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ENVIRONNEMENTAL ENGINEERING

Hong LIU and Zhaoming CHEN

Water Quality Systems Informatics

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Water Quality Systems Informatics

Hong LIU and Zhaoming CHEN

This book presents an innovative integration of Water Quality Engineering with Systems Science and Information Science, offering a comprehensive theoretical framework alongside practical guidance to address the increasingly complex challenges of water quality management. The content is structured into three main parts: (1) Information and Signals in Water Quality Systems; (2) Linear Water Quality Systems; and (3) Nonlinear Water Quality Systems.

Adopting a novel perspective rooted in information space, the book provides a clear and accessible introduction to the fundamental theories and principles of system control in water quality systems. It equips readers with essential methodologies for data acquisition, signal analysis, and the development of precise and intelligent control strategies.

This work is intended as both a textbook and a reference for advanced undergraduate and graduate students in Environmental Engineering and Systems Engineering. It also serves as a valuable resource for researchers, professionals, and engineers working in Information Science and related technological fields.

Hong LIU is a Professor at the Chongqing Institute of Green and Intelligent technology, Chinese Academy of Sciences. His research focuses on environmental electrochemistry and wastewater treatment technologies.

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Acknowledgments

This book is dedicated to the memory and in honour of Academician Professor Cao Chunan (1930–2020), who served as the doctoral supervisor and intellectual guide for the primary author of this book. From 1996 to 1999, under Academician Cao's mentorship, the primary author pursued his doctoral studies, focusing on the development of an impedance spectroscopy model for the photocatalytic reaction associated with pollutant kinetics in water. This endeavour marked the beginning of his engagement with the application of mathematical language and definitional rules to address and solve problems within environmental engineering. Throughout the decade devoted to the composition of this book, both authors faced numerous challenges. They drew inspiration and perseverance from Academician Cao's integration of theory and practice, his meticulous and rigorous academic standards, his concise and potent scholarly style, and his commitment to truth and innovation.

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Preface

This book synthesizes the foundational theories and recent advancements in Water Quality Engineering Science, System Science and Information Science. By constructing a conceptual framework centred around water quality and water quality systems, it endeavours to apply mathematical language and definitional or structural rules to transform the study of water quality from a focus on unit processes and operations into a framework of system equilibrium and control. The former approach concentrates on the laws governing material and energy flows within individual components and processes, whereas the latter emphasizes the dynamic dependencies of information and signal flows across various components and processes.

This transformation deepens our understanding of the laws governing material and energy flows in water quality systems and offers new methods and strategies for analysing and controlling the flow of information and signals. This shift from a unit process and operational paradigm to one of system equilibrium and control represents a significant leap forward, aiding us to solve complex problems in water quality management and advancing the theoretical and technical aspects of Water Quality Engineering Science.

The concepts of water quality and water quality systems are central to this book and indeed form the theoretical foundation of the entire text.

Water quality is hereinafter defined as a mapping relationship between the state of water contamination and the time variable. This definition, as a time-domain function, not only reveals the physicochemical characteristics of water quality but also reflects its mathematical and informatics attributes. In essence, water quality is a time-domain function with signal characteristics, acting as a bridge between the physicochemical and informational spaces. This conceptualization serves as the theoretical cornerstone for transformative paradigms in the field of water quality engineering science. Furthermore, this definition allows for independent mathematical operations on water quality signals, facilitating the establishment of differential equations and state-space representations for water quality systems. This, in turn, lays down the theoretical and technical foundation for the control of water quality systems.

Water quality systems are defined in this book as a cohesive whole comprising interdependent parts and functions that persist (or evolve) over time. The study of

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water quality systems focuses on the dynamic interdependencies among various components and stages. While the processes and mechanisms within individual components and stages remain the core of water quality engineering and the micro-foundations of systems control theory, this book also theoretically explores the intrinsic connections between systems control theory and the theory of unit operations. Nevertheless, the primary focus remains on the theoretical underpinnings and control methodologies of water quality systems science.

Water quality systems are the structures and venues where water quality signals exhibit their dynamic changes. The rate of change of water quality signals, represented by the first derivative of the time-domain function, serves as a fundamental physical quantity for assessing the dynamic relationships among different parts and stages of water quality systems. Water quality information reflects the specific physical, chemical and biological laws of water quality, whereas water quality signals are the physical manifestations or carriers of this information, in electrical or optical forms, for example. The mathematical expressions of water quality signals transcend the original meanings of water quality information and form the theoretical basis for effective control of water quality systems. Both water quality information and signals occupy a special and significant place in this book.

This book delineates five fundamental signals within water quality systems and provides a detailed discussion based on these signals and their various combinations. The methods of analysing water quality signals, including time-domain, frequency-domain and complex frequency-domain analyses, represent the most recent applications of traditional signal analysis techniques in water quality systems. The control theory for water quality systems is also established on the mathematical operations of water quality signals.

The foundational approach of this book consists of establishing a conceptual framework for water quality systems based on the fundamental concepts of water quality. Drawing on physical, chemical and biological information within water quality systems, the book develops differential equations and state-space representations to describe signal variations in linear water quality systems, thereby establishing transfer function-based control methods. For non-linear water quality systems, the discussion primarily revolves around the describing function approach, phase-plane methods and includes several algorithms for intelligent control. Finally, in conjunction with common issues encountered in real-world water quality systems, the book discusses methods for analysing stochastic signals within these systems.

Methodologically, this book transforms the information on material and energy flows within water quality systems into mathematical equations for the purposes of further, specialized studies. These equations extend beyond the specifics of the information content, allowing for independent mathematical operations.

Integrating the contents of this book, one of the challenges in controlling water quality systems lies in establishing these mathematical equations, particularly in capturing the characteristics of material and energy flow changes through structural coefficients. Another lies in mastering the observability and controllability of water quality systems, determined by the inherent chemical and biological characteristics of these systems and also constrained by our limited understanding of these fields. In the

future, developing theoretical insights into the observability and controllability of linear water quality systems and exploring innovative design strategies or even disruptive process design methods will allow for a significant direction in the advancement of informatics in water quality systems. Additionally, the principles and methods for analysing and utilizing non-linear water quality systems and stochastic water quality signals will pose future research challenges.

