dedicated to four important subjects: (1) hydrodynamics (Chapter 2), (2) sediment transport (Chapter 3), (3) pathogens and toxics (Chapter 4), and (4) water quality and eutrophication (Chapter 5). After external sources and total daily maximum load (TMDL) are discussed in Chapter 6, and mathematical modeling and statistical analyses in Chapter 7, the book is focused on different types of surface waterbodies: (1) rivers (Chapter 8), (2) lakes and reservoirs (Chapter 9), (3) estuaries and coastal waters (Chapter 10), and (4) wetlands (Chapter 11). The last chapter of this book, Chapter 12, presents risk analysis for environmental management.

Each chapter (after Chapter 1) introduces concepts, processes, and mathematical representations at a level sufficient to meet the modeling needs but elementary enough to allow the readers to have a good understanding of the topic. The organization of each chapter is similar: it begins by introducing basic concepts, proceeds to the discussions of physical, chemical, and/or biological processes and their mathematical representations, and concludes with case studies.

The best way to understand theories is via examples and case studies. This book (Chapters 2–12) presents a range of applications designed to be representative of surface water systems, including rivers, lakes, estuaries, and wetlands. Each chapter typically includes two case studies on two different waterbodies. The case studies are useful for understanding the theories and processes presented in the previous sections of that chapter. They detail key features of surface water systems and exhibit

Table 1.2 Waterbodies discussed in this book as case studies and examples.

Waterbody name	Waterbody type	Physical feature	Major problems	Chapters
Blackstone River, MA	Small river	Shallow (<1 m) Narrow (<20 m)	Sedimentation, Toxic metals	3, 8
Susquehanna River, PA	Deep river	Deep (>10 m)	Thermal pollution	8
Lake Okeechobee, FL	Lake	Large (1730 km^2) Shallow (3.2 m)	Phosphorus, Eutrophication	2, 3, 5, 7, 9
Lake Tenkiller, OK	Reservoir	Long (49 km) Deep (>45 m)	Eutrophication	9
Rockford Lake, NE	Reservoir	Small (0.6 km^2) Shallow (3.7 m)	Pathogens	4
St. Lucie Estuary and Indian River Lagoon, FL	Estuary–lagoon	Small (29 km^2) Shallow (2.4 m)	Salinity intrusion, Eutrophication	2, 4, 5, 10
Morro Bay, CA	Estuary	Small (8.5 km^2) Shallow (<2.5 m)	Sedimentation, Pathogen	10
Stormwater Treatment Area (Cells 3A/3B), FL	Wetland	Small (18 km^2) Shallow (0.40 m)	Aquatic vegetation, Nutrient removal	11

varying levels of complexity. They provide real-world examples of how models can be set up on a practical level, used to simulate surface waters, and applied to support decision making. A primary objective of presenting these case studies is that the modeling approaches, the analysis methods, and the discussions on processes in these case studies are useful for readers to conduct their own modeling studies on similar waterbodies.

The case studies have been carefully selected, so that they represent different types of waterbodies. All these case studies originated from real engineering projects. None of them is just an "idealized" exercise. The contents of these case studies are based on either published journal papers or technical reports. Physical features of these waterbodies and major problems addressed in the cases studies are summarized in Table 1.2. Electronic files of four examples (three case studies and one simplified case) are included in the modeling package.

1. *Tidal Channel*: Illustrates estuarine transport and stratification associated with salinity, sediment, and toxic metal.
2. *Blackstone River*: Describes the applications of hydrodynamics, sediment transport, and metals modeling.
3. *Lake Okeechobee*: Shows the modeling and applications of hydrodynamics, wind wave, sediment transport, water quality, and SAV.
4. *St. Lucie Estuary and Indian River Lagoon*: Presents the applications of hydrodynamics, sediment transport, toxic metal, and water quality.

These case studies demonstrate modeling applications to rivers, lakes, estuaries, and wetlands. Sample input files and output files of these studies are included in the modeling package. Readers can use these input files as templates for their own applications and avoid developing the entire input files from scratch.

2

Hydrodynamics

Hydrodynamics studies the motion of water and the forces acting on water. This chapter discusses the fundamentals of hydrodynamics in surface waters, such as rivers, lakes, estuaries, coastal waters, and wetlands. The materials presented in this chapter will be used throughout this book.

Hydrodynamics is the driving mechanism for the transport of sediments, toxics, and nutrients and is critical to the movement of pollutants through the environment. A hydrodynamic model can provide crucial information to sediment, toxic, and eutrophication models, including water velocities and circulation patterns, mixing and dispersion, water temperature, and density stratification. Therefore, it is necessary to have a good understanding of hydrodynamic processes in a water system before proceeding to the studies of sediment, toxic, and/or water quality.

In this book, Chapters 2–5 and 8–12 are organized in a similar manner. They typically have the following contents:

1. What this chapter is about and how the contents in this chapter relate to other chapters.
2. How the contents of this chapter are applicable to practical problems.
3. Basic concepts, theories, and processes.
4. Analytical solutions and/or simplified cases that are helpful for understanding the theories and processes.
5. Model parameters and data that are commonly used/adjusted in modeling.
6. Case studies.

In this chapter, the basic hydrodynamic processes are discussed in Section 2.1, and the governing hydrodynamic equations in one-, two, and three-dimensional (1D, 2D, and 3D) forms are presented in Section 2.2. Water temperature and thermal processes are discussed in Section 2.3. Hydrodynamic modeling is discussed in Section 2.4, in which major hydrodynamic model parameters, data required in hydrodynamic modeling, and case studies are presented. The two case studies described in this chapter are the modeling of Lake Okeechobee and of St. Lucie Estuary (SLE) and Indian River Lagoon (IRL). These two waterbodies are also used as cases studies in other chapters of this book.

2.1 Hydrodynamic Processes

Hydrodynamic processes are integral components of complex surface water systems. Water movements at different scales and of different types significantly affect not only the distribution of temperature, nutrients, and dissolved oxygen (DO) but also the aggregation and/or distribution of sediments, contaminants, and algae. Circulation, wave, and turbulent mixing are major influences on the distribution of biota and the productivity of natural waterbodies. This section illustrates the fundamental laws and basic processes in hydrodynamics.

2.1.1 Water Density

Water density has unique physical properties. Water is less dense as a solid than as a liquid. Consequently, ice floats on water. Water density does not monotonically decrease with increasing temperatures. Instead, water has its maximum density at 4 °C. Water becomes less dense as the temperature either increases or decreases from 4 °C. As a result, a lake in the summer tends to have a layer of warm water floating on the top of the denser, colder water below. Conversely, in the winter, if the lake's surface drops to <4 °C, it creates a layer of cold water that floats on the top of the denser, warmer (∼4 °C) water below. Further, the temperature–density relation is nonlinear. The density difference between 20 and 21 °C is approximately equal to the density difference between 5 and 10 °C. Besides, water density is also significantly influenced by salinity and sediment concentrations. These density differences between the surface water and the bottom water create stratifications and inhibit vertical mixing. Because of this density–temperature relationship, many lakes and estuaries tend to stratify, that is, they separate into distinct vertical layers.

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Companion Website: www.wiley.com/go/ji/hydrodynamics_water_quality

Water density is a basic parameter in hydrodynamic and water quality studies. Accurate hydrodynamic calculations require accurate water densities. The density is largely determined by three parameters: (1) temperature (T), (2) salinity (S), and (3) concentration of total suspended sediment (C). The relationship between the four variables, namely ρ, T, S, and C, can be written as

$$\rho = f(T, S, C) \tag{2.1}$$

and is referred to as the equation of state. The actual form of function f is established empirically.

It is convenient to express the equation of state in differential form as follows:

$$d\rho = \left(\frac{\partial \rho}{\partial T}\right)_{S,C} dT + \left(\frac{\partial \rho}{\partial S}\right)_{T,C} dS + \left(\frac{\partial \rho}{\partial C}\right)_{T,S} dC \tag{2.2}$$

Consequently, we have

$$\rho = \rho_T + \Delta\rho_S + \Delta\rho_C \tag{2.3}$$

where ρ_T = density of pure water as a function of temperature (kg/m^3), $\Delta\rho_S$ = density increment due to salinity (kg/m^3), and $\Delta\rho_C$ = density increment due to total suspended sediment (kg/m^3).

A variety of empirical equations have been proposed to describe the density of pure water as a function of temperature. The one presented by Gill (1982, p. 599) is commonly used in hydrodynamic modeling (e.g., Hamrick, 1992; Cole and Buchak, 1995):

$$\begin{aligned}\rho_T = {} & 999.842594 + 6.793952 \times 10^{-2} T \\ & - 9.095290 \times 10^{-3}\, T^2 + 1.001685 \times 10^{-4} T^3 \\ & - 1.120083 \times 10^{-6} T^4 + 6.536332 \times 10^{-9} T^5\end{aligned} \tag{2.4}$$

where T = water temperature (°C).

The water density increment due to salinity, $\Delta\rho_S$, is given by (Gill, 1982)

$$\begin{aligned}\Delta\rho_S = {} & S\,(0.824493 - 4.0899 \times 10^{-3} T \\ & + 7.6438 \times 10^{-5} T^2 - 8.2467 \times 10^{-7} T^3 \\ & + 5.3875 \times 10^{-9} T^4) + S^{3/2}(-5.72466 \times 10^{-3} \\ & + 1.0227 \times 10^{-4} T - 1.6546 \times 10^{-6} T^2) \\ & + S^2(4.8314 \times 10^{-4})\end{aligned} \tag{2.5}$$

where S = salinity (kg/m^3). Based on Eqs. (2.4) and (2.5), Fig. 2.1 gives the variations of water density with water temperature under salinity values of 0, 10, 20, 30, and 40 ppt (parts per trillion). It shows that the water density varies from 992.2 kg/m^3 at 40 °C and 0 ppt to 1032.1 kg/m^3 at 0 °C and 40 ppt.

The total suspended sediment, C, includes two parts: the total suspended solids (TSS) and the total dissolved solids (TDS). Ford and Johnson (1986) presented the following equation to calculate water density increment due to TSS and TDS:

$$\begin{aligned}\Delta\rho_C = {} & \mathrm{TSS}(1 - 1/\mathrm{SG}) \times 10^{-3} + \mathrm{TDS}(8.221 \times 10^{-4} \\ & - 3.87 \times 10^{-6} T + 4.99 \times 10^{-8} T^2)\end{aligned} \tag{2.6}$$

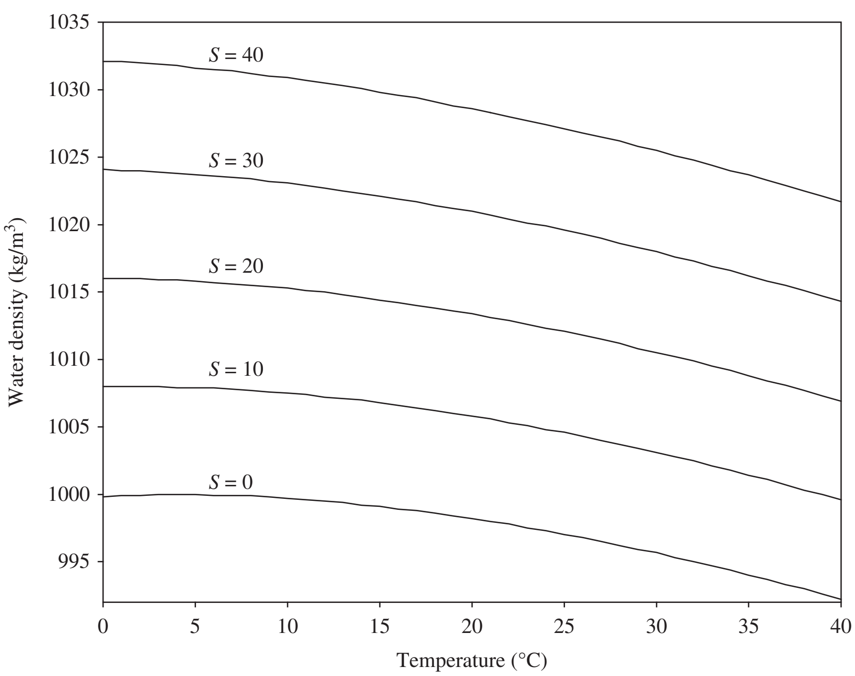

Figure 2.1 Variations of water density with water temperature under salinity values of 0, 10, 20, 30, and 40 ppt.

where TSS = total suspended solids concentration (g/m^3), TDS = total dissolved solid concentration (g/m^3), SG = specific gravity of TSS (=2.56). SG is the (dimensionless) ratio of the density of a fluid (or solid) to the density of pure water. As a rule of thumb, an increment of water density by one-tenth of one percent (0.1%) needs a decrease of ~5 °C or an increase of ~1.2 ppt salinity, that is, the change of 1 ppt salinity has a similar effect on water density variation as the change of 4 °C temperature.

