Chapter 5 Stream Water Quality Modelling Techniques

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Abstract Water quality in open channels plays a significant role in water resources planning and management. Water quality models are important decision support tools for water pollution control, the study of the aquatic ecosystems and the assessment of the effects of point and non-point (diffuse pollution) sources. Modelling of stream water quality is broadly used to assess current conditions and impacts of proposed measures in water quality management. The modelling is based on knowledge about parameters describing transport processes like hydrodynamic dispersion, advection and decay rates. According to the purpose, the scale of the studied area and the detail of solution various models of different levels are used. In this chapter, practical examples of screening, overall and detailed water quality studies applying modelling techniques are presented.

Keywords Watercourses · Water quality · Stream water quality modelling · Pollution sources

5.1 Introduction

In the worldwide context, and in the Czech Republic, the protection of waters is traditionally a complex activity consisting in the protection of both quantity and quality of surface and subsurface water. Water quality studies are integral part of research and tutorials focused on water management and environmental issues $[1–7]$ $[1–7]$ and others. In the Czech Republic, the water quality is dealt with according to the Czech law represented, namely, by the Water Act [\[8\]](#page-23-2) and by the European regulations, namely the Water Framework Directive [\[9\]](#page-23-3). The Directive [\[9\]](#page-23-3) aims at maintaining and improving the aquatic environment and primarily the quality of the waters concerned. In the Czech Republic, the responsible authorities are the Ministry of Agriculture and the Ministry of Environment who annually report the state of water management to the

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M. Zelenakova et al. (eds.), *Management of Water Quality and Quantity*, Springer Water, https://doi.org/10.1007/978-3-030-18359-2_5

government of the country. For the water quality assessment in the Czech Republic national decrees [\[10,](#page-23-4) [11\]](#page-23-5) supplement Water Act [\[8\]](#page-23-2) and incorporate European regulations into the Czech legislation system taking into account local conditions.

For the assessment of the long-term conditions of water quality in watercourses, periodic monitoring is carried out at 263 profiles located at significant streams in the Czech Republic (Fig. [5.1\)](#page-1-0). The frequency of the sampling is annually 12 or 24 samples. Normally, 78 water quality indicators are observed, however not at all sampling profiles. The monitoring programme [\[12\]](#page-23-6) was elaborated by the Czech Hydrometeorological Institute and was issued by the responsible ministries providing guidance on the methods and the extent of the monitoring. As a part of individual research projects, on-purpose monitoring is frequently carried out at locations of interest and during the limited period. This monitoring is sometimes organized as tracer experiments [\[1\]](#page-23-0).

In the European context, the European Water Framework [\[9\]](#page-23-3) formulates objectives concerning stream water quality. In the Czech Republic, the immission and emission standards for the release of both municipal and industrial effluents to the surface streams are specified in the $[10, 11]$ $[10, 11]$ $[10, 11]$. They are expressed in terms of maximum permissible concentration limits for individual water quality indicators like biochemical oxygen demand (BOD) and chemical oxygen demand (COD), nitrogen compounds and many others. In practice, the majority of permanent effluent discharges, for example, from waste water treatment plants (WWTP) are subject to periodic water quality checks carried out by authorized bodies. However, the limit values are not prescribed for instantaneous releases of sewage water from storm water overflows, which is mostly due to the difficulty of measuring released wastew-

Fig. 5.1 The location of monitoring profiles in the Czech Republic [\[16\]](#page-23-7)

ater during heavy rainfall [\[2\]](#page-23-8). For this type of effluents, permissible limits have to be specified individually based on the character and quantity of the released wastewater, on the water flow and quality in the receiving stream and its environmental value. Cost–benefit analysis is required to indicate the effectiveness of the measures proposed. During the last decades, numerous studies have dealt with both municipal and industrial effluents to the surface waters [\[3\]](#page-23-9) and others. Particular attention has been paid to water quality monitoring, measurement and contamination tracking in relation to drainage system $[4, 13, 14]$ $[4, 13, 14]$ $[4, 13, 14]$ $[4, 13, 14]$ $[4, 13, 14]$. Here, various pollution indicators and polluting agents have been studied. These were dissolved oxygen, $BOD₅$ and COD, nitrogen and phosphorus compounds, temperature, faecal contamination and many others.

The critical part of the stream water quality management is mathematical models, which may serve for the interpolation of monitoring data and are an essential decision tool. They enable optimization of proposed measures for stream water quality improvements like investments into the sewer systems or intensification of wastewater treatment plants (WWTP). Stream water quality models are used to be part of general water management plans of inhabited and outdoor areas as a base for the elaboration of urban plans namely of the municipalities. The results of coupled hydraulic and water quality modelling of sewer–watercourse may indicate the need for arrangements at the sewer network like surge chambers and storm water overflows separating part of wastewater during heavy rainfalls.