It is unequivocally necessary for readers of this book to possess a robust foundational knowledge in mathematics, encompassing areas such as trigonometry, complex numbers, calculus, linear algebra and mathematical statistics, as well as a methodological approach to mathematical modelling. Additionally, a comprehensive understanding of environmental engineering science, particularly in terms of the specialization of water quality engineering science, is indispensable. Furthermore, foundational knowledge in fields such as signal processing and control theory is also required.

Throughout the writing process, mathematical methods relevant to water quality systems are introduced and elucidated through practical application scenarios. This approach is deliberately adopted to circumvent the complexities and tedium of mathematical derivations and proofs, thereby enabling readers to use these mathematical tools to grasp the fundamental concepts, theories and technical methods of informatics in water quality systems.

Currently, the field of informatics in water quality systems is still in its infancy, involving a multidisciplinary integration of various academic disciplines. The need for knowledge and experience from multiple disciplines is paramount. Inevitably, there may be some omissions and inaccuracies in the book and readers are invited to offer their criticism and corrections to the authors.

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Introduction

(I) The issue at hand

Water, as a fundamental and strategic natural resource, plays a pivotal role in human life, production and socio-economic development.

A given quantity of water used for production, living, or as an ecological water body can be considered a mixture of water molecules and other substances. These substances, regarded as impurities, determine the quality of the water—its purity or level of pollution.

In the context of sustainable development strategies, it is imperative to gain a deeper understanding of the essence of water quality in order to more effectively manage and protect water environments, resources and ecosystems. Water quality systems, whether natural systems with defined spatial boundaries, engineered systems composed of constructed units, or task systems artificially defined with specific physical, chemical, or biological objectives, all aim to improve water quality. Thus, the water quality engineering systems described in this book can exist as natural systems, engineered systems, or artificially designated task systems.

In daily life, industrial activities and the construction of ecological civilizations, it is frequently necessary to engage in engineering operations on water quality systems to facilitate water quality transformation. Such engineering endeavours, typically comprising multiple interrelated components or stages, represent quintessential systematic projects. From a systems thinking perspective, understanding and controlling the dynamics of water quality transformation projects hinges on mastering the dynamic relationships between the various components and stages, while the internal material movement and mechanisms within any single component or stage may be disregarded. This approach aligns with fundamental concepts, perspectives and methodologies in systems science.

Currently, the theoretical framework for recognizing and managing water quality transformation from a systems science perspective remains in a nascent stage, characterized by vague empirical understandings, with a comprehensive theoretical system yet to be established. The prevailing research paradigms in water quality engineering science tend to focus on the process mechanisms and control within specific components of water quality systems, often overlooking the dynamic interdependencies among these components. A critical question arises: How can one

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approach water quality transformation engineering from a systems science perspective? Furthermore, how can a theoretical "bridge" be established between water quality engineering science and systems science? These questions have repeatedly surfaced in the development of environmental engineering disciplines, attracting significant attention but remaining unresolved at a theoretical level.

Further contemplation prompts inquiries into how the dynamic relationships among various parts of water quality systems can be quantified. How can the rich information embedded within these dynamic relationships be excavated and used? How should one manage both deterministic and uncertain information inherent in these relationships? These issues frequently present challenges in the practical implementation of water quality transformation projects and have long troubled professionals without a theoretical resolution.

In summary, to effectively manage water quality transformation projects, it is imperative to apply theoretical and methodological principles of systems thinking within an informational space to address the recognition and control issues in water quality engineering. Evidently, this book represents an integration of water quality engineering science with systems and information sciences, it is aptly titled "Informatics of Water Quality Systems."

(II) Problem resolution

The objective of this text is to employ systemic thinking within the realm of information spaces to theoretically elucidate solutions to two categories of problems, thereby establishing and advancing the nascent interdisciplinary field of water quality informatics.

Firstly, the text aims to construct a bridge between the scientific disciplines of water quality engineering and water quality information. It proposes shifting the research paradigm of water quality engineering science from a focus on unit processes and operations to a systems-oriented perspective emphasizing equilibrium and control.

The prevailing research paradigm in water quality engineering science primarily utilizes the fundamental principles and methodologies of physics, chemistry and biology to examine the laws governing the fluxes of materials and energy within mixtures of pollutants and water within defined boundaries. These theories are well-established and provide precise descriptions and control mechanisms for specific processes and stages.

In the design and operation of unit processes, the theoretical foundation is based on the laws of conservation of mass, energy and charge. The primary objective of these processes is to optimize the efficiency of material and energy utilization. The law of conservation of mass also encompasses aspects of chemical reaction kinetics, focusing primarily on the rate of material transformations to determine the operational duration of unit processes. Collectively, these theories fall under the purview of the law of conservation of mass and are typically expressed in forms such as chemical equations, algebraic equations and differential equations.

The study of informatics within water quality systems presents both similarities and differences when compared to the research paradigms of unit processes and operations.

Initially, let us examine the similarities:

(1) *Convergence of control objectives*

Both the control objectives of unit operations and those of system-wide controls aim to maintain the stable operation of water quality systems, enhance process efficiency and reduce operational costs.

(2) *Similarities in intrinsic motion laws*

A system comprises various units where the movement of materials within each unit adheres to the theories of unit operations. Consequently, the overall movement patterns of the system are necessarily constrained by the theories of unit processes and operations. If the phenomena exhibited by the system are viewed as holistic, then the physical, chemical and biological phenomena within individual units can be considered local phenomena. There is a connection between these holistic and local phenomena. This is further elucidated by the derivation process from the law of conservation of mass within individual units to the differential equations describing the system's dynamic equilibrium, revealing an inherent logical connection from local to holistic perspectives.

Now, let us consider the differences:

(1) *Different objects of concern*

Water quality engineering science focuses on the precise description and control of individual parts and stages. In contrast, informatics within water quality systems overlooks these specific processes and mechanisms within each part and stage (including individual units), focusing instead on the dynamic interdependencies among various parts and stages.