Because of the small variations in water density, it may be necessary to know the density to at least five decimal places in some modeling studies. A variable called σ_t is defined as

$$\sigma_t = \rho - 1000 \tag{2.7}$$

Both ρ and σ_t have the unit of kilograms per cubic meters (kg/m^3). When studying density variation and vertical stratification, it is sometimes more convenient to present σ_t than to directly present density. For example, Ahsan and Blumberg (1999) used σ_t to illustrate the seasonal variation of vertical density distributions in a lake.

2.1.2 Conservation Laws

The conservation laws that govern hydrodynamic processes include (1) the conservation of mass, (2) the conservation of energy, and (3) the conservation of momentum. These three conservation laws form the theoretical basis of hydrodynamics and are used routinely in the studies of hydrodynamics and water quality. While basic equations in hydrodynamic models are frequently manipulated, simplified, and renamed, they all come from the same conservation laws. The conservation of mass and the conservation of momentum are discussed here. The conservation of energy will be described in Section 2.3 when heat fluxes are presented.

2.1.2.1 Conservation of Mass

The law of conservation of mass states that mass can neither be produced nor destroyed. It is often expressed in a mass balance equation (also called continuity equation), which accounts for the flux of mass going into a defined area and the flux of mass leaving the defined area. For an incompressible fluid (which is a very accurate description of surface waters) in a defined area, the water flux in must equal the flux out. That is

$$\begin{aligned}\text{Mass accumulation} &= \text{mass in} - \text{mass out}\\ &\quad + \text{source} - \text{sink}\end{aligned} \tag{2.8}$$

In hydrodynamics, the equation for the conservation of mass is frequently illustrated in and applied to water columns. A water column is a portion of a waterbody, or a hypothetical "cylinder" of a waterbody, extending from the surface of a waterbody to the bottom. It is an imaginary vertical column of water used as a control volume for computational purposes. A control volume is a spatial domain for analysis separated from the rest of the spatial domain by a defined boundary. Variables may enter and leave this volume and be stored within it, but its shape and position in space remain unchanged. For a given water column, the inflow minus outflow must equal the volume change over time. Equation (2.8) can be restated as

$$dm = (m_{\text{in}} - m_{\text{out}} + m_r) \cdot dt \tag{2.9}$$

where dm = mass accumulation, m_{in} = the rate of mass in flux, m_{out} = the rate of mass out flux, m_r = the net rate of production from all source and sink terms, and dt = time increment. To develop an equation in terms of mass flux (the rate at which mass enters or leaves a water column), Eq. (2.9) is divided by the time increment dt. It yields the following mass balance equation for water (or a particular pollutant):

$$\frac{dm}{dt} = \frac{\partial m}{\partial t} + \nabla \cdot (m\vec{v}) = m_{\text{in}} - m_{\text{out}} + m_r \tag{2.10}$$

If other compounds react to form this pollutant, the net rate of production, m_r, will be positive. If this pollutant reacts to form some other compounds, resulting in a loss of this pollutant, m_r will be negative. Equation (2.10) is the basic equation for mass conservation and is used extensively in hydrodynamic and water quality studies.

If a pollutant increases in a waterbody (say, in a lake), it must be due to one (or both) of the following reasons:

1. There are external sources that have discharged into the lake.
2. There are in-lake chemical/biological reactions from other compounds that formed this pollutant.

If chemical/biological reactions caused the pollutant to increase, they must also have caused a corresponding decrease in some other compounds. Thus, the conservation of mass, as expressed in Eq. (2.10), provides a means of compiling a pollutant budget in the lake. This budget tracks the amount of the pollutant entering the lake and leaving the lake, as well as the amount formed or destroyed by chemical and biological reactions.

When the reactions and the inflow/outflow are neglected, the differential equation for the conservation of mass can be further derived from Eq. (2.10) as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\vec{v}) = 0 \tag{2.11}$$

where ρ = density of water, $\vec{v}$ = velocity vector, and ∇ = gradient operator. Equation (2.11) is also called the continuity equation. For incompressible flow ($d\rho/dt = 0$), the continuity equation simplifies to

$$\nabla \cdot \vec{v} = 0 \tag{2.12}$$

It means that the net rate of mass flow across any closed surface is zero. In Cartesian coordinates, Eq. (2.12) can be written as

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \tag{2.13}$$

where u, v, and w are velocity components in the x, y, and z directions, respectively.

2.1.2.2 Conservation of Momentum

The conservation of momentum can be derived from Newton's second law:

$$\vec{F} = m \cdot \vec{a} \tag{2.14}$$

where $\vec{F}$ = external force, m = mass of the object, and $\vec{a}$ = acceleration of the object.

In addition to external forces (e.g., wind), there are three forces important to hydrodynamics:

1. Gravitational force
2. Force from water pressure gradient
3. Viscous force.

Gravitational force is due to the gravitational attraction of the earth. Water pressure gradient is caused by the pressure gradient in a waterbody. Viscous force is due to water viscosity and turbulent mixing. Hence, the momentum equation, Eq. (2.14), can be expressed as

$$\rho\frac{d\vec{v}}{dt} = \frac{\partial \rho\vec{v}}{\partial t} + \nabla \cdot (\rho\vec{v}\vec{v}) = \rho\vec{g} - \nabla p + \vec{f}_{\text{vis}} \tag{2.15}$$

where $\vec{f}_{\text{vis}}$ = viscous force, p = water pressure, $\vec{g}$ = gravitational force, ρ = water density, and ∇ = gradient operator. Equation (2.15) does not include wind forcing, which can be incorporated as boundary conditions in Eq. (2.85). The negative sign for the pressure gradient is to indicate that the pressure gradient force is directed opposite to the gradient. For an incompressible Newtonian fluid, the viscous force can be expressed as

$$\vec{f}_{\text{vis}} = \nabla \cdot \vec{\tau} = \mu\nabla^2\vec{v} \tag{2.16}$$

where $\vec{\tau}$ = shear stress, μ = absolute (or dynamic) viscosity, which is assumed to be constant, and ∇^2 = the Laplacian operator.

A Newtonian fluid is one in which the stress is linearly proportional to the rate of deformation. Most common fluids are Newtonian, such as water, air, and gasoline. However, some fluids have a nonlinear relationship between stress and the rate of deformation. These fluids are called non-Newtonian. Examples of non-Newtonian fluids are toothpaste and butter.

In Cartesian coordinates, the water shear stress can be written as

$$\tau_{xy} = \mu\frac{dv}{dx} \tag{2.17}$$

$$\tau_{yx} = \mu\frac{du}{dy} \tag{2.18}$$

where u = velocity component in the x-direction and v = velocity component in the y-direction. Here, a double subscript notation is used to label the shear stress components (τ_{xy} and τ_{yx}). For example, the first subscript of τ_{xy} indicates the plane on which the stress acts (in this case, a surface perpendicular to the x-axis). The second subscript indicates the direction in which the stress acts.

When considering the rotation of the earth and external forces, Eq. (2.15) is changed to

$$\begin{aligned}\frac{d\vec{v}}{dt} &= \frac{\partial\vec{v}}{\partial t} + \nabla \cdot (\vec{v}\vec{v}) \\ &= \vec{g} - \frac{1}{\rho}\nabla p + \nu\nabla^2\vec{v} - 2\vec{\Omega} \times \vec{v} + \overrightarrow{F_{\text{fr}}}\end{aligned} \tag{2.19}$$

where $\vec{\Omega}$ = angular velocity of the earth, $\overrightarrow{F_{\text{fr}}}$ = external forces, and $\nu = \mu/\rho$ = kinematic viscosity. The angular velocity of the earth, $\vec{\Omega}$, is related to the Coriolis parameter f by the following:

$$f = 2\Omega\sin\varphi \tag{2.20}$$

where Ω = the magnitude of the earth's angular velocity $\vec{\Omega}$ (=$7.292 \times 10^{-5}\ \text{s}^{-1}$) and φ = the latitude.

Equation (2.19) is the Navier–Stokes equation, valid for incompressible Newtonian flows. The meanings of each term in Eq. (2.19) are as follows:

1. The acceleration term, $d\vec{v}/dt$, is composed of the local rate of change due to time variation ($\partial\vec{v}/\partial t$), plus the rate of change due to advection of the flow ($\nabla \cdot (\vec{v}\vec{v})$). It is the acceleration $\vec{a} = \vec{F}/m$ given in Eq. (2.14). The terms on the right-hand side of Eq. (2.19) are all the forces that cause this acceleration. One of the most important objectives in hydrodynamic studies is to find out how the currents change with time, which is specified by this term.
2. The gravitational force $\vec{g}$ acts toward the center of the earth.
3. The pressure gradient term, $-\frac{1}{\rho}\nabla p$, represents the effects of the spatial variation of water pressure. Pressure gradients cause the water to move. The two contributing factors to pressure gradients are water surface level slopes (the barotropic component) and changes in density (the baroclinic component).
4. The viscous term, $\nu\nabla^2\vec{v}$, includes the effects of water viscosity. This term can also be modified to represent turbulent mixing.

5. The Coriolis force term, $-2\vec{\Omega} \times \vec{v}$, represents the effect of the earth's rotation on water movement. It is significant only when large waterbodies are studied.
6. The external force term, $\overrightarrow{F_{\mathrm{fr}}}$, can be used to include wind forces.

There are no analytical solutions to the Navier–Stokes equation, Eq. (2.19). It is also too complex to be solved numerically for large domains over long periods. Further simplifications to the Navier–Stokes equation are needed in hydrodynamic models, which will be described in Section 2.2.1.

2.1.3 Advection and Dispersion

When a pollutant load is discharged into a waterbody, it is subject to fate and transport processes that modify its concentration. The principal factors determining the pollutant concentration are hydrodynamic transport and chemical/biological reactions.

All forms of aquatic life rely on the surrounding water for the transport of resources and the products of metabolic activity. Chemical/biological reactions play an important role in a pollutant's fate in the environment. An equally important aspect is the hydrodynamic transport of the pollutant. Hydrodynamic transport acts to move pollutants from the location at which they are generated, resulting in impacts that can be far away from the pollution source. On the other hand, some pollutants, such as wastewater discharges, can be degraded in the receiving waterbody if they are sufficiently diluted. For these pollutants, slow ambient water velocity and weak mixing can result in excessively high pollutant concentrations and lead to increased adverse impacts on the environment.

The processes that affect the transport of material to and from the surface of an organism include molecular and turbulent diffusion. However, since the viscosity of water is about 55 times that of air, the scales at which these processes occur are different. Hydrodynamic transport includes the following processes: (1) advection, (2) dispersion, and (3) vertical mixing and convection. Material in water can be transported by one or all of these processes. Collectively, these three processes are referred to as hydrodynamic transport. Both horizontal and vertical transport should be considered since, for flow fields with a complex spatial topography, material transport is usually three dimensional.

Advection refers to horizontal transport by flows that move patches of material around but do not significantly distort or dilute them. In rivers and estuaries, advection often represents the primary transport process of pollutant in the longitudinal direction. Lateral advection across a river is usually small. In a straight channel (Fig. 2.2), the velocity profile indicates that the maximum advection occurs in the middle of the channel and that the minimum advection occurs near the banks. The lateral velocity differences cause the flow at the center of the river moving faster than the flow near the banks. This lateral variation promotes dispersion across the river. In contrast to advection, convection refers to vertical transport of water and pollutants. Convection in rivers, lakes, and estuaries is usually very small. Vertical turbulent mixing and its mathematical description will be described in Section 2.2.3.

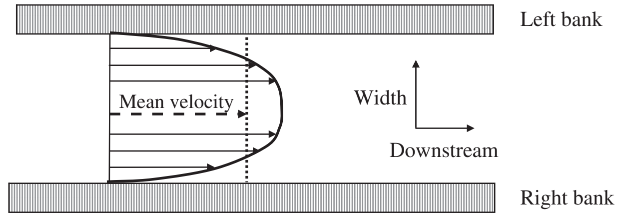

Figure 2.2 Velocity profile in a channel.

Dispersion is the horizontal spreading and mixing of water mass caused by turbulent mixing and molecular diffusion. Dispersion reduces the gradient of material concentration. This process involves not only an exchange of water mass, but also of any substance dissolved in it, such as salts and dissolved pollutants. Hence, in addition to hydrodynamic variables, such as temperature and salinity, dispersion processes are also of importance to the distributions of sediments, toxics, and nutrients in waterbodies. Dispersion in the direction of water flow is called longitudinal dispersion, and that perpendicular to the direction of flow is called lateral dispersion. Longitudinal dispersion is generally much stronger than lateral dispersion in rivers.