Due to one-dimensional (1D) character of open channels, the water quality models in streams are essentially proposed as 1D. According to the nature of the simulated problem, the water quality models may be steady state or transient in combination with steady-state or transient water flow.

5.2 Classification of Water Quality Models

Classification of stream water quality models may be carried out according to various factors. This may be according to the model level (global, basic, detailed), domain character (urban area, water courses related to river basin, models including surface and diffusion pollution) and time dependence of variables (steady state, transient).

5.2.1 Models According to Their Level

Global models, sometimes called as screening models, provide fast and general information about the state of water quality in large catchments. At the modelling fixed constants and parameters are used in the simplified governing equations. Such models usually do not reflect the interaction between individual environmental components, water quality indicators and pollution agents. Global models are used for the assessment of the relative effect of crucial measures at the catchment, forecasting of relative changes in water quality, evaluation of the impact of hydrological characteristics on water quality or for identification of dominating processes and variables in the catchment.

Basic models contain more detailed description of the most important processes governing stream water quality. The results provide a rough quantitative view on the concentration of individual indicators. Basic models enable evaluation of limit (maximum, minimum) concentrations at individual channel reaches, the approximative extent of potential accidents in river pollution and consequence of both accidental and permanent spills. Based on results of basic modelling, the areas for more detailed solution may be pinpointed.

Detailed models concern local water quality conditions, namely in particular areas and watercourses with significant pollution origin and spills where water quality may be permanently or temporarily harmed. Simulation of individual pollution indicators is possible, and interaction between the selected substances may be taken into account. All types of pollution sources like surface, linear and point are included either invariable or changing during the time.

Borders between single model types are not sharp; particulars of the models are governed by various factors like size of the river basin, number, and significance of pollution sources, the density of monitoring network, etc.

In this chapter, applications of three mentioned models are presented. The general location of individual models is shown in Fig. [5.2.](#page-3-0)

Fig. 5.2 Approximate location of individual models. Blue—global model, green—basic balance model, red—detailed model

5.2.2 Models According to the Regime of Pollution Release

Dynamic models concern situations when the pollution is suddenly released at river cross section. The pollution causes "wave" which propagates along the stream. Such pollution escape can be originated by controlled and uncontrolled releases from the wastewater treatment plant (WWTP), car crash or lack of discipline in the industrial, municipal or agricultural waste management. When solving the sudden release of the pollution to the stream, water quality management aims to the most effective protection and a decrease of injuries of human life, human health, property and real estates. The purpose of the modelling is to forecast time-spatial distribution of the pollution concentration along the watercourse downstream of the spillage point. The mathematical model is therefore based on the unsteady transport-dispersion equation. Due to relatively short time, conservative solids are usually assumed, and the decay of substances is not taken into account. The numerical model can be used as so-called "alarm model" compiled in advance for the given stream, calibrated and verified using the field injection test data obtained from tracing experiments.

Balance models are used for proposing solutions for the long-term pollution state. Also, they help to permanently taking care of the stream water quality improvement. This can be achieved by testing different scenarios such as reducing pollution sources by investments to remedial measures with the aim to reduce the pollution emission at the sources (WWTP intensification, landfill management, system of penalties, etc.). The main goal of the modelling is to evaluate scenarios tending to the overall stream water quality improvement. The target water quality is determined by the national and international water quality standards and directives, environmental demands (water organisms, plants) and by the manner of water use (drinking water). The quasi-steadystate balance stream water quality models serve for the evaluation of present water quality conditions at various flow and pollution scenarios and for the simulation of selected variants of water quality improvement (building or intensification of WWTP, erosion control, etc.) and optimization of the improvement based on cost–benefit analysis.

In general, two approaches mentioned above may be used as models of all three conceptual levels mentioned in the Sect [5.2.1.](#page-2-0) However, the dynamic approach is common at more detailed models (Sect. [5.7\)](#page-17-0) with boundary conditions and other state variables changing with time.

5.3 Input Data for the Modelling

Input data concern both watercourses network and corresponding river basin. For the analysis, integrated system of water courses is characteristic, and the subject of modelling is significant streams regarding the length, discharge conditions or pollution sources.

In general punctuality of input data should follow the aims of modelling and required accuracy. Before the modelling, the data should be completed, summarized, evaluated eventually corrected, completed and presented in tables, graphs and thematic maps. The structure of the data may be as follows:

- 1. General characteristics of the catchment like geographical data (location, altitude, management, land cover), morphology, cadastral and population data, protected areas with special water regime, river network topology, etc.
- 2. River data contain geometrical characteristics of the streams, water bodies (reservoirs, lakes), hydraulic structures, water management rules and arrangements (water diversions).
- 3. Hydrological and climatic data concerning precipitation, temperatures, discharges in streams and water quality data.
- 4. Pollution sources are classified according to their type (municipal, agricultural, industrial) and according to spatial character (point, linear, surface and diffuse sources).
- 5. Data from water quality monitoring serve for model calibration and verification. It concerns data from permanent long-term monitoring and from tracer experiments.