(2) *Different theoretical foundations*

The theoretical foundation of water quality engineering science is based on the law of conservation of mass. Meanwhile, the theoretical foundation of informatics within water quality systems integrates system theory, information theory and control theory with practical applications in water quality systems, namely theories of equilibrium and control within these systems. The focus here is on the dynamic relationships among different parts and stages of the water quality system. These relationships are quantitatively represented through differential equations, difference equations, or state-space representations, which are forms of mathematical models that describe the interrelationships between system inputs and outputs and input-state-output configurations.

(3) *Different methodologies in the utilization of information and signals:*

In the discipline of water quality engineering science, the application of information is primarily confined to the specific content of information within physical, chemical, or biological processes. Essentially, this involves studying the material and energy flows of systems. By contrast, informatics within water quality systems focuses on the analysis of information and signal flows within these systems, representing another significant aspect of objective phenomena. This information and signal flows can further evolve into physical signals that are carried and transmitted

by sensing and detection equipment. All theoretical and technical methods in water quality systems informatics revolve around the nature and control of these signals. Thus, water quality systems informatics constitutes a scientific field concerned with the patterns and control of information and signal flows within water quality systems, where information and signals hold a central position in the theoretical and technical framework.

Secondly, addressing the theoretical foundations of water quality systems control and the practical value of water quality systems theory and methodologies.

1. **Theoretical foundations of water quality system control**

Achieving efficient control of water quality systems represents the ultimate goal of water quality engineering. The theoretical foundation of water quality systems control not only encompasses the principles and methods of systems theory, information theory, and control theory, but also integrates the fundamental principles and methods of water quality engineering science. This integration signifies the latest development in the theoretical foundations of water quality engineering science, reflected in several aspects:

(1) *Changes in the concept of water quality*

Traditionally, water quality was understood in terms of static data. This conception has been elevated to include a temporal function and at times, a spatial function as well. This notable change in definition underscores the systemic attributes of water quality engineering: the value of the water quality function at any given moment, based purely on traditional concepts, represents only a specific value in this context. This value is intrinsically linked to its preceding and succeeding values, highlighting the essential nature of temporal connections within water quality systems. This enriches and deepens our understanding of the dynamic processes in water quality systems. Moreover, this revised definition facilitates mathematical operations such as differentiation, the establishment of differential equations and state-space representations, thereby forging an intrinsic link between the physicochemical space and the information space of water quality, enhancing both theoretical relevance and engineering practicality.

(2) *Changes in evaluation metrics*

In the discipline of water quality engineering science, the pivotal metrics for assessing the operational status of water quality systems are water quality parameters. These parameters include, but are not limited to, pH, dissolved oxygen (DO), chemical oxygen demand (COD) and biochemical oxygen demand (BOD). Within the realm of informatics applied to water quality systems, the key evaluation metrics not only encompass these data points but also the rates of change of these parameters over time, along with their derivatives of various orders. These derivatives provide additional insights into the trends of water quality changes. Consequently, the rational expansion of these evaluation metrics, particularly through the incorporation of dynamic indicators, facilitates a more profound understanding of the dynamic behaviours of water quality systems. In practical applications, by

constructing differential equations and state-space representations that describe the dynamic changes in water quality systems, real-time monitoring and prediction can be achieved, thereby offering technical support for the control of water quality systems.

(3) *Transformation in theoretical expression*

In water quality engineering science, system descriptions predominantly utilize the law of conservation of mass, typically articulated through (bio)chemical reaction equations or algebraic equations. Differential equations are also employed to capture the primary information of physical, chemical, or biochemical processes, representing the intrinsic properties of a "process toolbox". In contrast, within water quality system informatics, the primary modes of theoretical expression are differential equations, difference equations, or state-space representations. These modes aim to depict the flow of information and signal streams that characterize the dynamic interdependencies among various system components and stages. It is important to note that while these expressions can be derived from the law of conservation of mass, they transcend it by quantifying the dynamic relationships among different parts of the system. This approach to theoretical expression can further evolve into a variety of control methodologies for water quality systems, such as transfer functions, transfer function matrices, zero-pole maps, root locus techniques and phase plane diagrams, thus enriching the content significantly.

(4) *Changes in information dimensions*

As previously mentioned, the focus within the field of Water Quality Engineering Science on water quality information has traditionally been limited to various dimensions such as physical, chemical, or biochemical. This information aids in the understanding and control of their respective physical, chemical, or biochemical processes. Typically, this information is deterministic, meaning that it can be obtained through experiments and measurements with clear numerical values. In contrast, the information involved in the Informatics of Water Quality Systems reflects the dynamic interdependencies among different components and phases within the water quality systems. This encompasses both deterministic and probabilistic (or uncertain) information, such as the uncertainty in predicting water quality parameters and the randomness in system operations, thus enriching the dimensionality of the information. Any information that enhances the deterministic understanding of water quality systems is considered valuable. The expansion and transformation of these informational dimensions contribute to a more comprehensive understanding of the dynamic behaviour of water quality systems, predicting trends in water quality changes and optimizing water quality control strategies.

(5) *Changes in the role of water quality signals*

In the field of Water Quality Engineering Science, the focus has predominantly been on the information itself, rather than on the signals, which are the physical carriers of information. However, in the Informatics of Water Quality Systems, both water quality information and signals are enriched and hold a central position,

particularly the role of water quality signals has reached an unprecedented level, becoming a prerequisite and tool for the control of water quality engineering systems.

These changes profoundly demonstrate that the Informatics of Water Quality Systems possesses attributes of systems science and incorporates a rich content of information science, thereby achieving a qualitative leap in understanding. This can be summarized in table 1:

Tab. 1 – Comparative theoretical connotations of water quality engineering science and informatics of water quality systems.

Dimension	Water quality engineering science	Informatics of water quality systems	Remarks
Concept of water quality	Water quality as data	Water quality as a function of time	Advances in conceptual frameworks
Evaluation metrics	Water quality index parameters	Water quality index parameters and their rates of change	Reflects system dynamics
Mode of expression	Reaction equations, algebraic equations, etc.	Differential equations, difference equations, state-space representations, etc.	Reflects the dynamic interdependencies among system components and phases
Information dimensionality	Physical, chemical, and biological dimensions	Dimensions of dynamic relationships among system components and phases	More enriched, facilitating understanding and control of water quality system properties
Water quality signals	Utilization of localized signals	Core position	Prerequisite and tool for the control of water quality systems

2. Practical significance of water quality system theory and methodology

Water quality informatics represents a significant breakthrough in our understanding of water quality engineering systems, offering substantial practical engineering value.