Turbulent mixing is often the dominant component of dispersion in rivers, lakes, and estuaries, and is much more rapid than molecular diffusion. Turbulent mixing is the result of the momentum exchange between water parcels in a turbulent flow. It spreads chemical or biological constituents in various directions depending on the flow characteristics. Diffusion is a transport process at the microscopic level, owing to the scattering of particles by random molecular motions. Diffusion is the movement of material from an area of high concentration to an area of low concentration due to concentration gradients. If a drop of a colored dye is put into a bottle containing still water, the dye will spread in the water. Eventually, the bottle will contain uniformly colored water. The reason is that the dye tends to move from higher concentration areas to lower concentration areas, just as heat is transferred from a higher temperature to a lower temperature. Molecular diffusion occurs much more slowly and so is important only on a very small scale, such as right at the bottom of a lake. Diffusion can be described by Fick's law and the classical diffusion equation.

Advection and dispersion are the major processes by which dissolved materials are transported along and distributed throughout a river or an estuary (Fig. 2.2). As water flows along the river, it transports dissolved materials with it via advection. It leads to a net transport of dissolved materials from areas of high concentration to areas of low concentration via dispersion. Hence, horizontal transport of material consists of two components: (1) advective flux and (2) dispersive flux. Both fluxes are defined as the mass of concentration crossing a unit area per unit time, with units of mass/(time length^2) (M/T/L^2). The unit conventions are M for mass units, L for length units, and T for time units.

The movement of pollutant mass due to advective flux is in the same direction as the fluid flow, while the dispersive flux moves mass from areas of high concentration to areas of low concentration. The advective flux density ($\vec{J_a}$) depends on concentration (C) and flow velocity ($\vec{v}$):

$$\vec{J_a} = C \cdot \vec{v} \tag{2.21}$$

Note that it is the product of $\vec{v}$ and C that is important for mass transport rather than either the velocity or concentration alone. It is possible to generate the same value for $\vec{J_a}$ using different combinations of values for $\vec{v}$ and C.

About the dispersive flux, Fick's law states that the rate of mass movement resulting from molecular diffusion is inversely proportional to the gradient of mass concentration:

$$J = -D\frac{dC}{dx} \tag{2.22}$$

where J = the dispersive mass flux density (M/L^2/T), C = the concentration of mass in the water (M/L^3), D = diffusion coefficient (L^2/T), and x = the distance (L).

The negative sign indicates that the diffusing mass flows in the direction of decreasing concentration. Equation (2.22) states, in simple terms, that mass will naturally move from areas of high concentration to areas of low concentration and that the rate of that movement is greatest when the greatest change in concentration occurs over the shortest distance, that is, the greater the concentration gradient, the greater the mass flux density.

Turbulent mixing results from the random scattering of particles by turbulent flow and can be considered roughly analogous to molecular diffusion. It is assumed that dispersive flux also follows Fick's law, Eq. (2.22); only that the magnitude of the diffusion coefficient (D) is different. Dispersion by turbulent mixing typically results in much larger rates of diffusion and transport and often plays a dominant role in dispersive transport.

The total mass flux across a boundary can be calculated as

$$\frac{dm}{dt} = (J_a + J)A \tag{2.23}$$

where m = mass, J_a = the magnitude of advective flux $\vec{J_a}$ (M/L^2/T), and A = area of the boundary that perpendicular to the direction of the flow. In most natural waterbodies, the advective flux (J_a) is larger than the dispersive flux (J). When the flow velocity is very small, the advection flux becomes small and can be neglected. The conservation of mass described by Eq. (2.10) can then be simplified as

$$\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x} \tag{2.24}$$

Combining Eqs. (2.22) and (2.24) yields

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{2.25}$$

This is the classical diffusion equation from Fick's law. Its solution needs one initial condition and two boundary conditions. Two simple solutions to Fick's law are described below.

Constant Release: This case has the following conditions:

$$\text{Initial condition:}\quad C(x,0) = 0 \tag{2.26a}$$

$$\text{Boundary condition:}\quad C(0,t) = C_0 \tag{2.26b}$$

$$C(\infty,t) = 0 \tag{2.26c}$$

This is the case where a source with constant concentration C_0 at $x = 0$ is added in a river, starting from $t = 0$. The solution toFick's law under these conditions is

$$C(x,t) = C_0 \,\mathrm{erfc}\left[\frac{x}{2\sqrt{Dt}}\right] \tag{2.27}$$

where the complementary error function, erfc(x), equals 1 minus the error function, erf(x). That is

$$\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-u^2}du \tag{2.28}$$

The complementary error function, erfc(x), has the following properties:

1. erfc(0) = 1
2. erfc(∞) = 0
3. erfc(r) is monotonically decreasing with x.

Figure 2.3 gives the values of erf(x) and erfc(x).

Instantaneous Release: If a slug is released into a river at $t = 0$ and $x = 0$, the initial condition and boundary conditions are as follows:

$$\text{Initial condition:}\quad C(x,0) = 0 \tag{2.29}$$

$$\text{Boundary condition:}\quad \int C(x,t)dx = M \tag{2.30}$$

$$C(x,\infty) = 0 \tag{2.31}$$

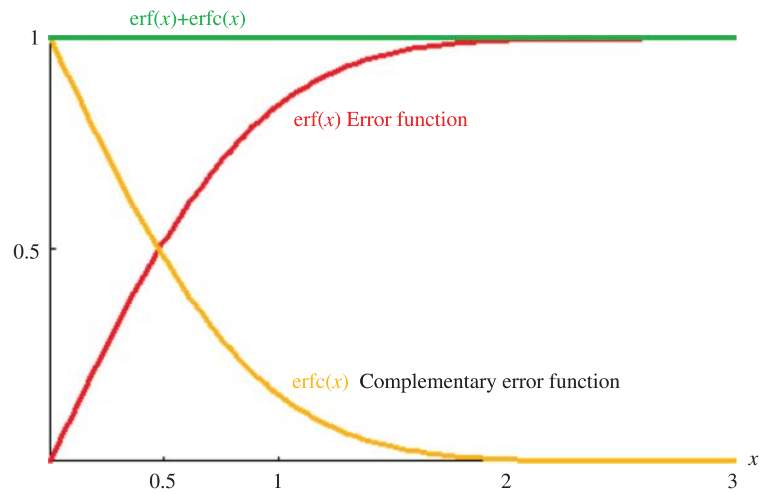

Figure 2.3 Error function and complementary error function.

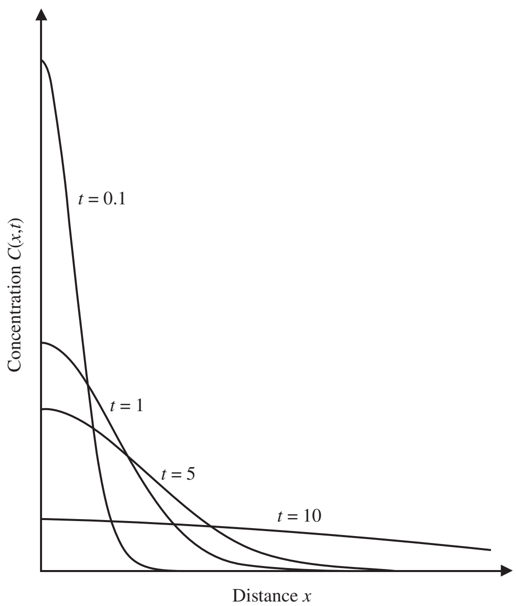

Figure 2.4 Longitudinal distribution of contaminant deposited instantaneously at $x = 0$, according to Eq. (2.32).

where M is the mass initially deposited at $x = 0$. Equation (2.30) does not actually specify a boundary value but requires that the total dye mass at any time t should be equal to the dye mass initially released at $t = 0$. In this case, the solution to Eq. (2.25) is

$$C(x,t) = \frac{M}{\sqrt{\pi D t}} e^{\left(-\frac{x^2}{4Dt}\right)} \tag{2.32}$$

Figure 2.4 expresses the solution (2.32) graphically.

2.1.4 Mass Balance Equation

Based on the principle of conservation of mass, the concentration change of a reactant can be calculated using the mass balance equation (2.10), which is simply an accounting of mass inputs, outputs, reactions, and net change. Its 1D form can be simplified as (Ji, 2000a)

$$\underbrace{\frac{\partial C}{\partial t}}_{\text{Net change of concentration}} = \underbrace{-U\frac{\partial C}{\partial x}}_{\text{Advection}} + \underbrace{\frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right)}_{\text{Dispersion}} + \underbrace{S}_{\text{Settling}} + \underbrace{R}_{\text{Reactivity}} + \underbrace{Q}_{\text{Load}} \tag{2.33}$$

where C = reactant concentration, t = time, x = distance, U = advection velocity in the x-direction, D = mixing and dispersion coefficient, S = sources and sinks due to settling and resuspension, R = reactivity of chemical and biological processes, and Q = external loadings to the aquatic system from point and nonpoint sources. Equation (2.33) indicates that net changes of pollutants in water involve five main processes:

1. The advection term accounts for the mass inputs and outputs by water current and specifies the movement of the pollutant with waters as it flows downstream.
2. The dispersion term describes the spreading of the pollutant that occurs due to turbulent mixing and molecular diffusion.
3. The settling term represents the particle settling to and getting resuspended from the bed, which will be discussed in Chapter 3.
4. The reactivity term refers to chemical and/or biological processes that take place within the water column, which will be described in Chapters 4 and 5.
5. The load term indicates external sources, which will be presented in Chapter 6.

It is evident that the diffusion equation from the Fick's law, Eq. (2.25), is just a special case of the mass balance equation when the terms of advection, settling, reactivity, and external load are neglected in Eq. (2.33). In addition to the two analytical solutions, namely Eqs. (2.27) and (2.32), another two solutions to the mass balance equations are given below.

Instantaneous Release with Mean Flow: The case of instantaneous release without mean flow is already discussed with the diffusion equation, and the solution is given by Eq. (2.32). For an instantaneous release with mean flow, Eq. (2.33) is

$$\frac{\partial C}{\partial t} = -U\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} \tag{2.34}$$

In the case of the instantaneous point source (slug injection) described by Eqs. (2.29)–(2.31), the solution to Eq. (2.34) is

$$C(x,t) = \frac{M}{B\sqrt{4\pi Dt}}e^{\left(-\frac{(x-Ut)^2}{4Dt}\right)} \tag{2.35}$$

where $C(x, t)$ = cross-sectional averaged tracer concentration, M = mass of tracer injected at $x = 0$ and $t = 0$, and B = cross-sectional area of the channel. If the initial concentration is a Gaussian distribution

$$C(x,0) = \frac{M}{\sqrt{2\pi\sigma}}\exp\left(-\frac{x^2}{2\sigma^2}\right) \tag{2.36}$$

where σ is the standard deviation of the Gaussian distribution, the solution to Eq. (2.34) is

$$C(x,t) = \frac{M}{\sqrt{2\pi(\sigma^2 + 2Dt)}}\exp\left(-\frac{(x-Ut)^2}{2(\sigma^2 + 2Dt)}\right) \tag{2.37}$$

Figure 2.5 shows the downstream travel of the dye concentrations at different times. In field studies, Eq. (2.37) can be helpful in estimating the values of the dispersion coefficient (D) in a river. Equation (2.37) can also be valuable in evaluating the accuracy of a numerical model in a simple channel test.

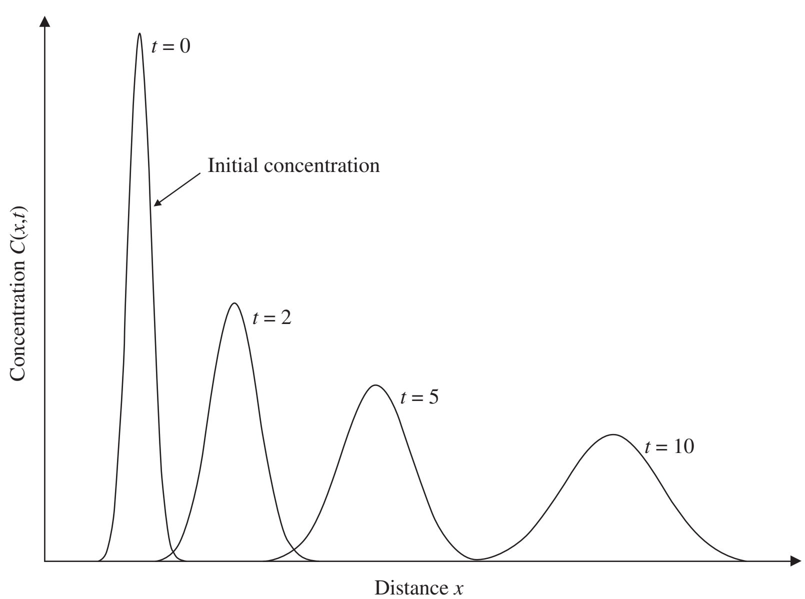

Figure 2.5 Spreading of contaminant in time and space in a steady uniform flow.