Sometimes, it is desirable to aggregate basic data into groups according to their acquisition, a method of processing or method of their incorporation into the model. It is important to relate all data to the unique global coordinate system (e.g. using GIS) or to the river stationing which may, however, differ in time with the gradual morphological processes and technical interventions like shortening of streams by cutting meanders.

The data acquisition represents considerable financial means and needs sufficient time reserve. In case of newly established monitoring for long-term pollution balance modelling, its duration exceeds several years to obtain seasonal water quality variations for selected indicators.

The data are acquired from diverse sources. The first information may be taken from the maps, in the Czech Republic comprehensive water management maps in scale 1:50,000, and also other river and catchment data are freely available from weboriented hydroecological information system [\[15\]](#page-23-13). Hydrological and climatic data and data from monitoring provides the Czech Hydrometeorological Institute [\[16\]](#page-23-7). More detailed river data and information about hydraulic structures are managed by river authorities. The pollution data should be provided by competent representatives of relevant sources like water companies managing WWTPs, industrial or agricultural facilities. It is recommended to check and verify reported data using population (population equivalent) data and other traditional and empirical knowledge about pollution sources and their treatment $[17, 18]$ $[17, 18]$ $[17, 18]$. The worst identifiable pollution amounts are spills from storm water overflows. These may be estimated only indirectly using calibrated sewer hydraulic and pollution models. In all cases, site investigation is necessary.

Data analysis usually contains basic statistical analysis, regression methods, time series analysis and comparison of monitoring data with water quality limits. It is

also necessary to adjust data to appropriate form suitable for the numerical model. For the model calibration and verification, temporally homogeneous data should be provided. The homogeneity refers to the river topology and geometry, hydrology and also water quality where all data from measurements, site investigation, hydrological and water quality monitoring should correspond to the same period. This may be difficult especially when processing long-term water quality monitoring data when during the period changes may occur in the catchment, streams and pollution sources.

5.4 Mathematical Formulation

The transport processes in open channels are traditionally described by onedimensional (1D) convection-diffusion Eq. [\(5.1\)](#page-6-0) expressing mass conservation law of the studied matter $[19-21]$ $[19-21]$. In such models, the density of polluted water is assumed to be constant and similar to "clean" water density, the substance is well mixed over the cross section, and only longitudinal hydrodynamic dispersion is taken into account. The basic Eq. [\(5.1\)](#page-6-0) expresses the time change of the mass (expressed via concentration *c*) as the function of advection, dispersion, dilution, constituent reactions and interactions, sources and sinks [\[19\]](#page-23-16):

$$
\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} - \frac{\partial}{\partial x} (D_{L} \frac{\partial c}{\partial x}) = R + \frac{S}{A}, \quad u = \frac{Q}{A}, \tag{5.1}
$$

where *c* is concentration, *u* is cross-sectional mean velocity, *A* is flow area, *O* is discharge, $D_{\rm L}$ is longitudinal hydrodynamic dispersion coefficient, R expresses constitutional changes of matter (e.g. retardation, sedimentation and degradation), *S* is source/sink per reach length, *t* is time, and *x* is spatial coordinate along the centre line of the channel.

The boundary conditions are defined as the known concentration at the upstream end $x = 0$:

$$
c(0, t) = c_0(t) \tag{5.2}
$$

and zero concentration gradient in the downstream end $x = x_L$,

$$
\frac{\partial c(x_{\rm L}, t)}{\partial x} = 0\tag{5.3}
$$

An initial condition is defined as known concentration along the assessed reach at time $t_0 = 0$.

$$
c(x, t_0) = c_I(x) \tag{5.4}
$$

In Eq. [\(5.1\)](#page-6-0), the key parameters are flow velocity *u* and coefficient of longitudinal dispersion D_L , which both generally change in time and along the stream axis. Basically, the flow velocity $u(x, t)$ is determined by hydrodynamic modelling [\[7\]](#page-23-1). In practical applications, the dispersion coefficient D_L is frequently assumed to be constant in time and along the typical river reaches. The longitudinal dispersion coefficient D_L is related to the hydraulic and geometric characteristics of a given open channel and also to fluid properties [\[1,](#page-23-0) [22\]](#page-23-18). Its value may be determined using empirical formulae published by various authors. The best fit verified by tracing experiments $[1]$ provide following Eq. (5.5) $[20]$ and Eq. (5.6) $[23]$:

$$
D_{\rm L} = 0.011 \frac{C w^2}{h \sqrt{g}} u,
$$
\n(5.5)

$$
D_{\rm L} = \frac{2.0h\sqrt{g}}{C} \left(\frac{w}{h}\right)^{3/2} u \tag{5.6}
$$

For the solution of Eq. (5.1) with boundary and initial conditions, appropriate numerical methods are used. These are finite difference method, finite elements method, a method of characteristics, random walk procedures and others.

