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Marcello Benedini George Tsakiris

Water Quality Modelling for Rivers and Streams



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Water Quality Modelling for Rivers and Streams



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To Anna and Mary

Preface

The idea of writing this book originated several years ago; however, due to certain factors it got delayed, and we have now finally been able to realise it. The objective of this book is to explain the computational methods that deal with the complex problem of water quality modelling in rivers and streams. The book provides in-depth coverage of computational open channel hydraulics as well as water quality issues and describes scientifically sound synthesised procedures that are relatively simple to use and fundamental for simulation purposes so that practical results can be achieved.

It was not our intention to replace any of the comprehensive books on numerical open channel hydraulics and water quality. The knowledge gathered in these two scientific areas over the last 50 years is so vast that it is impossible to review it comprehensively in a volume of this type.

On the contrary, the objective of the book is to address some fundamental problems of water quality in rivers and streams by integrating methods and procedures from these scientific fields. Our intention is thus to describe modelling fundamentals that will assist potential developers and users in devising the new generation of models, which will serve specific requirements in keeping with new legislation in many areas of the world, the Water Framework Directive in Europe being the principal reference.

Readers who would like to acquire deeper knowledge of the methods presented briefly in this book are recommended to refer to the following scientific literature on computational hydraulics: *Practical Aspects of Computational River Hydraulics*, by J. Cunge, F. Holly and A. Verwey; *Computational Hydraulics – Elements of the Theory of Free Surface Flow*, by M.B. Abbott; *Computational Techniques for Fluid Dynamics*, by C.A. Fletcher; and the recently published *Numerical Modelling in Open Channel Hydraulics*, by R. Szymkiewicz.

Readers can also refer to the following books on water quality science: Aquatic Chemistry, by W. Stumm and J. Morgan; Surface Water-Quality Modeling, by S.C. Chapra; Hydrodynamics and Water Quality: Modelling Rivers, Lakes and Estuaries, by J. Zhen-Gang; and Quality Assurance for Water Analysis, by P. Quevauviller.

Since this book is didactic, readers can consult even the more fundamental texts in river hydraulics, such as *Open Channel Hydraulics*, by V.T. Chow, and *Open Channel Flow*, by F.M. Henderson, which were the first introductory books on the subject published several years ago.

In view of the continuous advance in numerical techniques and computing facilities, there is an increasing production and circulation of ready-made software packages, which young engineers tend to use extensively. In light of this, it is also the aim of this book to explain the theoretical background for the simulation of the physical processes described, as well as the principles and limitations of these models, so that they can be applied effectively and safely to a variety of practical water quality problems.

It should be borne in mind that no model can offer useful results if it is not extensively calibrated and validated. Further, it should be remembered that successful model users are those who have the so-called engineering judgement.

The book is organised in 21 chapters and an appendix.

The first four chapters present introductory material related to the state of the art, the basics of pollution transport and the fundamental hydrodynamic processes.

Chapters 5, 6, 7, and 8 explain biochemical pollution and describe the most frequent pollutants in a river system.

Chapters 9, 10, 11, 12, 13, 14, and 15 are devoted to analytical and numerical methods, which can be used for simulating the pollution transport in rivers and streams.

Chapter 16 addresses thermal pollution and its simulation.

Chapters 17, 18, 19, and 20 are concerned with optimisation problems and the general processes of calibration and validation. They also deal with data acquisition and retrieval as well as with model reliability and measurement uncertainty.

Chapter 21 covers future trends and perspectives.

Last but not least, the appendix provides a short description of some widely used commercial ready-made packages.

We would like to express our gratitude to a number of people who assisted us in improving the content and the presentation of this book, in particular Prof. Mario Rosati of the University "La Sapienza" of Rome for his valuable suggestions and remarks in fundamental and applied mathematics. We would also like to thank Dr. D. Alexakis of the National Technical University of Athens for his assistance on quality issues and PhD candidate V. Bellos of the same university for running the numerical models with significant examples.

We would like to acknowledge the encouragement provided by members of the Permanent Working Group on "Water Quality" of the European Water Resources Association during the preparation of the book.