2.1.5 Atmospheric Forcings

The description of a surface water system is usually premised on the identification and understanding of external forcings to the system. Surface waters are subjected to forcings over a broad range of periods, from hourly to seasonal variations. Major external forcings to surface waters include (1) atmospheric forcings, (2) point and nonpoint sources, and (3) forcings from open boundaries. Atmospheric forcings will be discussed in this section. Point and nonpoint sources will be described in Section 6.1. Forcings from the open boundary will be presented in Section 10.5, where estuarine and coastal modeling is discussed.

Major atmospheric forcings include (1) wind, (2) air temperature, (3) solar radiation, and (4) precipitation. Besides, the atmospheric humidity, cloud cover, and atmospheric pressure can also affect a surface water system via evaporation and heat flux transfer on the air–water interface. As an example, Fig. 2.6 shows a photo of Station LZ40 in Lake Okeechobee, FL. The data measured at LZ40 are frequently used in the Lake Okeechobee modeling, and the modeling results are discussed extensively in this book.

Wind is usually a major source of energy in large lakes, coastal waters, and some estuaries. Wind exerts a drag on the water surface and pulls floating objects in the wind direction. The Coriolis force can deflect the movement of floating objects. Wind-driven currents are a major mechanism in the transport and distribution of floating pollutants, such as oil spills. If the distance

Figure 2.6 Sampling station LZ40 in Lake Okeechobee, FL. Its location in the lake is shown in Fig. 2.25. The data measured at LZ40 are used extensively in this book. *Source:* Photograph by Zhen-Gang Ji.

over which the wind blows and the wind duration are favorable, wind-driven surface currents can approach a velocity equal to 2–4% of the wind speed. But, given the lengths of open water found in most rivers, lakes, and estuaries, it is likely that the resulting current velocity will be less than this. For example, currents in a narrow estuary may be predominantly tidal, and wind has only minimum impact on the flow in the long run. On the other hand, if the estuary is wide, wind stresses can generate considerable currents. Wind may modify the circulation and become a major force on occasions, but wind cannot be responsible for the mean circulation over extended periods.

Winds vary on a variety of time scales, including diurnal variations (sea/land breeze), the time scale of weather systems (a few days), and the seasonal change in prevailing winds. The sea/land breeze is a phenomenon caused by the different heat capacities between land and large waterbodies (e.g., oceans and large lakes). Surface water can respond to an applied wind stress within a few hours and to the cessation of the wind in about the same time frame. Wind forcings can generate waves and storm surges. Seasonal weather patterns in a particular area can generate persistent circulation patterns in a particular water system.

For example, wind is the dominant force in driving the circulation and in generating turbulent mixing in Lake Okeechobee, FL. Because of the wind forcing, the lake circulations are typically dominated by a two-gyre pattern, especially in the winter (Ji and Jin, 2006). Wind-driven circulation has a time scale of a few days, the same as the period of local weather systems. Figure 2.7 gives the measured wind in the lake between October 1, 1999 and September 30, 2000. It shows that wind patterns in the summer and the winter are quite different, causing different effects on Lake Okeechobee. Early summer winds generally are caused by differential heating of land and water, exhibiting a diurnal pattern. Winter winds are associated with cold fronts passing through the area and are much stronger and more persistent than summer winds. These winds constantly mix the water columns.

Strong winds may also cause storm surge in surface waters. Storm surge is simply the phenomenon where water is pushed toward the shore by the winds. Strom surges can cause large water level fluctuation, which can have devastating effects on low-lying coastal regions. Both local and remote winds can play a large role in storm surges in coastal regions. For large lakes, such Lake Okeechobee, storm surges are also a significant threat to the local areas (SFWMD, 2002). Strong storms cause large flows as well as increased transport and mixing in surface water systems. For example, Jin and Ji (2004) reported that, although the typical mean flow in Lake Okeechobee is <5 cm/s, episodic storm currents can be >30 cm/s and last for several days.

Air temperature affects surface waters via heat flux and evaporation exchange between the air and the water. The temperature differences between air and water strongly influence the exchange of heat flux and moisture between the two. Figure 2.8 is the measured air temperature in Lake Okeechobee between October 1, 1999 and September 30, 2000, the same period as the one shown in Fig. 2.7. The wind velocity in Fig. 2.7 and the air temperature in Fig. 2.8 are frequently mentioned in the case studies in modeling Lake Okeechobee. In addition to diurnal changes, the air temperature has strong seasonal variations. Figure 2.8 shows that the air temperatures in the lake area can be $>30\,°C$ in the summer and a few degrees centigrade in the winter, but never $<0\,°C$.

Solar radiation is often the most important heat flux component that acts as a heat source to a waterbody. Detailed discussions on solar radiation, heat fluxes, and evaporation will be presented in Section 2.3, where thermal processes are described. Precipitation is usually treated as an input of freshwater to a waterbody. For

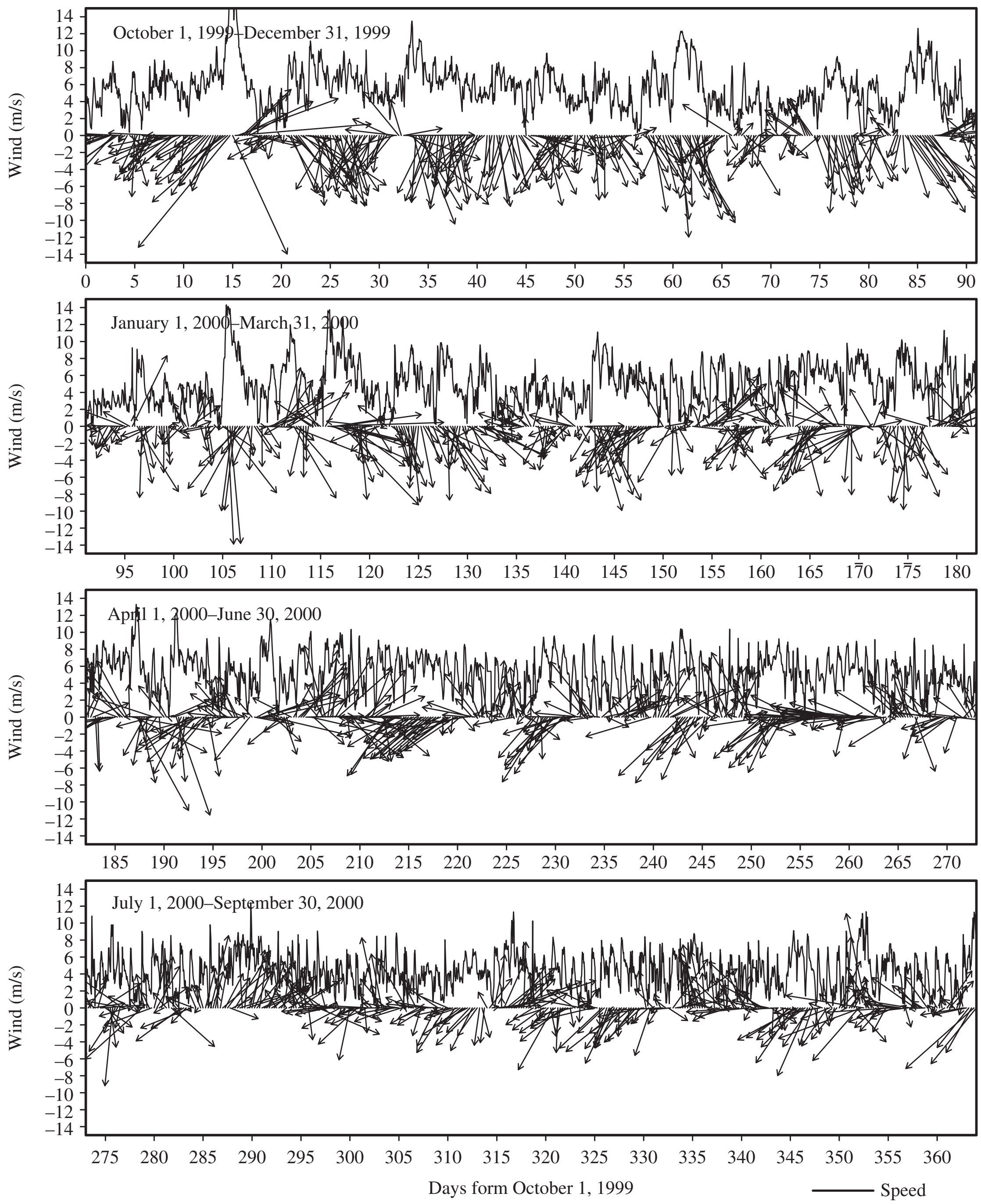

Figure 2.7 Measured wind at Station LZ40 in Lake Okeechobee, FL.

large subtropical lakes like Lake Okeechobee, direct rainfall on the lake surface is one of the major water sources. For water systems with relatively small surface water areas, such as rivers, the direct precipitation can be insignificant compared to inflows from tributaries and runoffs.

For coastal waters, atmospheric pressure affects sea level through the "inverse barometer effect," where low atmospheric pressure causes the sea level to be higher than normal (~1 cm/mbar). This effect, coinciding with storm surge, wind waves, and tides, can cause severe flooding in coastal areas. For most rivers, lakes, and estuaries, however, the hydrodynamic impacts of atmospheric pressure changes are usually small.

Wind stress is the tangential force per unit area due to the horizontal movement of the wind over the water

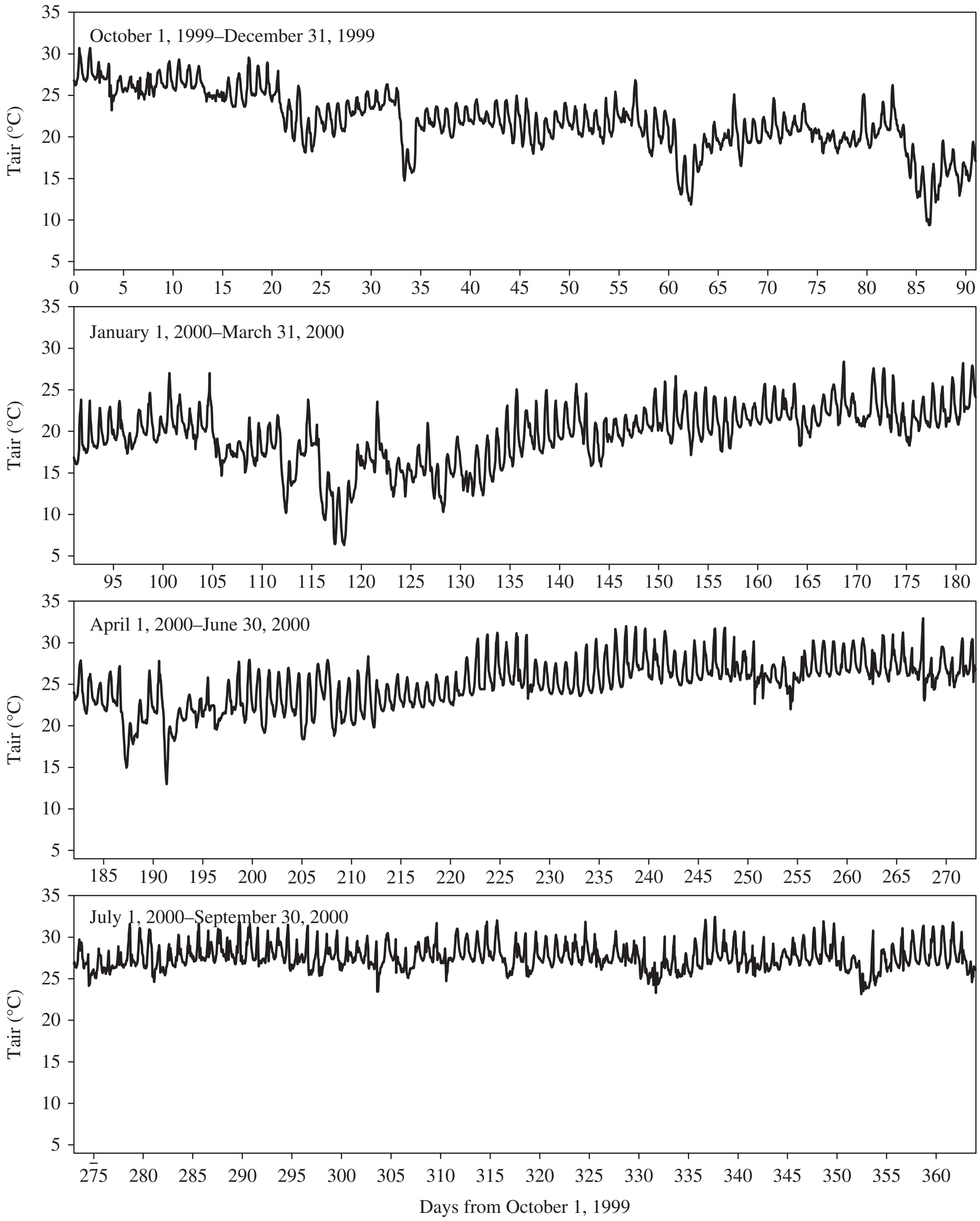

Figure 2.8 Measured air temperature at LZ40 in Lake Okeechobee, FL.