(1) *Theoretical guidance for traditional process operation methods*

In the field of water quality engineering science, traditional process operation methods, such as consistent dosing, intermittent dosing and unstable dosing within a certain fluctuation range, are common. However, these methods often lack precision when applied on a large scale. Within water quality informatics, these

operational methods can be translated into mathematical language, such as step functions, rectangular pulse functions and sine and cosine functions. Mathematical modelling and systems analysis further reveal that the unit impulse function is an ideal mode of material dosing. This theoretical model can more accurately describe and predict the response of water quality systems to material dosing, thereby providing targeted theoretical support for water quality transformation projects. For example, this approach can elucidate numerous existing engineering practices, such as the effects of pulse nano-bubbles on dissolved oxygen. It also provides guidance for the development of more efficient dosing equipment based on the unit impulse function, thus advancing technological innovation in the field of water quality engineering.

(2) *Guidance on design concept of water quality engineering units*

Analysis of water quality systems yields a critical parameter: the time constant of the water quality system. The time constant of a first-order water quality system, which includes indicators such as pollutant load and microbial activity, typically correlates directly with pollutant load and inversely with microbial activity. Higher-order water quality systems feature more complex indicators in their time constants. The value of the time constant determines the time required for the system to return to a stable state, leading to the development of new concepts such as critical load or microbial activity thresholds. These insights provide a theoretical basis and technical guidance for the design of water quality engineering units.

(3) *Theoretical guidance for state parameter selection of water quality systems*

In the realm of water quality engineering science, the state parameters predominantly encompass various water quality parameters. The selection of these parameters is principally guided by the requirements of regulatory management or determined by empirical knowledge and operational conditions. However, there are several issues associated with this approach: the data are often sparse, delayed, costly and lack shareability. It is generally recognized that the selection of water quality parameters should be scientifically grounded. The fundamental criteria include representativeness, whereby the parameters should reflect the overall state of the water quality systems, indicating the basic characteristics of the water body, the level of pollution and the health of the aquatic ecosystem. Additionally, these parameters should exhibit high sensitivity to changes within the water quality systems, enabling rapid and accurate responses to the presence of pollutants, environmental shifts, or external disturbances, thereby facilitating timely monitoring and early warning of changes in the water body. From the perspective of information science in water quality systems, it is imperative to select a minimal and complete set of state parameters that are not linearly representable by each other and are independent of input time functions.

(4) *Transformation in water quality state control mode*

The traditional control paradigm in water quality engineering predominantly relies on PID control using mechanical devices, employing relatively simplistic

technological approaches. In contrast, the control methods in informatics for water quality systems entail multidimensional control. These methods are grounded in the theoretical frameworks of transfer functions and root loci for water quality systems, which offer a richer theoretical content and more diverse technological approaches tailored to the control of water quality information systems.

The transformation brought about by this new control paradigm is significant. For instance, consider the control of a second-order water quality system. Traditional methods in water quality engineering science might involve using blowers, aeration equipment, or chemical dosing devices, where control is achieved by monitoring water quality data and providing feedback to subsequently adjust operational parameters of the equipment. However, in the realm of informatics for water quality systems, control can be executed based on the zeros of the transfer function derived from the differential equations of the second-order water quality system. By altering the zero parameters, one can more flexibly modulate the system's dynamic response characteristics, timely adjust control strategies to adapt to varying operational conditions and environmental demands, thereby ensuring the continuity and stability of water quality treatment. Moreover, the control paradigm in water quality informatics not only depends on mathematical models but also integrates modern information technologies such as big data analytics and artificial intelligence, enhancing the intelligence of control strategies. Through real-time monitoring and analysis of extensive water quality data, it is possible to predict trends in water quality changes, thereby enabling more precise control of water quality.

(5) *Guidance on new process research*

Informatics in water quality systems is not only applicable to the operational control and technological retrofitting of existing processes to enhance quality and efficiency, but it also plays a potential role in guiding the development of new processes. For instance, by applying the theoretical frameworks and methodologies of water quality systems informatics, one can establish mathematical descriptors for precise and intelligent control. This facilitates the bridging of the linguistic gap between water quality engineering science, informatics and control science. Consequently, it enables the establishment of water quality system models, the simulation of processes and the development of new process methodologies aimed at multi-objective optimization. These methodologies facilitate the effective recovery and utilization of resources (such as organics, nitrogen, phosphorus) and energy (such as bioenergy, thermal energy) in the wastewater treatment process.

3. Similarities and differences between water quality system and other systems

Water quality systems, when compared to other systems such as electromechanical systems, electrical circuit systems and engineering systems, share fundamental characteristics inherent to systems in general. These characteristics include dynamism, the principles of superposition and homogeneity in linear systems and the mathematical expressions used to describe these systems. However, distinct differences arise when focusing specifically on water quality systems. These systems are primarily concerned with the behaviour and patterns of water quality transformation, emphasizing factors directly related to water quality. The mathematical

formulations of water quality systems are derived from mass conservation laws pertinent to pollutants. Consequently, the specific parameters within these expressions are closely tied to the structural properties, initial conditions and boundary constraints of the water quality systems, dictated by the physical, chemical and biological specifics of the system.

Moreover, the input-output response of water quality systems, or the time required to return to a new equilibrium state following perturbations, is generally slow, particularly in systems involving biochemical reactions. For instance, in a first-order biochemical system, the time constant is inversely proportional to microbial activity. In a first-order chemical system, it is inversely proportional to the Gibbs free energy of the reaction; in a first-order electrochemical reaction system, it corresponds inversely to the Nernst potential. It is critical to note, however, that the relative speed of response in water quality systems can vary. Compared to ecological systems or some complex large systems, the response time of water quality systems may be considered relatively fast.