We would like to express our thanks to Ms. P. Van Steenbergen from Springer and to Prof. V.P. Singh, editor-in-chief of the series in which this book is included, for their suggestions during the finalisation of our work. We are also grateful to Ms. H. Vloemans, who helped us in preparing the text. Preface

Finally, we would like to thank Prof. G. Viggiani of the University of Palermo and Prof. V.A. Tsihrintzis of the Democritus University of Thrace for their critical review of the manuscript and the encouraging appreciation of our work.

We hope that the reader will find the book practical, easy to follow and useful in professional life.

Rome, Italy Athens, Greece Marcello Benedini George Tsakiris

About the Authors

Marcello Benedini graduated in civil engineering at the University of Padua, Italy, where he spent several years as an assistant to the chair of hydraulics, obtaining the official degree of professor. In 1969, he joined the Water Research Institute of the National Research Council and was appointed director of the water management sector. He carried out research on the advanced methods for the integrated use of water and environment protection, in collaboration with national authorities responsible for water management and with many other scientific institutions worldwide.

Benedini is active in Italian and international scientific organisations dedicated to water management problems.

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Chapter 1 Water Quality in the Context of Water Resources Management

Abstract Water resources management refers to all types of actions aiming at creating more favourable conditions for all water bodies in the future. This fundamental objective included in recent legislation, such as the Water Framework Directive of the European Union, brings water quality issues in the centre of interest of the water sector. Monitoring systems are now built in all European countries to produce original water quality data characterising the water bodies. Modelling techniques are complementary tools of great importance for assessing management decisions, which aim to improve the health of the water bodies. This book gives emphasis on innovative and classical methods useful for devising new comprehensive water quality models.

1.1 The Progress in Water Resources Management

Water is essential for life and for all human activities but also for preserving the environment and its resources. Rapidly growing population, intensification of agriculture, industrialisation, urbanisation, development of any kind and climatic factors are the main reasons for water scarcity conditions in many countries of the world.

The other side of the problem is the deterioration of water quality. Billions of people even today do not have access to safe water for drinking or other uses. The United Nations estimate that about 3,800 children die every day as a direct result of unsafe water and lack of sanitation.

Since gradually the available water is getting scarce, less food will be produced, more diseases will emerge and widespread poverty and hardship will prevail, sparking water conflicts in several regions of the world.

Water resources management is the scientific field that can assist in a rational equitable and efficient way of water resources development, treatment and use, safeguarding the sustainability of water resources and the environment.

Sustainability, or *sustainable development*, has become household word since the report of the Brundtland Commission (World Commission on Environment and Development: Our common future, 1987), which states that the "Sustainable Development aims at ensuring that humanity meets its present needs without compromising the ability of future generations to meet their own needs". In short "sustainable development" implies that limitations should be imposed concerning the ability of the environment to fulfil the ever-increasing uses of resources so that "development" is able to last.

It is interesting to note that some decades ago countries and governments based their development on the approach of single-purpose planning. Each sector used its own criteria without considering the consequences of its decisions to the other sectors. Following this short-eyed approach, projects have been implemented having very negative consequences in other sectors, impeding the development. Even in the water sector, projects and measures have been decided creating catastrophic effects on other activities of the same sector.

As known, the definition of water resources management in the 1980s was referring to all activities aiming to fulfil the present and future water requirements with water of sufficient quantity and appropriate quality. This definition is lacking to secure the protection of the environment from any kind of abuses or natural hazards, since the main target is the fulfilment of demands. In other words, this led water resources management to become demand driven.

Focusing on water resources, it is evident that during the past decades some form of integration was attempted and adopted in development plans of most industrialised countries. The danger of destroying the environment led policymakers and authorities to introduce (apart from the economic criteria) some rather vague environmental limitations of water abstractions and exploitation. Integration was also attempted in the process of management. The planning and construction phases were incorporated in the management process, whereas distinction was made between strategic and operational management.

In the late 1980s, the majority of parties concerned with the water sector (e.g. scientists, nongovernmental organisations, policymakers, river managers, authorities and all stakeholders) have adopted procedures presented as "integrated or comprehensive water resources management (IWRM)". Most laws and regulations of developed countries, in one form or the other, are influenced by the ideas of integration. As a logical consequence, water management systems became multi-objective using a series of criteria (e.g. economic, environmental, social). However, the most striking change in the new approach adopted in water resources management is the direct inclusion of water quality (or water pollution) in the management models (Quentin Grafton and Hussey 2011).