surface. It is determined by the wind speed, wind direction, and factors transforming the wind speed into wind stress. The latter is usually described by a drag coefficient and is estimated using several water and air parameters. The wind speed is the dominant parameter determining wind stress:

$$\tau = C_D \rho_A U^2 \tag{2.38}$$

where U = the wind speed at 10 m above the water surface (m/s), ρ_A = the density of the air (kg/m^3), C_D = the wind stress coefficient (dimensionless), and τ = wind stress (N/m^2). The density of air varies with temperature, pressure, and humidity, with typical values being 1.2–1.3 kg/m^3. The wind stress coefficient C_D generally increases with the wind speed. Hicks (1972) found that C_D is equal to 1.0×10^{-3} for wind speeds up to 5 m/s and increases linearly to 1.5×10^{-3} for a wind speed of

15 m/s. For wind speeds between 6 and 22 m/s, Smith (1980) suggested

$$C_D = (0.61 + 0.063 \cdot U) \times 10^{-3} \tag{2.39}$$

Hamrick (1992) used the following formulas for calculating wind stress in hydrodynamic models:

$$\tau_x = 1.2 \times 10^{-6}\,(0.8 + 0.065U) \cdot U \cdot u \tag{2.40}$$

$$\tau_y = 1.2 \times 10^{-6}\,(0.8 + 0.065U) \cdot U \cdot v \tag{2.41}$$

where τ_x = wind stress in the x-direction (N/m^2), τ_y = wind stress in the y-direction (N/m^2), u = wind speed in the x-direction (m/s), and v = wind speed in the y-direction (m/s).

For shallow waterbodies (less than a few meters), the longer water waves will not be able to develop fully and the water surface will remain smoother. Hicks et al. (1974) showed that under such conditions, C_D remains close to 1.0×10^{-3} for all wind speeds. Fischer et al. (1979) reported that the stability of the air column also has a strong influence on the value of C_D. Warm winds blowing over a cold waterbody are stabilized by the temperature difference, which in turn results in less friction. The value of C_D can be reduced by as much as 40% for stable conditions and increased equally by up to 40% for very unstable air flows. Lake Okeechobee is a large lake with a mean depth ~3 m. The longwaves in this shallow lake cannot fully develop, and the lake should have a relatively smoother surface. AEE (2005) used the following wind stress formulas for the lake modeling:

$$\tau_x = 1.2 \times 10^{-6}\,(0.8 + 0.065U) \cdot \alpha \cdot U \cdot u \tag{2.42}$$

$$\tau_y = 1.2 \times 10^{-6}\,(0.8 + 0.065U) \cdot \alpha \cdot U \cdot v \tag{2.43}$$

where α is an empirical coefficient for including the shallow water effects reported by Fischer et al. (1979) and Hicks et al. (1974). AEE (2005) reported that by setting $\alpha = 0.8$, the modeled currents follwed the measured data well. It should be mentioned that Eqs. (2.39)–(2.43) are all empirical formulas, and there are other formulas (e.g., Mellor, 1998; Sheng, 1986) that are similar to but slightly different from the ones presented here.

2.1.6 Coriolis Force and Geostrophic Flow

The Coriolis force term in Eq. (2.19), $-2\vec{\Omega} \times \vec{v}$, represents the effects of the earth's rotation. It was first described by the nineteenth-century French engineer–mathematician Gaspard-Gustave de Coriolis in 1835. Coriolis force is significant only when the spatial scale of the study area is very large, such as the Great Lakes and the Chesapeake Bay. Jin et al. (2002) reported that Coriolis force can be significant to circulations in Lake Okeechobee, which is a subtropical lake with spatial scale of 50 km. In hydrodynamic studies, the Coriolis parameter, $f = 2\Omega \sin\varphi$, can be treated as a constant, and its variation with latitude (φ) is often insignificant.

The Coriolis force (1) becomes evident in large waterbodies due to earth's rotation, (2) deflects motion to the right (left) in the Northern (Southern) Hemisphere, (3) allows geostrophic flow, and (4) leads to inertial oscillations. Owing to the Coriolis force, moving objects are deflected a few degrees to the right in the Northern Hemisphere and to the left in the Southern Hemisphere. In estuaries that are wide enough to be affected by this force, the effect is to deflect the seaward flow (freshwater flow) to the right side (looking toward the sea) of the estuary and landward flow (seawater flow) to the left. If the effect is strong, the net flow averaged over time can produce a secondary circulation, with a persistent seaward flow of freshwater along the right bank and a landward flow of seawater along the left bank.

When frictional forces are neglected, the steady-state flow is determined by the balance between the pressure gradient force and the Coriolis force. Equation (2.19) can be simplified to

$$2\vec{\Omega} \times \vec{v} = -\frac{1}{\rho}\nabla p \tag{2.44}$$

In Cartesian coordinates, we have

$$-fv = -\frac{1}{\rho}\frac{\partial p}{\partial x} \tag{2.45}$$

$$fu = -\frac{1}{\rho}\frac{\partial p}{\partial y} \tag{2.46}$$

This balance is known as geostrophic flow. As shown in Fig. 2.9, particles in the geostrophic flow move along the lines of constant pressure, with high pressure on their right (left) in the Northern (Southern) Hemisphere (looking in the direction of the flow). The geostrophic flow can be computed from these equations using the pressure gradient obtained by integrating the hydrostatic equation

$$\rho g = -\frac{\partial p}{\partial z} \tag{2.47}$$

which in turn uses the density calculated from temperature and salinity.

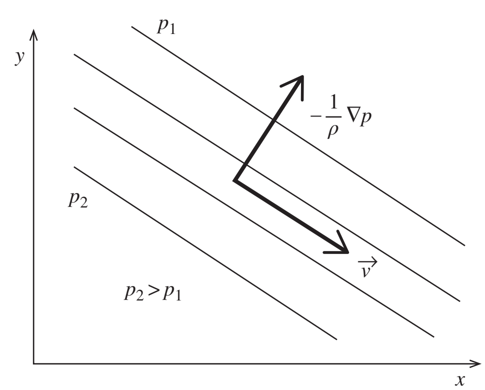

Figure 2.9 Pressure gradient and geostrophic flow.

Equation (2.19) can also be simplified to describe inertial oscillations:

$$\frac{\partial u}{\partial t} - fv = 0 \tag{2.48}$$

$$\frac{\partial v}{\partial t} + fu = 0 \tag{2.49}$$

These momentum equations have the following solution:

$$u = A \sin ft \tag{2.50}$$

$$v = A \cos ft \tag{2.51}$$

Equations (2.50) and (2.51) indicate that the inertial oscillations with amplitude A have the current vector rotating clockwise with the inertial period

$$T_f = \frac{2\pi}{f} \tag{2.52}$$

The inertial period T_f frequently dominates in current observations in the interior of large basins. T_f is equal to 18.6 h at 40°N.

The importance of Coriolis force can be estimated using a dimensionless Kelvin number, K, which is defined as the ratio of the domain size to the Rossby radius:

$$K = \frac{B}{R_0} \tag{2.53}$$

where the Rossby radius is given by

$$R_0 = \frac{C_0}{f} = \frac{\sqrt{gH}}{f} \tag{2.54}$$

In Eqs. (2.53) and (2.54), B is the domain size, f is the Coriolis parameter, R_0 is the external Rossby radius, C_0 ($= \sqrt{gH}$) is the phase speed of external gravity wave, and H is an average depth. For lakes and estuaries with $K \sim$ (or $>$) 1.0, the earth's rotation becomes important and the effects of Coriolis force should be considered. The opposite is also true: the Coriolis force can be neglected when K is much less than 1.0. For Lake Okeechobee, $B = 50$ km, $H = 3.2$ m, and $\varphi = 27$ °N, which yields $K = 0.6$. Therefore, Coriolis force can be significant to the lake circulations. The geostrophic flow in Lake Okeechobee will be discussed in Section 2.4.2, where the hydrodynamic modeling of the lake is presented as a case study.

The internal structure of a deep lake or estuary can be more responsive to the Coriolis force, because it is controlled by motions with smaller phase speeds. In this case, the Rossby radius is calculated using a reduced gravity:

$$R_0 = \frac{C_i}{f} \tag{2.55}$$

where C_i is the phase speed of the first baroclinic wave produced as a result of the density difference. A rough estimate for C_i is 1–2 m/s, corresponding to a water depth of 20 m and a density difference of 5–20 kg/m^3. For a mid-latitude estuary with f of 10^{-4} s^{-1}, the Rossby radius is equal to 10–20 km.

2.2 Governing Equations

This section describes the governing equations in hydrodynamic models. After introducing the commonly used assumptions in hydrodynamic modeling, the governing equations in one, two, and three dimensions are presented. Initial and boundary conditions for the governing equations are also discussed in this section.

2.2.1 Basic Approximations

As discussed earlier in this chapter, the conservation of momentum, mass, and energy provides the fundamental principles needed to develop hydrodynamic models. Even with advanced computers, these conservation equations are too complex to be solved numerically for large domains over long periods. Therefore, further simplifications are needed. This section discusses the approximations that are widely used in the studies of surface water systems: (1) the Boussinesq approximation, (2) the hydrostatic approximation, and (3) the quasi-3D approximation. These approximations are commonly used in the development and application of hydrodynamic models. It is essential to keep these approximations in mind when applying models to solve practical problems.

A widely used approximation in the studies of river, lakes, estuaries, and coastal waters is the so-called shallow water approximation. The shallow water (or longwave) approximation assumes that the horizontal scales of interest are much larger than the depth of water. When the water depth is much smaller than the wavelength, we have

$$H \ll \frac{1}{k} = \frac{L}{2\pi} \tag{2.56}$$

where H = water depth, k = wave number, and L = wavelength. Under the shallow water approximation, the surface gravity wave speed, c, depends only on the water depth and has the form of

$$c = \sqrt{gH} \tag{2.57}$$

In this case, the wave is nondispersive and the wave speed does not depend on wave number ($k = 2\pi/\mathrm{L}$). Similarly, the shallow water approximation in hydrodynamics states that the horizontal scale of motion, L, is much larger than the vertical scale of motion, H, that is,

$$\frac{H}{L} \ll 1 \tag{2.58}$$

This approximation is justified for most hydrodynamic processes in rivers, lakes, estuaries, and coastal waters, but not for studies such as jet plume modeling. The shallow water approximation is often assumed to be valid when $\frac{H}{L} \leq 0.05$. The Boussinesq approximation, the hydrostatic approximation, and the quasi-3D approximation represent different aspects of a shallow water system.

2.2.1.1 Boussinesq Approximation

A good approximation for describing surface water systems is to assume that the flows are incompressible, which means that the water density does not change with water pressure. The Boussinesq approximation is used to represent buoyancy in an incompressible fluid in which the density is not related to water pressure. In the Boussinesq approximation, variations in water density are ignored except when the gravitational force and buoyancy are considered.

The Boussinesq approximation is justified for most surface waters on the basis of small variations in density within the waterbodies. Typically, the density varies less than a few percent in a water column. The Boussinesq approximation does not depend on the shallow water approximation. Density changes due to local pressure gradients in the horizontal momentum equations are negligible. The water is treated as incompressible. The Boussinesq approximation excludes sound and shock waves in surface waters.

2.2.1.2 Hydrostatic Approximation

Many surface waters exhibit a common feature: their ratio of horizontal scale to water depth is very large (shallow water approximation). This leads to a widely used approximation in hydrodynamics, meteorology, and oceanography: the hydrostatic approximation. The hydrostatic approximation assumes that the vertical pressure gradient is almost balanced by the forcing due to buoyancy excess. The vertical acceleration then is a much smaller term and can be omitted.