Part I

Information and Signals in Water Quality Systems

Progressing from the theory of unit operations in water quality engineering science to the equilibrium and control theories of water quality systems calls for a fundamental breakthrough in our understanding of these systems. The key here lies in shifting the focus from precise descriptions and control of internal process mechanisms within various components of water quality systems to recognizing and controlling the dynamic interdependencies between components. Expressing these dynamic relationships begins with the extraction of information from the internal processes of water quality systems, which is then developed into physical signals for system analysis and control. It is essential to understand that the foundational theories and technical principles established based on water quality signals transcend the specific information content of the individual components, thus enabling mathematical operations and further technical developments.

Part I initially establishes a basic conceptual framework in order to construct a theoretical foundation for bolstering our understanding of water quality systems. It then goes on to discuss the physical carriers of water quality information—water quality signals—including their mathematical representation, signal decomposition and transformational processing, which are fundamental methods for handling water quality information. Although time-domain methods of analysing water quality signals are simple and effective, complex water quality signals require resorting to Fourier Transforms to shift the analysis from the time to the frequency domain. For exponential growth signals such as $x(t) = e^{\alpha t}u(t)$(where $\alpha > 0$), which do not satisfy the conditions for a Fourier Transform, it becomes necessary to process these signals in the complex frequency domain through the application of the Laplace or Z-Transforms. The contents of this first chapter aim to recognize and understand the fundamental properties of water quality systems, thereby laying the theoretical groundwork for studying the dynamic characteristics and control methods of these systems.

Chapter 1

Introduction

This chapter initially introduces several basic concepts in order to establish an understanding of water quality systems. It then explores the dynamic attributes of water quality systems and discusses the contents involved in their analysis and management. Following this, chapter 1 goes on to define the informatics of water quality systems scientifically, clarifying the inherent interdisciplinary nature and importance of the field.

1.1 Fundamental Concepts

The theoretical foundation and disciplinary inception of Water Quality Engineering Science are rooted in a set of fundamental concepts characterized by their unique disciplinary features. These factors include COD, BOD,[1] Ammonia Nitrogen, Total Nitrogen and Total Phosphorus, among others. As an emerging interdisciplinary field, Water Quality Systems Informatics (WQSI) also calls for the definition of a series of basic concepts.

Water Quality: It is defined as the characteristics of water necessary to fulfil specific functions and uses. It is described by functions that characterize physical, chemical, biological and ecological attributes and their temporal evolution. Here, water quality, also referred to as water quality parameters of water, can be represented either as a single time-domain function, $x(t)$, or as a collection of multiple time-domain functions, denoted as $\{x_i(t), i = 1, 2, \ldots, n\}$, where n is the total number of water quality functions. These functions may be *univariate*, describing the variation of a single water quality indicator over time, or multivariate, describing the relationships among multiple indicators or their changes over time. Additionally, the expressions of water quality parameters can also take the form of vectors or

[1]BOD = Biochemical Oxygen Demand, is the amount of dissolved oxygen needed (*i.e.*, demanded) by aerobic biological organisms to break down organic material present in a given water sample at certain temperature over a specific time period. COD = Chemical Oxygen Demand, is an indicative measure of the amount of oxygen that can be consumed by reactions in a measured solution.

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matrices, especially when it is necessary to consider multiple indicators simultaneously or analyse water quality data within a multidimensional space.

Defining water quality in the mathematical form of time functions, rather than as isolated data points, represents a significant breakthrough and progress in our understanding of the intrinsic properties of water quality. This time-function-based definition of water quality enables mathematical operations such as differentiation and the development of differential equations and state-space representations, which are foundational for advancing related technological methods. From a mathematical perspective, water quality represents a mapping relationship between the information on the state of water contamination and the time variable.

Typically, water quality refers to the concentration of a substance in water, representing its chemical nature and the resulting quality of the water, such as BOD, COD, heavy metal content and organic pollutants. Frequently, water quality also includes physical state indicators of the water body, such as transparency, colour, temperature and solids in suspension.

In summary, water quality reflects the chemical, biological, or physical state of water and its evolutionary process. Its mathematical essence is a time-domain function, representing a dynamic mapping relationship between the state of water contamination and the time variable.

Water Quality Systems: These are comprehensive entities composed of various interconnected components and processes within the continuum or transformation of water quality, each reliant on (and contributing to) the specific functionalities of the whole. Water quality systems encompass a range of scales and types, from microscale experimental setups to larger, engineered systems such as municipal pipeline networks and wastewater1 treatment reactors. They also include both artificial and natural aquatic systems like rivers, channels, ponds and reservoirs in urban and rural settings, as well as task-specific systems designed for specific processes or stages, such as nitrogen removal in wastewater, phosphorus removal systems, anaerobic systems, aerobic systems, nitrification systems and denitrification systems. Several smaller water quality systems can be integrated to form larger, more complex systems, or a vast and intricate system can be subdivided into smaller, simpler subsystems that are easier to manage.

State of Water Quality Systems: This refers to the characterization of the dynamic state of water quality systems as described by a minimal set of time-domain variables that cannot be linearly represented in relation to each other. The state reflects the ongoing dynamics of the system, influenced by both internal process factors and external inputs, and is expressed as: $S(t+1) = f[S(t), I_r(t), P_c(t)]$, where $S(t)$ represents the state of the water quality system at the time t; $f(\cdot)$ denotes the system function, describing the interdependencies among the various components and processes. $I_r(t)$ represents external inputs, where $r = 1, 2, \ldots \alpha$, such as pollutant loads or operational parameters, and $P_c(t)$ represents internal process variables, where $c = 1, 2, \ldots \beta$, including characteristics of biological degradation, chemical reactions, carbon removal and nitrogen transformation processes. This set of independent variables that describes the state of water quality systems as a function of time is known as **the state variables of the system**.

In the context of a specific water quality system, the selection of state variables is not predetermined but must adhere to several essential criteria: (1) State variables are functions of time rather than frequency; (2) State variables must be linearly independent and cannot be expressed in terms of each other; (3) State variables should not include input functions or their derivatives but may encompass output functions and their derivatives; (4) Typically, the outputs of key structures or reaction units within the water quality system are selected as state variables; (5) The minimal number of state variables should equal the number of independent key structures or reaction units within the system, which can be referred to as **the order of the water quality system**. Choosing different state variables may result in diverse models of the water quality system, each corresponding to different descriptions of system behaviour and control strategies. In practical applications, it is advisable to select the smallest set of complete state variables to describe the system. This approach facilitates simplification of the system model, reduces the complexity of system control and decreases computational and implementation costs.