Methods now exist, incorporated in comprehensive management models, which can find the best possible development scenario by evaluating all accountable effects associated with it. Spatially, water resources management is applied to the entire river basin or watershed. According to Dzurik (1996), integrated water resources management is a specific application of the more general notion of integrated environmental management, which seeks to deal holistically with the natural environment.

Nowadays, it is widely understood that activities and processes in the watershed are linked close together in a continuum, which should be carefully modelled in order to assess any development scenario incorporating all the important activities related directly or indirectly to water resources and their quality. Perhaps the term water resources management does not clearly represent the new ideas that could be better represented by a term such as *Watershed Management*.

Points of water availability, centres of water consumption, lakes and rivers fragile environmental zones and ecosystems, sources of pollution and any other point of interest are linked together. The management aim is to achieve a favourable and stable relation between all these players.

In an even wider definition, the Watershed Management is replaced by the management of the water system, which comprises human, physical, biological and biochemical components (e.g. Craswell et al. 2007).

It should be stressed that sustainability is not another criterion in the multiobjective planning of the past. It is an extra requirement for the behaviour of the already existing criteria. Time series of criteria should be examined together with the additional limitation of being sustainable and covering all the above three components of the water system.

1.2 The Water Framework Directive

One of the most remarkable developments in the field of water resources management is no doubt the Water Framework Directive of the European Union, which has affected the legislation of many countries in the world (European Commission 2000).

The 2000/60 Directive establishes a framework for the protection of all waters (including surface waters, transitional and coastal waters and groundwaters).

This is achieved by:

- 1. Preventing further deterioration, protecting and improving the status of water resources
- 2. Promoting sustainable water use based on long-term protection of water resources
- 3. Protecting and improving the aquatic environments through reduction of discharges, emissions and losses of priority substances, and cessation or phasing out of discharges, emissions and losses of hazardous substances
- 4. Reducing the pollution of groundwater and preventing its further pollution
- 5. Mitigating the effects of floods and droughts

The key actions that the member states have taken for implementing the Water Framework Directive are:

- (a) Identification of the river basins and formation of the river basin districts by spatial integration of adjacent river basins. Identification of responsible authorities (deadline 2003)
- (b) Characterisation of river basin districts in terms of pressures, impacts and economics of water uses together with a register of protected areas (deadline 2004)
- (c) Intercalibration of the ecological status classification systems (deadline 2006)
- (d) Monitoring networks in operational mode (deadline 2006)
- (e) Formulation of a programme of measures for achieving the environmental objectives of WFD in a cost-effective manner (deadline 2009)
- (f) Presentation of River Basin Management Plans for each river basin district, including the designation of heavily modified water bodies (deadline 2009)
- (g) Implementation of water pricing policies (deadline 2010)
- (h) Rationalisation of the measures of the programme (deadline 2012)
- (i) Implementation of programme of measures and achievement of environmental objectives (deadline 2015)

1.3 EU Directives Related to Water Quality Issues

As key factor in water resources management, the Water Framework Directive has favoured the implementation of measures so that the water quality in all water bodies is improved. Obviously the European Union has implemented a number of directives related to water quality and water pollution over the last decades. For informative reasons, the list of directives related to water quality issues follows. This information will assist any interested reader searching for specific data and criteria of water quality, applied in Europe and many other countries of the world:

- Official journal of the European Communities, No. L 010: Directive of the European Parliament and of the council of 9 December 1996 on the control of major-accident hazards involving dangerous substances (96/82/EC).
- Official journal of the European Communities, No. L 020: Council directive of 17 December 1979 on the protection of groundwater (80/68/EEC).
- Official journal of the European Communities, No. L 031: Council directive of 16 June 1975 concerning the quality of bathing water (76/160/EEC).
- Official journal of the European Communities No. L 103: Council directive of 2 April 1979 on the conservation of wild birds (79/409/EEC).