From Eq. (2.19), a vertical momentum equation is typically written as

$$\frac{dw}{dt} + g + \frac{1}{\rho}\frac{\partial p}{\partial z} = 0 \tag{2.59}$$

where w = vertical velocity, g = gravitational acceleration, ρ = density, p = water pressure, t = time, and z = vertical coordinate. The hydrostatic approximation omits the term dw/dt and leads to the hydrostatic equation

$$\frac{1}{\rho}\frac{\partial p}{\partial z} = -g \tag{2.60}$$

The hydrostatic equation relates the vertical pressure gradient to the vertical distribution of density. Most of the 2D (vertical plane) and 3D hydrodynamic models use this approximation (e.g., Blumberg and Mellor, 1987; Hamrick, 1992). In these models, the vertical momentum equation is reduced to the hydrostatic equation (2.60).

The hydrostatic approximation implies that vertical pressure gradients are due only to density. When the horizontal scales are much greater than the vertical scales, the hydrostatic approximation is justified and, in fact, is identical to the shallow water approximation for continuously stratified waters. Given that the horizontal scale of natural waterbodies, such as river, lakes, and estuaries, is very much greater than their depth, this is generally a valid approximation. However, when the vertical scale of motion approaches the horizontal scale, the hydrostatic approximation becomes no longer valid. At these scales, the pressure at some point in the waterbody is also a function of the water velocity. For example, convective plumes from wastewater discharge diffusers are non-hydrostatic motions (Blumberg et al., 1996).

2.2.1.3 Quasi-3D Approximation

An alternative to deriving a fully 3D model is to treat the system as a set of horizontal layers that interact via source/sink terms representing water exchanges with overlying and underlying layers. This approach allows the elimination of the momentum equation in the vertical direction. For most surface water applications, the quasi-3D approximation ensures computational efficiency and model accuracy.

Most 3D hydrodynamic models used in rivers, lakes, and estuaries are actually quasi-3D models (e.g., Blumberg and Mellor, 1987; Hamrick, 1992). By using the hydrostatic approximation, the models have momentum equations only in the horizontal direction; and the vertical momentum equation is simplified to the hydrostatic equation, Eq. (2.60). This often prevents the application of these models to near-field problems, where a high degree of turbulence occurs. For example, a model that does not include vertical momentum equation cannot resolve momentum transfer due to a submerged jet. Except when jet plumes are simulated, the quasi-3D approximation is frequently used in hydrodynamic studies with sufficient computational accuracy. In most 2D laterally averaged models (e.g., Cole and Wells, 2000), a similar approach is also used so that the vertical momentum equation is not computed.

2.2.2 Equations in Cartesian Coordinates

Based on the Navier–Stokes equation presented in Section 2.1, the governing equations under the Cartesian coordinates in 1D and 2D are described. After introducing the sigma coordinate, this section also gives the 3D governing equations with the Cartesian coordinates in the horizontal and the sigma coordinate in the vertical.

Natural waterbodies are all three dimensional. The hydrodynamic and water quality variables in these systems have spatial variations over their length, width, and depth. There are instances in which a simplification in the governing equations is permissible. The relevant equations can then be reduced from three to two dimensions, or even to one dimension. Justifiable reductions in the dimensionality result in savings in model development, simulation, and analysis costs. A numerical model developed for a waterbody should only include the dimension(s) in which spatial variations affect the water quality analysis significantly.

A numerical model can be

1. zero-dimensional (0D),
2. one-dimensional (1D),
3. two-dimensional (2D), or
4. three-dimensional (3D).

Zero-dimensional models assume a well-mixed waterbody and do not have spatial variations. A small lake or pond that is completely mixed in all directions is a good example. Zero-dimensional models calculate water quality variables based on the conservation of mass. They may be used in preliminary estimations of water quality conditions in lakes.

One-dimensional models simulate the spatial change over a single dimension, typically oriented longitudinally down the length of a river or a narrow estuary. A 1D model in the vertical may also be applicable to a small, but well stratified lake. Two-dimensional models consider spatial variations in the lateral and longitudinal directions (in the horizontal plane) or in vertical and longitudinal directions (in the vertical plane). Three-dimensional models describe changes that occur over all three spatial dimensions and provide the most detailed assessment of pollutant distributions.

A 3D model should be easily applicable to 1D or 2D studies by using only a 1D or 2D model grid with little changes to the 3D model. For example, with a single layer in the vertical dimension, a 3D model can be reduced to a 2D model and can be applied to shallow, well-mixed waterbodies (e.g., Ji et al., 2001). Again, with a single cell in the lateral direction, the 3D model can be further reduced to a 1D model and can then be applied to shallow and narrow rivers (e.g., Ji et al., 2002a).

Eliminating a dimension in a numerical model implies neglecting the spatial variation in that dimension. For example, use of a 1D model in the longitudinal direction implies small deviations in concentrations from the cross-sectional mean, both laterally and vertically. The transport behavior of the river (or estuary) studied and the objectives of the study are the two major factors determining the dimensionality of the model needed.

2.2.2.1 1D Equations

The 1D model is defined with one space coordinate, that is, the model state variables are averaged over the other two directions. The use of a 1D model implies that the variation in directions perpendicular to the main channel is either neglected or not computed. It assumes well-mixed properties in the vertical, zero velocity across the main channel, and so on. These models describe flow and water quality concentrations in the direction of flow. One-dimensional models are often well suited to river flow problems but are less suited to lake/estuarine problems. The most likely application is for run of the river. This kind of free-flowing rivers is shallow and has high velocity, and is characterized by steep hydraulic profiles. They may have low-head dams or locks along the river. The Blackstone River, MA, is a typical one, and will be described in Chapters 3 and 4 as case studies (Ji et al., 2002a).

After neglecting the Coriolis force, the 1D continuity and momentum equations can be derved as

$$\frac{\partial H}{\partial t} + \frac{\partial (Hu)}{\partial x} = Q_H \tag{2.61}$$

$$\frac{\partial (Hu)}{\partial t} + \frac{\partial (Huu)}{\partial x} = -gH\frac{\partial \eta}{\partial x} - C_B|u|u + \frac{\partial}{\partial x}\left(HA_H\frac{\partial u}{\partial x}\right) + \tau_x \tag{2.62}$$

where $H = h + \eta$ = total water depth, h = the equilibrium water depth, η = surface displacement from equilibrium, u = water velocity in the x-direction, $|u|$ = water speed, Q_H = water inflow/outflow from the external sources, C_B = bottom drag coefficient, A_H = horizontal eddy viscosity, g = gravity acceleration, and τ_x = wind stress in the x-direction. In Eq. (2.62), the first term represents the time rate of change of horizontal momentum, and the second term is the horizontal advection of momentum in the x-direction. The first term on the right-hand side (RHS) of Eq. (2.62) is the force due to the horizontal pressure gradient. The second term on the RHS is the force due to bottom friction, and the third term on the RHS is the horizontal dispersion of momentum in the x-direction. The last term on the RHS is the wind forcing, which was already discussed in Section 2.1.5.

In hydrodynamic models, the subgrid-scale influence of turbulent mixing is parameterized using horizontal and vertical eddy diffusivity coefficients. The horizontal eddy viscosity represents the internal shear forces created by the transfer of momentum between faster and slower regions of flow by means of turbulent mixing. Its value cannot be directly measured or observed. It affects the velocity distributions and should be calibrated based on measured velocity data. In general, the higher its value, the more uniform the velocity distribution.

The horizontal eddy viscosity is not only related to the turbulence in the flow but also influenced by the way that

Eq. (2.19) or (2.62) is solved. Greater numerical dispersion results in lower horizontal eddy viscosity needed in a numerical model when Eq. (2.19) or (2.62) is solved using a coarser grid or averaged over longer time periods. The horizontal eddy viscosity A_H can be calculated using the Smagorinsky subgrid scale scheme (Smagorinsky, 1963), which can be generally written in 2D Cartesian coordinates as

$$A_H = C \,\triangle x \,\triangle y \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right]^{1/2} \tag{2.63}$$

where C = horizontal mixing constant, $\triangle x$ = model grid size in the x-direction, and $\triangle y$ = model grid size in the y-direction. The parameter C has typical values between 0.10 and 0.20. The Smagorinsky formula links numerical models' horizontal mixing to current shear and model grid size. The horizontal eddy viscosity A_H is small if the velocity gradients are small. If the horizontal spatial resolution ($\triangle x$ and $\triangle y$) is sufficiently fine so that major features of the bottom topography and the horizontal advection can be resolved in the model, the horizontal eddy viscosity A_H will be very small. Accordingly, the horizontal dispersion transport associated with A_H will be very small and can be neglected. For coarse spatial resolution, horizontal diffusion should be retained to represent the unresolved advective mixing and transport processes. Horizontal diffusion in a numerical model is also closely related to the numerical scheme used. Both the flow condition and the numerical scheme affect the horizontal dispersion in a numerical model.

Friction accounts for the dissipation of energy by small-scale turbulent motion. Frictional forces retard or change the direction of water flow. Frictional terms are included in momentum equations to parameterize the turbulent transfer of momentum within the water column or between the water and the boundaries, such as between the atmosphere and the water (the wind stress τ_x term in Eq. (2.62)) or between the water and the bottom (the term $-C_B|u|u$). In Eq. (2.62), the bottom drag coefficient C_B can be a spatially varying parameter. It represents the effects of bottom roughness on energy losses in flowing water. In addition to C_B, the Manning roughness coefficient is another commonly used parameter to represent bottom friction. The two can be linked together with the following formula (Johnson et al., 1991):

$$C_B = \frac{gn^2}{H^{7/3}} \tag{2.64}$$

where n = Manning roughness coefficient.

The 1D mass transport equation of a material concentration is

$$\frac{\partial (HC)}{\partial t} + \frac{\partial (uHC)}{\partial x} = \frac{\partial}{\partial x} \left(HA_C \frac{\partial C}{\partial x} \right) + S + R + Q_C \tag{2.65}$$

where C = concentration of a vertically and laterally averaged constituent, A_C = horizontal eddy diffusivity for mass transport, which is often set to equal to A_H, S = sources or sinks due to settling and resuspension, R = reactivity of chemical and biological processes, and Q_C = external loadings to the system from point and nonpoint sources.

2.2.2.2 2D Vertically Averaged Equations

Two-dimensional models are defined along two spatial coordinates, and the model state variables are averaged over the third remaining spatial coordinate. They can be either 2D vertically averaged or 2D laterally averaged. The 2D vertically averaged equations are presented here. The 2D laterally averaged equations are described next.

In shallow waterbodies, such as broad and well-mixed lakes and estuaries, a weak vertical stratification allows strong coupling of surface wind stresses and bottom friction stresses. The vigorous mixing minimizes vertical gradients in the water column. Physical transport is dominated by essentially depth-uniform horizontal advection. These conditions allow the general 3D equations to be approximated by 2D vertically integrated equations and eliminate all vertical structure (e.g., Hayter et al., 1998). Shallow and broad lakes, lagoons, and bays may be well represented with 2D vertically averaged models. Morro Bay, CA, is a good example of vertically mixed waterbody (Ji et al., 2001). Its simulation will be presented later in Section 10.5.2 as a case study.

The 2D vertically averaged conservation of mass and momentum equations can be expressed as

$$\frac{\partial H}{\partial t} + \frac{\partial (uH)}{\partial x} + \frac{\partial (vH)}{\partial y} = Q_H \tag{2.66}$$

$$\frac{\partial (uH)}{\partial t} + \frac{\partial (u^2 H)}{\partial x} + \frac{\partial (uvH)}{\partial y} - fHv = -gH\frac{\partial \eta}{\partial x} - C_B|u|u + \frac{\partial}{\partial x}\left(HA_H \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y}\left(HA_H \frac{\partial u}{\partial y} \right) + \tau_x \tag{2.67}$$

$$\frac{\partial (vH)}{\partial t} + \frac{\partial (uvH)}{\partial x} + \frac{\partial (v^2 H)}{\partial y} + fHu = -gH\frac{\partial \eta}{\partial y} - C_B|u|v + \frac{\partial}{\partial x}\left(HA_H \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y}\left(HA_H \frac{\partial v}{\partial y} \right) + \tau_y \tag{2.68}$$

where v = velocity in the y-direction, $|u| = \sqrt{u^2 + v^2}$ = water speed, and τ_y = wind stress in the y-direction. In Eq. (2.67), the first term represents the time rate of change of horizontal momentum, and the second and third terms are the horizontal advection of momentum in the x- and y-direction, respectively. The fourth term represents the Coriolis force. The first term on the RHS of Eq. (2.67) is the force imposed by the horizontal pressure gradient. The second term on the RHS is the force due to bottom friction, and the third and fourth terms on the RHS are the horizontal dispersion of momentum in x- and y-direction, respectively. The last term on the RHS is the wind forcing whose formulas are presented in Section 2.1.5. The terms in Eq. (2.68) have meanings similar to the ones in Eq. (2.67). The Smagorinsky formula, Eq. (2.63), can be used to calculate the horizontal eddy viscosity A_H.