Water Quality Information: This constitutes an objective expression of the state and dynamic processes of water quality within a system, reflecting the motion and changes of water quality under specific temporal and spatial conditions. This information includes not only quantitative data on water quality but also encompasses the physical, chemical and biochemical reactions, mechanisms and effects associated with changes in water quality, as well as the dynamic interdependencies among various components and segments of the water quality system.

Typically, water quality information can be classified into *state information* and *process information*. The former refers to data describing the dynamic changes of the water quality system as it reaches a steady or equilibrium state, while the latter relates to information relevant before the system settles into these states. Analysing water quality information can enhance the certainty of understanding the water quality system and the precision of managing its current state. Water quality information is available in multiple forms, including data, text, images, audio and video.

The characteristics of water quality information can be delineated as follows. (1) **Spatiotemporal Dynamics**: Water quality information typically reflects the continuous variations of water quality states over time and space, as well as the dynamic responses of water quality processes. (2) **Quantitative Nature**: This type of information encompasses specific numerical values obtained through the measurement of various physical properties, chemical components and biological activities. (3) **Descriptive Nature**: Water quality information can describe physical attributes such as temperature, colour, odour, clarity and turbidity of the water. It also encompasses chemical properties like pH, dissolved oxygen levels, conductivity, total dissolved solids (TDS), total suspended solids (TSS) and dissolved inorganic substances (*e.g.,* iron, manganese, sulphur). Additionally, it can detail biological characteristics, including the presence of algae, bacteria and pathogens in the water. (4) **Material Nature**: Water quality information typically includes the types and concentrations of pollutants such as heavy metals, organic pollutants and chemical residues. These characteristics are interrelated and collectively form the multidimensional features of water quality information, providing critical support for the cognition and management decision-making of water quality systems.

Water Quality Information Space: A concept which refers to an aggregate formation where water quality information and its interrelationships coexist, representing the modes and manifestations of information within the field. Traditionally, the domain of water quality engineering science could be regarded as the physicochemical space of water quality systems, encompassing the physical, chemical and biological information manifestations. However, once the field of water quality engineering science extends into the information space, it signifies a comprehensive shift in research perspectives. Within this water quality information space, it becomes possible to collect and integrate water quality data, conduct analyses and processing of water quality information, utilize mathematical methods to construct predictive models of water quality systems and provide scientific foundations and decision-making support for the management of complex water quality systems.

Water Quality Signals: Water quality signals refer to the physical manifestations or expressions of water quality information, such as electrical, optical, acoustic, or thermal forms. These signals function as variables dependent on time and/or space. For non-electrical water quality signals, conversion into electrical signals is necessary to facilitate their analysis and utilization. Water quality signals serve as the physical carriers of information within water quality systems, providing the essential prerequisites and mathematical tools for understanding and controlling these systems. Water quality information, conveyed by these signals, represents a multidimensional reflection of the state of water quality systems. Water quality information and signals occupy a fundamental and central role within these systems. The conversion of diverse water quality information within these systems into signals recognizable by instrumental apparatus often becomes a critical aspect in the development of control technologies for water quality systems. Thus, water quality signals act as a "bridge" between the physicochemical space and the informational space of water quality.

Water quality signals typically include both analogue and digital formats. Analogue water quality signals are continuous-time signals recognized and captured by various sensors and detection instruments, representing parameters such as dissolved oxygen, pH levels and turbidity as functions of time, denoted as $x(t)$. When water quality signals possess defined values only at specific, discontinuous moments and are undefined at other times, they are referred to as discrete water quality signals, denoted as $x(n)$, where n is an index. Analogue water quality signals are converted into a special type of discrete signal, termed digital water quality signals, through processes of sampling, holding, quantization and encoding. These signals are usually represented in binary form to facilitate storage, transmission and processing by computer systems.

1.2 Dynamic Attributes of Water Quality Systems

Water quality systems are characterized by their dynamic and evolving nature, where the interdependencies among various components and processes form dynamic relationships. The understanding and control of these systems are

mediated through water quality signals. In essence, water quality systems are the venues and mechanisms for the dynamic transformation of these signals. Therefore, the dynamic attributes of water quality systems are expressed through the dynamic properties of the water quality signals.

1.2.1 The Dynamics of Water Quality Signals and Their Mathematical Representation

In the study of the dynamics of any entity, the primary focus is placed on its trajectory. The most intuitive trajectory one might consider is linear motion. However, purely linear motion is rare or virtually non-existent in Nature. For instance, vehicles on highways do not move in a straight line over extended periods but rather follow a curved trajectory. A more detailed examination of the movement patterns of snakes or worms reveals a distinctly curvilinear form. Thus, the inherent trajectory of objects is curved, with linear trajectories being a special case of curved ones.

Experience suggests that water quality signals, which carry water quality information, are subject to dynamic changes and often manifest in a curvilinear state. Consequently, it is reasonable to hypothesize that a typical, ideal and simple curvilinear trajectory can be represented by a sinusoidal curve. This leads to the question of whether sinusoidal functions such as sine and cosine could be employed to model the trajectory of these movements.

A sine function can be expressed as a cosine function offset by an angle of $\frac{\pi}{2}$:

$$\sin\left(\omega t + \frac{\pi}{2}\right) = \cos(\omega t) \tag{1.2.1}$$

where ω represents the angular velocity, indicating the rate of angle change during sinusoidal motion and t denotes time; their product ωt is the angle θ.