- Official journal of the European Communities, No. L 123: Directive of the European Parliament and of the Council of 16 February 1998 on the placing of biocidal products on the market (98/8/EC).
- Official journal of the European Communities, No. L 129: Council directive of 4 May 1976 concerning pollution caused by certain dangerous substances discharged in the aquatic environment of the Community (76/464/EEC).
- Official journal of the European Communities, No. L 135: Council directive of 21 May 1991 concerning urban waste water treatment (91/271/EEC).
- Official journal of the European Communities, No. L 162: Council directive of 21 May 1992 on the conservation of natural habitats and of wild fauna and flora (92/43/EEC).
- Official journal of the European Communities No. L 182: Directive of the European Parliament and of the Council Ministers concerning waste landfills (99/31/EC).
- Official journal of the European Communities, No. L 192: Commission decision of 17 July 2000 on the implementation of a European pollutant emission register (EPER) according to Article 15 of Council Directive 96/61/EC concerning integrated pollution prevention and control (IPPC) (2000/479/EC).
- Official journal of the European Communities, No. L 194: Council directive of 16 June 1975 concerning the quality required of surface water intended for the abstraction of drinking water in the member states (75/440/EEC).
- Official journal of the European Communities, No. L 222: Council directive of 18 June 1978 concerning the quality of fresh waters needing protection or improvement in order to support fish life (78/659/EEC).
- Official journal of the European Communities, No. L 229: Council directive of 15 July 1980 relating to the quality of water intended for human consumption (80/778/EEC).
- Official journal of the European Communities, No. L 230: Council directive of 15 July 1991 concerning the placing of plant protection products on the market (91/414/EEC).
- Official journal of the European Communities, No. L 257: Directive of the European Parliament and of the council of 4 May 1976 concerning integrated pollution prevention and control (IPPC) (96/61/EC).
- Official journal of the European Communities, No. L 281: Council directive of 30 October 1979 on the quality required of shellfish waters (79/923/EEC).
- Official journal of the European Communities, No. L 327: Decision of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy (2000/60/EC).
- Official journal of the European Communities, No. L 330/32: Council directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption.
- Official journal of the European Communities, No. L 375: Council directive of 12 December 1991 concerning the protection of waters against pollution caused by nitrates from agricultural sources (91/676/EEC).

1.4 From Pressures to Impacts

The WFD focuses on the pressures and impacts in Article 5, which requires for each river basin district:

- (a) An analysis of its characteristics
- (b) A review of the impacts of human activities on the status of surface waters and groundwater
- (c) An economic analysis of water use

All the required tasks have been completed by many member states by 2004. Revision of those tasks is expected by 2013 and subsequently every 6 years. WFD initiated a process of assessment, iteration and refinement starting from the current conditions of each water body and forecasting the conditions at the end of the initial period (2015).

According to Annex II of WFD, the required review process is summarised in five tasks related to surface water bodies:

- 1. Characterisation of surface water body types
- 2. Definition of ecoregions and surface water body types
- 3. Establishment of reference conditions for each type of surface water body
- 4. Identification of pressures
- 5. Assessment of impacts

For a successful analysis of pressures and impacts, some prerequisites are required as shown in Fig. 1.1.

As anthropogenic pressures, WFD examines:

- 1. Point pollution sources
- 2. Diffuse pollution sources
- 3. Modification of flow regime (through abstraction or regulation)
- 4. Morphological alterations



Fig. 1.1 The basic prerequisites for a successful development and application of appropriate mathematical models

In regard to the impact assessment, apart from the information derived from the pressures, additional information is needed (e.g. from environmental monitoring systems and/or necessary modelling procedures) to determine the most probable status of the surface water body in the future versus the set of environmental quality objectives and whether additional monitoring or a programme of measures is required.

All tasks related to pressures and impacts and the establishment of the resulting programme of measures (where it was required) had as the deadline the year 2009.

Although the impacts are the result of pressures, in many cases a systematic analytical framework is required for linking pressures and impacts. According to several researchers (e.g. CIS for WFD Guidance doc, no. 3) the DPSIR (driver, pressure, state, impact, response) analytical framework is already widely accepted and used.