The mass transport equation is

$$\frac{\partial(HC)}{\partial t} + \frac{\partial(uHC)}{\partial x} + \frac{\partial(vHC)}{\partial y} = \frac{\partial}{\partial x}\left(HA_C\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(HA_C\frac{\partial C}{\partial y}\right) + S + R + Q_C \tag{2.69}$$

where C = concentration of a vertically averaged constituent.

The vertically integrated models are relatively straightforward to program and can produce physically interesting results with only modest computational demands. Their major deficiencies are the absence of any vertical structure and the need for a simplistic parameterization of the bottom stress. Besides, in many 2D studies on rivers, the models usually have fixed river width at any particular river section and do not allow river width change with flow rates. Therefore, the flow is confined within the bounds of the 2D numerical grid, and the riverbanks are considered to be solid vertical walls. To realistically simulate this kind of riverbank flooding events, the model should have the so-called wetting and drying capability (e.g., Ji et al., 2001).

2.2.2.3 2D Laterally Averaged Equations

The other type of 2D models is the laterally averaged model. In narrow and deep lakes, reservoirs, and estuaries (especially fjords), the effects of narrow width may result in near-uniform distributions of hydrodynamic and water quality variables in the lateral direction. The primary transport in these systems is longitudinal advection and vertical mixing. These systems may be represented well with a 2D laterally averaged model.

As shown in Fig. 2.10, the x-coordinate represents the horizontal variation and the z-coordinate represents the vertical variation. The bathymetry slope shown in Fig. 2.10a is approximately represented by "stairs" in the Cartesian (x, z) coordinates in Fig. 2.10b. By neglecting the Coriolis force, the laterally averaged momentum equation can be derived from the Navier–Stokes equation:

$$\frac{\partial \eta}{\partial t} + \frac{\partial(uB)}{\partial x} + \frac{\partial(wB)}{\partial z} = Q_H \tag{2.70}$$

$$\frac{\partial(uB)}{\partial t} + \frac{\partial(u^2B)}{\partial x} + \frac{\partial(uwB)}{\partial z} = -\frac{1}{\rho}\frac{\partial Bp}{\partial x} + \frac{\partial}{\partial x}\left(BA_H\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial z}\left(BA_v\frac{\partial u}{\partial z}\right) + \tau_x \tag{2.71}$$

where B = water width, z = vertical Cartesian coordinate, w = vertical velocity, p = water pressure, and A_v = vertical

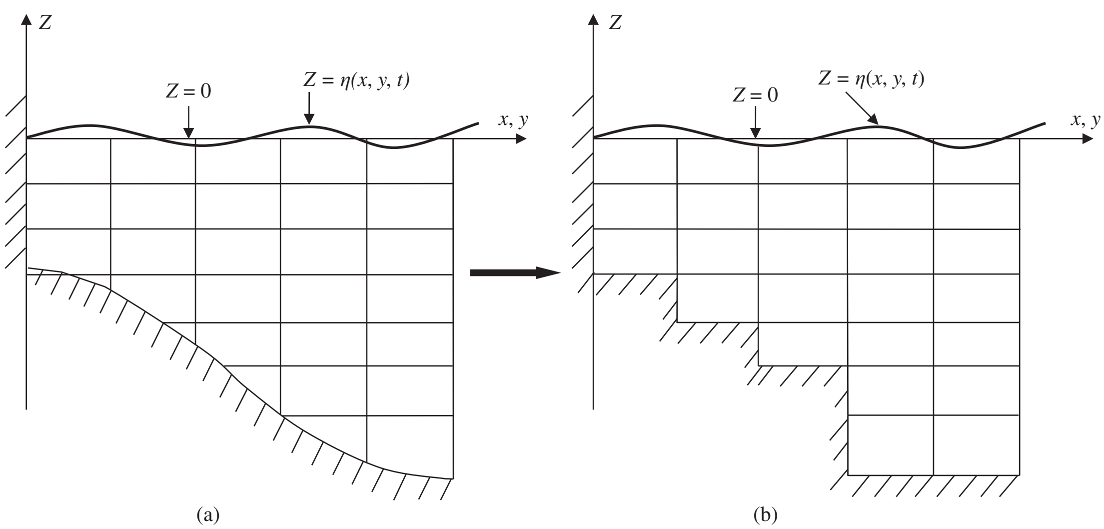

Figure 2.10 *x–z* Coordinates.

turbulent momentum mixing coefficient. In Eq. (2.71), the first term represents the time rate of change of horizontal momentum, and the second and third terms are the horizontal and vertical advection of momentum. The first term on the RHS of Eq. (2.71) is the force imposed by the horizontal pressure gradient. The second term on the RHS is the horizontal dispersion of momentum, and the third term is the vertical dispersion of momentum due to turbulent eddy mixing. The last term on the RHS is the wind forcing. The calculation of A_v will be discussed in Section 2.2.3.

The mass transport equation is

$$\frac{\partial(BC)}{\partial t} + \frac{\partial(uBC)}{\partial x} + \frac{\partial(wBC)}{\partial z} = \frac{\partial}{\partial x}\left(BA_H\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial z}\left(BA_b\frac{\partial C}{\partial z}\right) + S + R + Q \tag{2.72}$$

The free water surface elevation has

$$\frac{\partial(B_s\eta)}{\partial t} = \frac{\partial}{\partial x}\int_{-h}^{\eta} uB\,dz - \int_{-h}^{\eta} Q_H B\,dz \tag{2.73}$$

where B_s = surface water width, $-h$ = coordinate of the water bottom, η = coordinate of the water surface, Q_H = lateral boundary inflow/outflow, and A_b = vertical turbulent mass mixing coefficient.

2.2.2.4 3D Equations in Sigma Coordinate

In deep surface waters, vertical density stratification can suppress vertical turbulent mixing, resulting in significant vertical variations of hydrodynamic and water quality variables. These systems are most appropriately modeled with 3D models. A 3D model is defined along three spatial coordinates (length, width, and depth), under which the hydrodynamic and water quality variables vary over all three spatial coordinates. A 3D model is the most physically realistic representation for a waterbody, in which water quality variables have significant gradients in the longitudinal, lateral, and vertical dimensions. Deep and large lakes, reservoirs, estuaries, and coastal waters commonly need a 3D representation.

In hydrodynamic modeling, 3D equations are often written in the Cartesian coordinate in the horizontal directions and a sigma coordinate in the vertical direction. Therefore, before the 3D equations are presented, it is necessary to introduce the sigma coordinate.

2.2.2.4.1 Sigma Coordinate To provide uniform resolution in the vertical, a time-variable mapping or stretching transformation is desirable. The mapping or stretching is given by

$$z = \frac{z^* + h}{\eta + h} \tag{2.74}$$

where z = the stretched dimensionless vertical coordinate or so-called sigma coordinate, and z^* = the physical vertical coordinate or the Cartesian coordinate.

In Eq. (2.74) and in Fig. 2.11, "*" denotes the original physical vertical coordinates and $-h$ and η are the physical vertical coordinates of the bottom topography and the free surface respectively. That is

$$z = 0 \text{ at bottom topography } z^* = -h$$
$$z = 1 \text{ at free surface } z^* = \eta$$

This so-called sigma coordinate was originally outlined by Phillips (1957). As shown in Fig. 2.11, the sigma coordinate allows smooth representation of the bathymetry and same order of accuracy in shallow and deep waters. Water depths are divided into same number of layers in the sigma coordinate. The bottom is transformed into $z = 0$ plane, and the unknown water-surface elevation is exactly transformed into the $z = 1$ plane, which is fixed in the computational plane. With such transformation, the equations are transformed from the x–y–z^* into the x–y–z coordinate systems. Details of the transformation may be found in Vinokur (1974) or Blumberg and Mellor (1987). Free surface boundary condition allows the air–water interface to evolve freely. One advantage of the sigma coordinate is that, even under free surface boundary conditions, the water surface is always at $z = 1$, which is very convenient in numerical modeling. Figure 2.12 shows a water column with three sigma layers. Variable locations in a numerical model are also indicated in Fig. 2.12.

As shown in Fig. 2.11, the sigma coordinate has the same number of vertical layers, no matter what the water depths are. The thickness of each vertical layer for each grid cell is variable, since the thickness is computed from the number of vertical layers and the water column depth at each grid cell. This kind of terrain-following coordinate has computational efficiency and is able to present currents with a uniform number of vertical layers. However, when the topography is very steep, large bathymetry gradient could lead to extra dissipation between the grid cells in shallow waters and the ones in deep waters. In this case, special attention should be given to avoid large model truncation errors and artificial vertical mixing from the sigma coordinate. In deep water areas, the sigma coordinate might lead to insufficient vertical resolution in representing the surface mixing in the mixing layer. Besides, the vertical velocity in the sigma coordinate should be transferred back to the real vertical velocity in the Cartesian coordinate before it is used for model–data comparisons.

2.2.2.4.2 3D Equations in Sigma Coordinate The 3D mass and momentum equations in sigma coordinate are

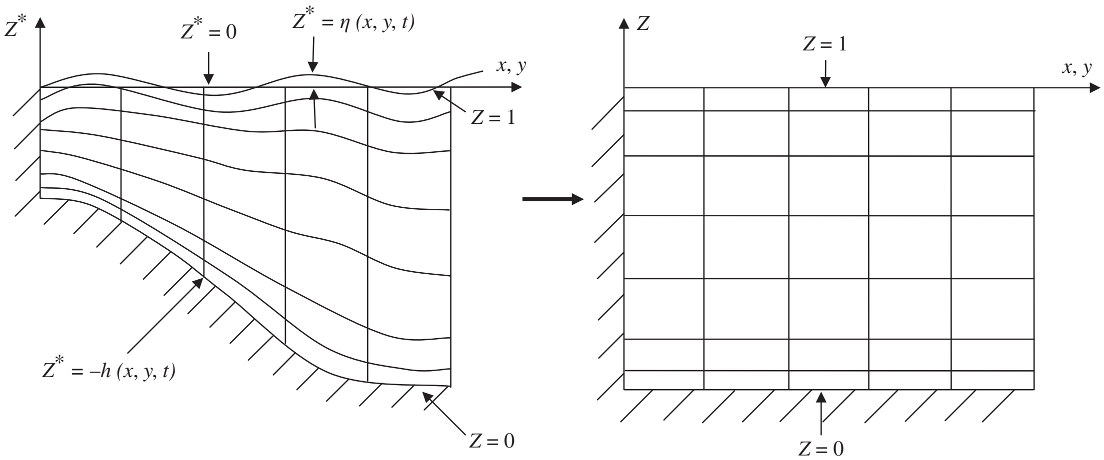

Figure 2.11 Vertical sigma coordinate system. z^* = Cartesian coordinate in the vertical direction, z = the sigma coordinate, and (x, y) = Cartesian coordinates in the horizontal directions.

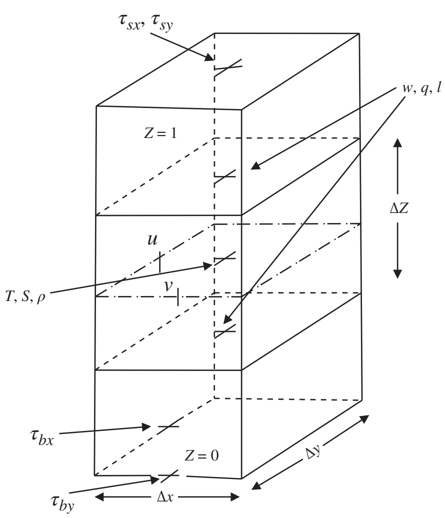

Figure 2.12 Sigma coordinate and variable locations.