For any given water quality signal $x(t)$, it can be represented using a cosine function:

$$x(t) = A\cos(\omega t + \theta) \tag{1.2.2}$$

Let A be the amplitude, for simplicity, set $A = 1$. If the motion trajectory of a water quality signal follows a cosine function, it completes one circular motion, equivalent to one period $T(T = 2\pi)$. Within a unit circle $(A = 1)$, the trajectory is illustrated as follows:

At any given moment, the coordinates of the signal point can be represented by the vector $\overrightarrow{c}$:

$$\overrightarrow{c} = a + bj \tag{1.2.3}$$

where j is the unit imaginary number. Noting that $a = \cos\theta$ and $b = \sin\theta$, we have:

$$\overrightarrow{c} = \cos\theta + j\sin\theta \tag{1.2.4}$$

According to Euler's formula, the vector $\overrightarrow{c}$ can also be transformed into $e^{j\theta}$, as:

$$e^{j\theta} = \cos\theta + j\sin\theta \tag{1.2.5}$$

Therefore, the motion trajectory of an ideal simple water quality signal can also be represented as a combination of complex numbers and trigonometric functions:

$$x(t) = \cos(\omega t) + j\sin(\omega t) \tag{1.2.6}$$

1.2.2 Rate and Frequency of Movement in Water Quality Signals

All moving entities possess a definite *rate of motion*, which, like the motion trajectory, serves as a vital piece of information about the motion. For any given water quality signal $x(t)$, as depicted in figure 1.2.1, its rate v can be described as the derivative of $x(t)$ at a particular moment, expressed as follows:

$$v = \frac{dx(t)}{dt} \tag{1.2.7}$$

Subsequent analyses will demonstrate that the mathematical equations describing linear water quality systems are constituted by the function $x(t)$ and its derivatives, underscoring the significance of the rate of motion of water quality signals.

For water quality signals characterized by sine and cosine functions, the angular velocity of their motion can be denoted by ω. Notably, this angular velocity is independent of the circle's radius. Given that ωt equals the angle θ, its differential form is:

$$\omega = \frac{d\theta}{dt} \tag{1.2.8}$$

Furthermore, the period T of a cosine function, representing the time required to uniformly complete one circular path, can be calculated by dividing the circle's radian measure by T, yielding the angular velocity ω:

$$\omega = \frac{2\pi}{T} \tag{1.2.9}$$

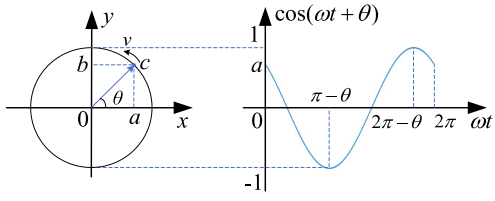


FIG. 1.2.1 – Trajectory of a cosine function signal within a unit circle over one period.

The reciprocal of the period T defines the frequency, $f = \frac{1}{T}$, indicating the number of cycles completed per unit time:

$$\omega = 2\pi f \tag{1.2.10}$$

Thus, the angular velocity of circular motion is equivalent to the angular frequency. *Frequency* is an inherent characteristic of water quality signals and, in many scenarios, it is of greater interest than the rate of motion.

The discussion above pertains to a general characteristic of signal motion, namely that it can be represented using sine and cosine functions, encompassing motion trajectory, rate and frequency. Equation (1.2.6) illustrates the relationship between sinusoidal signals and complex exponential signals. Further discussion will now enable us to explore the complex description of water quality signals.

1.2.3 Complex Representation of Water Quality Signals

In water quality systems, employing a complex representation of water quality signals facilitates the simplification of signal analysis and processing, particularly when addressing complex periodic signals. Utilizing the complex form of signals enables straightforward operations such as superposition, decomposition and transformation.

In the complex number $c = a + jb = |c|e^{j\theta}$, by setting $a = \cos\theta$ and $b = \sin\theta$, we obtain:

$$\cos\theta + j\sin\theta = e^{j\theta} \tag{1.2.11}$$

Equation (1.2.11) is recognized as Euler's formula, which plays a crucial role in simplifying the computation of complex water quality signals. A brief proof follows, utilizing the Taylor series expansion:

$$\cos\theta = 1 - \frac{\theta^2}{2} + \frac{\theta^4}{4} - \frac{\theta^6}{6} + \cdots \tag{1.2.12}$$

$$\sin\theta = \theta - \frac{\theta^3}{3} + \frac{\theta^5}{5} - \frac{\theta^7}{7} + \cdots \tag{1.2.13}$$

Similarly, expanding $e^{j\theta}$ yields:

$$\begin{aligned} e^{j\theta} &= 1 + \frac{j\theta}{1!} + \frac{(j\theta)^2}{2!} + \frac{(j\theta)^3}{3!} + \cdots \\ &= 1 - \frac{\theta^2}{2} + \frac{\theta^4}{4} - \frac{\theta^6}{6} + \cdots + j\left(\theta - \frac{\theta^3}{3} + \frac{\theta^5}{5} - \frac{\theta^7}{7} + \cdots\right) = \cos\theta + j\sin\theta \end{aligned}$$

By substituting $-\theta$ for θ in equation (1.2.10), we derive:

$$\cos\theta - j\sin\theta = e^{-j\theta} \tag{1.2.14}$$

Adding equations (1.2.11) and (1.2.14) results in:

$$e^{j\theta} + e^{-j\theta} = (\cos\theta + j\sin\theta) + (\cos\theta - j\sin\theta) = 2\cos\theta os\theta = \frac{1}{2}(e^{j\theta} + e^{-j\theta}) \quad (1.2.15)$$

Similarly:

$$e^{j\theta} - e^{-j\theta} = 2j\sin\theta,$$

Therefore:

$$\sin\theta = \frac{1}{2j}(e^{j\theta} - e^{-j\theta}) \quad (1.2.16)$$

For water quality signals represented by sine and cosine functions, which are time-varying, we can set $\theta = \omega t$ and substitute into equations (1.2.15) and (1.2.16) to obtain the complex expression of water quality signals:

$$\cos\omega t = \frac{1}{2}(e^{j\omega t} + e^{-j\omega t}) \quad (1.2.17)$$

$$\sin\omega t = \frac{1}{2j}(e^{j\omega t} - e^{-j\omega t}) \quad (1.2.18)$$

As time t varies, the mapping relationship between the complex exponential signal $e^{j\omega t}$ and the sine and cosine signals $\sin\omega t$ and $\cos\omega t$ is illustrated in figure 1.2.2.