An explanation of the DPSIR framework may be achieved through the explanation of terms included in the analysis:

y)
llution

An illustration of the DPSIR analytical framework appears in Fig. 1.2.



Fig. 1.2 An example of DPSIR (Modified from CIS WFD Guidance document no. 3)

The WFD defines three types of objectives for surface water bodies, namely, ecological status (for river, lakes transitional and coastal waters), ecological potential (for heavily modified or artificial water bodies) and chemical status (for all surface water bodies).

The categories of driving forces, pressures and impacts are presented in detail in CIS Guidance doc. 3. In the same document, a list of possible impacts or changes in state of surface water bodies that can be identified from monitoring data is presented as follows:

- Biological quality elements: macrophytes, phytoplankton, planktonic blooms, benthic invertebrates, fish, eutrophication
- Hydromorphological quality elements: hydrological regime, tidal, regime, river continuity, morphology
- Chemical and physicochemical quality elements: transparency, thermal conditions, oxygenation conditions, conductivity, salinity, nutrients status, acid-ification status, priority substances, other pollutants

The monitoring system at each water body can collect data on the quality items. However, no monitoring system can produce data of the appropriate density in space and time. To secure that data can be produced where they are needed, modelling techniques can be implemented as complementary tools to monitored data from the water body.

In particular, for the river system, numerous modelling attempts have been made since the original work of Streeter and Phelps in 1925. Although many of such river models suffer from the limitation that they use discrete point pollution sources instead of diffuse source inputs, they are still very important in contributing to the assessment of the water quality at each river segment. Although today there is a tendency for modelling not only the river system but the whole watershed, this book insists on giving emphasis on the processes and their modelling in the river system.

It can be easily understood that the new legislation on water resources management is very demanding and its application requires new advanced models to be devised and implemented in the river systems and the other water bodies.

As known, models provide the context in which decisions are made. Since the book is concerned with modelling, the limitations of the use of models should be always considered before they are used as decision support systems (Elms and Brown 2012a, b).

Examples of existing water quality models are included in the Appendix of this book. Unfortunately, existing models focus on classical pollution issues that can be computed and modelled. As explained, the main aim of this book is to analyse innovative and classical techniques and methods for devising future comprehensive water quality models for rivers and streams. According to some authors, rivers are among the most valuable but also the most abused resources on earth (Smits et al. 2000).

When reading this book, the basic knowledge on water quality issues is a prerequisite. Concerning the wide spectrum of topics related to water quality, the reader is advised to consult some of the numerous books on the subject (e.g. Stumm and Morgan 1996; Trimble et al. 2007; AWWA 1995; USEPA 2006).

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Chapter 2 Basic Notions

Abstract Mathematical models are now essential tools in water resources management and are currently applied for the solution of environmental problems including those of polluting discharge into surface and underground water bodies. Following the development of computational facilities and mathematical procedures, the models can provide reliable solutions, provided that they use proper data and are operated by competent professionals.

2.1 Modelling and Water Quality Problems

The progress of computer technology and mathematical procedures has introduced tools that are now essential for any activity of human life. This quite general and global aspect includes also the problems of water quality protection. The advantage of applying these tools for water quality control in rivers, lakes and aquifers is now appreciated by all scientists and professionals working in this field.

A tool that promises enormous power to address the water quality problems and give rational solutions is the mathematical model. According to Cox (2003), a water quality model *can mean anything from a single empirical relationship through a set of mass balance equations, to a complex software piece*. Much work has been done during the past decades, and today several mechanisms are available, not only in the scientific field but also in the flourishing software market. The use of mathematical models is now in the reach of any person who has a sufficient professional background to understand and deal with water quality problems. The mathematical models belong to a large family of models that is not new in the daily practice of water resources management and protection.

Because many aspects and variables have to be taken into account simultaneously dealing with water, the models are becoming more and more important in order to achieve reliable solutions in practical problems. The model acts as a representation of the reality and allows its problems to be handled without directly interfering with it. Verifying a solution directly in natural entities requires costly and complex engineering interventions, very often destructive. Vice versa, if the model represents correctly the reality and all its related phenomena, it can allow a solution to be examined in a short time and at a much lower cost.

As known, three types of models are currently used to solve water-related problems, namely, the hydraulic, the analogical and the mathematical models.