(Hamrick, 1992)

$$\frac{\partial H}{\partial t} + \frac{\partial Hu}{\partial x} + \frac{\partial Hv}{\partial y} + \frac{\partial w}{\partial z} = Q_H \tag{2.75}$$

$$\begin{aligned}\frac{\partial (Hu)}{\partial t} + \frac{\partial (Huu)}{\partial x} + \frac{\partial (Huv)}{\partial y} + \frac{\partial (uw)}{\partial z} - fHv \\ = -H\frac{\partial (p+g\eta)}{\partial x} + \left(-\frac{\partial h}{\partial x} + z\frac{\partial H}{\partial x}\right)\frac{\partial p}{\partial z} \\ + \frac{\partial}{\partial z}\left(\frac{A_v}{H}\frac{\partial u}{\partial z}\right) + Q_u\end{aligned} \tag{2.76}$$

$$\begin{aligned}\frac{\partial (Hv)}{\partial t} + \frac{\partial (Huv)}{\partial x} + \frac{\partial (Hvv)}{\partial y} + \frac{\partial (vw)}{\partial z} + fHu \\ = -H\frac{\partial (g\eta + p)}{\partial y} + \left(-\frac{\partial h}{\partial y} + z\frac{\partial H}{\partial y}\right)\frac{\partial p}{\partial z} \\ + \frac{\partial}{\partial z}\left(\frac{A_v}{H}\frac{\partial v}{\partial z}\right) + Q_v\end{aligned} \tag{2.77}$$

$$\frac{\partial p}{\partial z} = -gH\frac{(\rho - \rho_0)}{\rho_0} = -gHb \tag{2.78}$$

$$(\tau_{xz}, \tau_{yz}) = \frac{A_v}{H}\frac{\partial}{\partial z}(u, v) \tag{2.79}$$

where p is the excess water column hydrostatic pressure, b is the buoyancy, and τ_{xz} and τ_{yz} are vertical shear stresses in the x- and y-direction, respectively.

The total depth, $H = h + \eta$, is the sum of the depth below and the free surface displacement relative to the undisturbed physical vertical coordinate origin, $z^* = 0$. The pressure p is the physical pressure in excess of the reference density hydrostatic pressure, $\rho_0 gH(1-z)$, divided by the reference density ρ_0:

$$p = \frac{\rho_0 gH(1-z)}{\rho_0} = gH(1-z) \tag{2.80}$$

The 3D temperature transport equation is

$$\begin{aligned}\frac{\partial (HT)}{\partial t} + \frac{\partial (HuT)}{\partial x} + \frac{\partial (HvT)}{\partial y} + \frac{\partial (wT)}{\partial z} \\ = \frac{\partial}{\partial z}\left(\frac{A_b}{H}\frac{\partial T}{\partial z}\right) + HR_T + Q_T\end{aligned} \tag{2.81}$$

where R_T = heating due to solar radiation, and Q_T = horizontal turbulent diffusion and external sources/sinks. As will be discussed in Section 2.3, solar radiation at the water surface attenuates with depth through the water column. The vertical velocity in the sigma coordinate (w) is related to the physical vertical velocity w^* by

$$\begin{aligned}w = w^* - z(\partial_t \eta + u\partial_x \eta + v\partial_y \eta) \\ + (1-z)(u\partial_x h + v\partial_y h)\end{aligned} \tag{2.82}$$

The mass balance equation for salinity (or a pollutant) is similar to Eq. (2.81) for temperature. The only difference is that the former should exclude the solar radiation term in Eq. (2.81).

2.2.2.4.3 Vertical Boundary Conditions in Sigma Coordinate

The vertical boundary conditions for vertical velocity are

$$w(0) = w(1) = 0 \tag{2.83}$$

which means that the vertical velocity at the surface and at the bottom is zero (Fig. 2.12).

Vertical boundary conditions for the momentum equations are kinematic shear stresses at the water bottom ($z = 0$) and the water surface ($z = 1$). Expressions for shear stresses are

$$\begin{aligned} A_v H^{-1} \partial_z (u, v)_{z=0} &= (\tau_{bx}, \tau_{by}) \\ &= C_B \sqrt{u_{\mathrm{bl}}^2 + v_{\mathrm{bl}}^2}\,(u_{\mathrm{bl}}, v_{\mathrm{bl}}) \end{aligned} \tag{2.84}$$

$$\begin{aligned} A_v H^{-1} \partial_z (u, v)_{z=1} &= (\tau_{sx}, \tau_{sy}) \\ &= C_D \sqrt{U_w^2 + V_w^2}\,(U_w, V_w) \end{aligned} \tag{2.85}$$

where τ_{bx} and τ_{by} = shear stresses at the bottom ($z = 0$), τ_{sx} and τ_{sy} = shear stresses at the surface ($z = 1$), U_w and V_w = wind velocity components at 10 m above the water surface, C_B = bottom drag coefficient, C_D = wind stress coefficient, and the subscript *bl* refers to the water velocity at the midpoint of the bottom layer. In a sigma coordinate model, the bottom drag coefficient C_B is usually calculated using (Mellor, 1998)

$$C_B = \frac{\kappa^2}{(\ln(\Delta z_b / 2z_0))^2} \tag{2.86}$$

where $\kappa = 0.4$ = the von Karman constant, Δz_b = the dimensionless thickness of the bottom layer, $z_0 = z_0^* / H$ = the dimensionless roughness height, and z_0^* = the bottom roughness height. Numerically, Eq. (2.86) is applied to the first sigma grid points nearest to the bottom. When the bottom of a water system is not well resolved by the vertical model layers, $\Delta z_b / 2z_0$ can be very large and lead to very small C_B. In this case, C_B is set to be a constant equal to 0.0025 in a numerical model (Blumberg and Mellor, 1987).

The wind stress coefficient C_D has a format similar to that discussed in Section 2.1.5:

$$C_D = 1.2 \times 10^{-6} \left(0.8 + 0.065 \sqrt{U_w^2 + V_w^2}\right) \tag{2.87}$$

where U_w and V_w are the wind velocity components (m/s).

The vertical boundary conditions on temperature and salinity are

$$\frac{A_v}{H} \left(\frac{\partial T}{\partial z}, \frac{\partial S}{\partial z} \right) = -\left(\langle wT(1) \rangle,\ \langle wS(1) \rangle \right), \quad z \to 1 \tag{2.88}$$

$$\frac{A_v}{H} \left(\frac{\partial T}{\partial z}, \frac{\partial S}{\partial z} \right) = 0, \quad z \to 0 \tag{2.89}$$

where $<wT(0)>$ = temperature flux at the surface (m/s °C) and $<wS(0)>$ = salinity flux at the surface (m/s ppt).

More discussions on temperature modeling and the related boundary conditions will be presented in Section 2.3. It is important to mention that the 3D equations can be simplified to 2D laterally averaged equations by eliminating terms associated with differentiations of x or y. The 2D vertically averaged equations can also be derived from the 3D equations. A 3D model should be easily applied to 1D or 2D studies by simply using a 1D or 2D model grid.

2.2.3 Vertical Mixing and Turbulence Models

Turbulence plays a critical role in vertical mixing and in the functioning of aquatic systems. It provides the energy required to carry nutrients from deeper waters (where they tend to accumulate) to surface waters (where they could be used in photosynthesis). Plant productivity is generally limited by the supply of nutrients. The greater the depth of water, the greater is the energy required to bring up the nutrients. Hence, shallow waters are generally more productive than deep waters.

Shallow waters, including rivers, lakes, estuaries, and coastal waters, have turbulence generated at the bottom or surface of the water. Vertical transport by turbulent diffusion can be sufficient to completely mix the water column. To accurately calculate the vertical turbulent mixing coefficients A_v and A_b in the equations of momentum and mass transport, it is necessary to have turbulence models that can represent the vertical mixing realistically. Only the basic concepts and theories that are commonly used in hydrodynamic models are presented here. For detailed discussions on turbulence theories, the reader is referred to the numerous books and papers on this topic (e.g., Canuto et al., 2001, 2002).

Turbulent flow is characterized by irregular and random velocity fluctuations. In turbulent mixing, mass is transferred through the mixing of turbulent eddies within the water system. It is the random motion of the water that does the mixing. This is fundamentally different from the process of molecular diffusion, which is caused by the random motion of molecules. In natural surface waters, turbulent diffusion is usually much stronger than molecular diffusion. Turbulence generated by vertical shear in the flow tends to mix dissolved constituents and acts to reduce sharp vertical gradients. Major turbulence-generating mechanisms include the following:

1. Water velocity shear
2. Wave breaking due to high wind and/or bathymetry change
3. Tides in estuaries and coastal areas
4. Inflows/outflows, such as rivers entering lakes or estuaries and water releases from reservoirs.

Some other mechanisms may also affect turbulence in a waterbody, but they are often negligible. For example, swimming fish may increase local dissipation rates by 10-fold compared to background levels (Farmer et al., 1987) and phytoplankton exudates can increase seawater viscosity and suppress turbulent dissipation rates (Jenkinson, 1986).

Generally, the stronger the flow, the more turbulent is the water column. In a lake environment, vertical mixing is generally caused by wind's action on the surface, through which eddy turbulence is transmitted to the lower portion of the water columns by shear stresses. The flow-through action in deep reservoirs also causes internal mixing. In estuaries, typically the vertical mixing is induced by the internal turbulence driven by the tidal flows, in addition to surface wind effects. In each environment, however, the amount of vertical mixing is controlled, to a large extent, by the density stratification in the waterbody, with strong vertical stratification inhibiting vertical mixing. Vertical stratification can be measured by the gradient Richardson number, which represents the ratio of the buoyancy force to the vertical velocity shear:

$$R_i = -\frac{g}{\rho}\frac{\frac{\partial \rho}{\partial z}}{\left(\frac{\partial v}{\partial z}\right)^2} \tag{2.90}$$

where R_i = gradient Richardson number (dimensionless), $\partial\rho/\partial z$ = vertical gradient of density (kg/m^4), and $\partial v/\partial z$ = vertical gradient of velocity (s^{-1}). The gradient Richardson number provides quantitative information on the relation between the stabilizing effect of buoyancy and the destabilizing effect of velocity shear. It indicates the tendency of the water column to either mix (weak stratification) or resist mixing (strong stratification). Large values of the gradient Richardson number indicate strong stratification, while small values are indicative of weakly stratified, well-mixed conditions.

If $R_i > 0$, the flow is stably stratified with lighter water floating over denser water, especially when $R_i \gg 0$. As the gradient Richardson number increases, the resistance to mixing increases. Generally, a value of $R_i = 10$ often indicates the presence of strong vertical stratification and almost complete inhibition of vertical mixing. As a result of strong stratification in a waterbody, for example, significant depletion of DO may occur at the bottom. The mixing of atmospheric oxygen at the bottom is restricted by the strong stratification. If $R_i < 0.25$, mixing occurs between the stratified layers. As R_i approaches zero, the flow approaches a neutral condition and the density is the same throughout the water column. If $R_i < 0$, flows are unstable, and heavier water overlies lighter water. Many lakes and reservoirs destratify during fall, as the result of colder air and decreased solar radiation. When the upper cooler layers are denser than the lower layers, lake overturning occurs, which causes rapid mixing of nutrient-laden bottom waters throughout the water column.

In numerical models, turbulent transport and mixing with spatial scales smaller than the model grid resolution are represented by vertical and horizontal turbulent dispersion. Horizontal dispersion, for example, can be represented by the Smagorinsky scheme in Eq. (2.63). Treatment of vertical mixing in mathematical models is generally achieved through the vertical eddy viscosity. The simplest approach is to represent turbulent mixing using empirical relationships to specify a constant mixing coefficient. Advanced hydrodynamic models, such as those of Blumberg and Mellor (1987), Hamrick (1992), and Sheng (1986), employ two-equation closure methods to provide internal calculations of vertical eddy diffusivity. The closure models provide the vertical turbulent diffusion coefficients necessary to represent vertical diffusive mass transport. There is a tradeoff between the complexity of the turbulence closure and the computational cost. In the 2D laterally averaged equations and the 3D equations, there are two parameters representing the vertical mixing: (1) the vertical turbulent momentum mixing coefficient A_v, and (2) the vertical turbulent mass mixing coefficient A_b. These two parameters can be calculated using turbulence models.

The original Navier–Stokes equations, such as Eq. (2.19), include all details of turbulence fluctuations and can be solved only by introducing time-averaged mean quantities. To account for the transport and history of eddy effects, two variables related to turbulence features in a two-equation turbulence model can be derived from the Navier–Stokes equations. Such models usually have turbulence variables such as turbulence kinetic energy and diffusivity (k–ε model) (e.g., Jones and Launder, 1972) or turbulence kinetic energy and turbulence length scale (k–l) (e.g., Mellor and Yamada, 1982). The turbulence closure scheme calculates the vertical turbulent momentum diffusion (A_v) and the mass diffusion (A_b) coefficients. The turbulence model described here was developed by Mellor and Yamada (1982) and modified by Galperin et al. (1988) and Blumberg et al. (1992). The model relates A_v and A_b to vertical turbulence intensity (q), turbulence length scale (l), and the Richardson number (R_q) by

$$A_v = \phi_v q l = 0.4\frac{(1 + 8R_q)ql}{(1 + 36R_q)(1 + 6R_q)} \tag{2.91}$$

$$A_b = \phi_b q l = \frac{0.5ql}{(1 + 36R_q)} \tag{2.92}$$