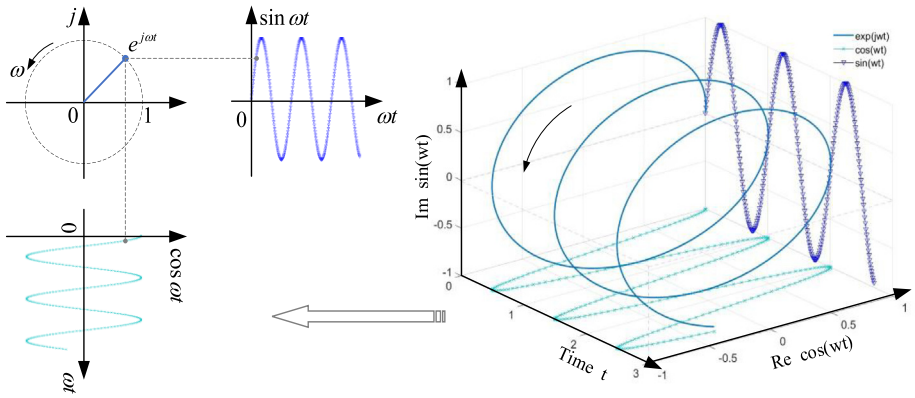


FIG. 1.2.2 – Relationship between the complex exponential signal and sine and cosine signals.

It is noteworthy that the motion trajectory of signals is often complex and in practical water quality transformation engineering, it is challenging to encounter water quality signals as simple as individual sine or cosine signals. How, then, can

such complex water quality signals be represented? In reality, any complex water quality signal can be expressed as a *weighted sum* or integral of a set of sine and cosine functions. This concept underlies the Fourier Transform of signals, which will be analysed in detail in this book.

1.3 Analysis and Management of Water Quality Systems

1.3.1 Input–Output Mapping

As previously discussed, water quality systems essentially serve as mechanisms through which water quality signals are transmitted and transformed. Therefore, understanding and controlling these systems can begin by establishing a mapping relationship between input (signals) and output (signals), as illustrated in figure 1.3.1.

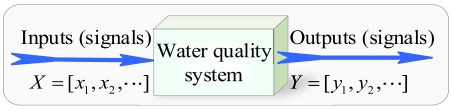


FIG. 1.3.1 – Schematic of the input–output mapping in water quality systems.

Input signals consist of materials, energy, or certain physical forms of stimulus or perturbations imposed externally on the water quality systems, while output signals are the responses exhibited by the water quality systems under the influence of input signals, in terms of materials, energy, or some physical forms. Output signals may also include random perturbations unrelated to the input signals. Only those signals that produce significant alterations in the water quality systems, such as changes in the thermodynamic state or kinetic rate-controlling steps of chemical or biochemical reactions, qualify as input signals. These include variations in process parameters such as dosage amounts, influent flow rates, aeration volumes and recirculation ratios. The function describing the change in state parameters or other predetermined physical quantities in the water quality systems due to the stimulation of input signals constitutes the output signals. A common example is the time-domain function of some water quality parameter or the function of the oxidation–reduction potential.

Input and output signals are typically described using time-domain functions. These can be transformed into frequency-domain functions through signal transformation, facilitating frequency-domain analysis. The correspondence between inputs and outputs in water quality systems, determined by functional relationships, predefined rules, or models, constitutes the input–output mapping of these systems. Direct mapping can be established between inputs and outputs to provide an external description of the water quality systems, or indirect mapping can be established through the systems' dynamic states for an internal description. For any

given water quality system, the input–output mapping comprises both linear and non-linear mappings.

1.3.2 Linear-Non-Linear Analysis

In essence, all water quality systems are inherently non-linear. To simplify our analysis, while preserving the primary physical significance, water quality systems are often treated as linear systems. Mathematically, a linear water quality system is defined by its physical, chemical and biological processes reaching a steady state, where the equations or models describing the system satisfy both *homogeneity* and *superposition* principles. *Homogeneity* implies that if the input signal $x(t)$ to the water quality system is scaled by a constant k, the output response $y(t)$ also scales by the same factor, that is, $x(t) \rightarrow y(t)$ leads to $kx(t) \rightarrow ky(t)$. *Superposition* means that the response produced by multiple input signals acting on the water quality system equals the sum of the responses that each input signal would produce independently, *i.e.*, $x_1(t) \rightarrow y_1(t), x_2(t) \rightarrow y_2(t)$ imply $x_1(t) + x_2(t) \rightarrow y_1(t) + y_2(t)$. Linear water quality systems include both single-input single-output and multiple-input multiple-output configurations. In practical engineering, if a wastewater treatment reactor follows first-order reaction kinetics, it often behaves as a linear system; if it follows second-order kinetics, it behaves as a non-linear system. There is no absolute demarcation between linear and non-linear systems; they can often be transformed into one another and can also be artificially delineated based on engineering objectives.

A water quality system that includes a single input $x(t)$ and a single output $y(t)$ and satisfies linear characteristics, is termed a single-input single-output linear water quality system $h(t)$, where $x(t)$, $y(t)$ and $h(t)$ are time-domain functions (*cf.*, figure 1.3.2). If the input and output signals also satisfy time-invariance, meaning the output does not change with the time origin of the input, the system can be further simplified to a linear time-invariant water quality system.

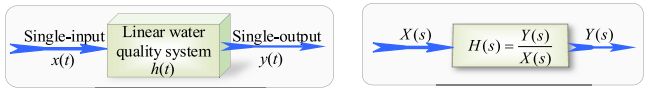


FIG. 1.3.2 – Schematic of a single-input single-output linear water quality system.

For continuous-time linear water quality systems, based on the law of conservation of mass, the following ordinary constant coefficient linear differential equation can be derived to quantitatively describe the dynamic relationships between the input and output:

$$\begin{aligned} & a_n \frac{d^n}{dt^n} y(t) + a_{n-1} \frac{d^{n-1}}{dt^{n-1}} y(t) + \cdots + a_1 \frac{d}{dt} y(t) + a_0 y(t) \\ & = b_m \frac{d^m}{dt^m} x(t) + \cdots + b_1 \frac{d}{dt} x(t) + b_0 x(t) \end{aligned} \tag{1.3.1}$$