The *hydraulic (physical)* model consists of a reality at a different scale: a river stretch is reproduced by means of a duct having the same geometrical and morphological characteristics but in a size easy to be accommodated in the narrow space of the laboratory. With this model, the phenomena to analyse are the same as in reality (a flow in reality is reproduced by a flow in the model), and there is a plain correspondence between the various components (level, velocity, forces...), according to well-known *laws of similitude*.

The *analogical* models are based on a formal identity of the mathematical expressions that interpret different phenomena. Typical is the case of groundwater, for which the water flow is expressed by the Darcy law, formally identical to the Ohm law that interprets the electric current in a conducting line. After a suitable *scale of correspondence*, the behaviour of an aquifer, somewhat very difficult to analyse directly in the field, can be understood by the behaviour of an electric network having appropriate resistances and capacities.

The *mathematical models* interpret the reality by means of the numerical values that can be adopted to quantify the various phenomena and their components.

It is worthwhile to point out that the first two types of models just mentioned encounter now some drawback and are progressively abandoned in favour of the mathematical models, which are in fact more and more predominant. In the field of water quality, they are now probably the only effective tool.

Nevertheless, a lack of confidence still persists among several people, who think that the mathematical model is a too sophisticated mechanism, useful only for academic exercises but not in the real-world practice, where it has very often undergone unsuccessful outcomes.

To some extent, the use of mathematical model is a complex task, but it can assist in discovering the insight of a process if it is fed with reliable and proper data. The numerous successes during the last years have confirmed that when the mathematical model is in the hands of a skilled person with appropriate professional knowledge, it can give quite successful results. The mathematical model becomes then a device that helps the interested people to abide, step by step, with the ordinary way of thinking and to put into practice what they have learned with their daily experience.

2.2 How to Interpret the Water Quality

A typical incorrect use of water resources, which can cause dangerous effects to humans and other species, is the uncontrolled discharge of sewage into rivers and streams. It destroys the aquatic life and makes the water useless for any other use. **Table 2.1** The most significant quality indicators

1 – Temperature
2 – pH
3 – Dissolved oxygen (DO)
4 – Turbidity
5 – Conductivity
6 – Total organic carbon (TOC)
7 – Bacteria
8 – Viruses
9 – Chemical oxygen demand (COD)
10 - Biochemical oxygen demand (BOD)
11 - Metals and non-metals (Cr, Cd, Ni, As, Hg, Na, Br)
12 – Phosphates
13 – Nitrogen compounds
14 – Organic compounds

- 15 Suspended solids
- 16 Salts (total dissolved salts)

Expensive treatments are then necessary, the cost of which becomes a burden for the whole community involved. Deterioration of river water has eventually an effect on the environment, on the human health and the economy.

The concept of water quality can be introduced by adopting some characteristic terms (generally called *parameters* or, better, *quality indicators*), which can be measured in the natural bodies and in the discharged water and are also characteristics of the water use. Table 2.1 lists some of the most important indicators, keeping in mind that such a list must be considered always open to introduce further terms that can be identified and detected by the research in progress. Each indicator can be measured, requires specific techniques of detection and analysis and imposes specific tasks for its control. Any use of water has its minimum and maximum values, determined after proper considerations.

As it will be better explained in the following chapters, the water quality in a river or stream depends on the quantity of water in which the pollutants are contained. It is, therefore, necessary that any action related to water quality is accompanied by accurate evaluations of the hydraulic conditions of the water body. In particular, water flow, level and velocity, which are determinant of pollutant behaviour, are to be carefully and frequently measured in the representative points of the water body. Moreover, the pollutants in water can be affected by rainwater and evaporation, and therefore, suitable measurements of the climatic and hydrological conditions are also of importance. Because the water quality in a natural or artificial body is a consequence of anthropogenic activities, the existing conditions of economic development, or the foreseeable trends, must be taken into consideration, with appropriate evaluation of all the terms to which a quality situation can be referred. Furthermore, water quality is controlled by natural factors that include geology and lithology of the watersheds and aquifers, the residence time, the reactions that take place within the aquifer and the type of land uses (Alexakis 2011).