5.5 Global Models

Global models serve for obtaining preliminary, general and fast information about water quality in larger catchments and river networks and for the rough estimate of effects of intended remedial measures within stream water quality management. The global models are characterized by only general data without more detailed data about stream geometry, hydrology of the catchment and pollution sources. Usually, the studies are "short term" with relatively low budget. The algorithm is simple with beforehand set model parameters. The assessment has more or less qualitative nature rather than quantitative one. As an example, the study [\[6\]](#page-23-21) may be mentioned at which global model comprised about 1000 km of water courses in the Dyje river basin. The main goal of the study was to assess an impact of technical improvements on sewers and wastewater treatment facilities financed from European sources on the water quality of the Dyje river which at its lower part is a boundary stream with Austria.

The structure of necessary data generally corresponds to the Sect. [5.3.](#page-4-0) However, only rough and generalized data are provided about watercourses and water bodies mostly using water management maps 1:50,000 [\[15\]](#page-23-13) and general water management plans. Quasi-steady-state hydrological and hydraulical conditions are assumed, the solved scenarios usually deal with average annual discharges and also low discharges with exceedance 270, 330 or 355 days. Long-term (usually not exceeding 5 years) averages of pollution sources and monitoring results are used.

One of the goals of global river pollution studies is a qualified estimate of total present and a future mass load of individual polluting agents. This is focused on total averages and on unfavourable conditions at low discharges during dry spells.

As the survey into all pollution sources over large catchments may be time demanding, quite expensive and hardly realized, many times only sources which are subject to improvements are credibly taken into account in the analysis. The model is set up via present water quality identified by long-term monitoring by introducing "fictive" pollution sources and constitutive changes following monitored water quality. By changing real pollution sources, qualitative rate of improvement may be modelled along the system of the concerned streams. Both mass flow and concentrations are simulated for individual water quality indicators.

It can be seen that numerous simplifying assumptions are taken into account at global models. These come mostly from the lack of more detailed and reliable data. For given scenario constant mass flow not changing with time is anticipated; change of concentration is given only by changing the discharge in streams (average, various exceedance). Constitutive changes may be approximated by the kinetics of the firstorder [\[24\]](#page-23-22) with constants estimated using an analogy with similar catchments and river systems.

From previous studies $[25]$, it comes that at the steady-state approach the effect of hydrodynamic dispersion may be neglected. Thus, Eq. [\(5.1\)](#page-6-0) may be rearranged using $Q = u.A$ and $R = -K.c$ as follows:

$$
\frac{d(Q \cdot c)}{dx} - S + A \cdot K \cdot c = 0 \tag{5.7}
$$

with boundary condition $c(0) = c_0$ expressing known concentration at the uppermost profiles of the domain. *K* is a first-order rate constant which in natural streams varies between 0 and 15 (1/day) for different open channels and flow conditions, type of water quality indicator and intensity of the processes in the streams.

The mass flow (kg/s) is defined as follows:

$$
L = c \cdot Q = A.u. Q \tag{5.8}
$$

For the numerical solution, simple explicit difference scheme was applied (Fig. [5.3\)](#page-8-0).

Denoting L_i , L_k mass flow in nodes *j*, *k*, the sum of all pollution sources along the reach with the length Δx is denoted $L_i = S \Delta x$ where *S* is a pollution source along the river reach. Then, Eq. (5.7) may be rewritten in terms of differences:

Fig. 5.3 The scheme of the computational river reach

$$
L_k - L_j - L_i + A.K.c.\Delta x = 0 \tag{5.9}
$$

Constitutive changes in Eq. [\(5.9\)](#page-9-0) may be expressed using detention time Δt along the reach Δx :

$$
A.K.c.\Delta x = K.\Delta t.L_j,\tag{5.10}
$$

and after some manipulation:

$$
L_k = L_j + L_i - L_j.K.\Delta t = 0.
$$
 (5.11)

The pollution "input" L_i along the reach length Δx is expressed for the present state (subscript *S*) and improved state after realizing anticipated measures (subscript *O*). The present mass flow L_{S_k} in the node *k* may be expressed via average discharge Q_{Sk} and concentration c_{Sk} taken from river monitoring:

$$
L_{Sk} = Q_{Sk} \cdot c_{Sk} \tag{5.12}
$$

Mass flow L_{Sk} thus represents terms in Eq. (5.11) , i.e. mass inflow from upper catchment L_{Si} , pollution sources along the reach L_{Si} and the effect of constitutional changes along the reach between nodes *j* and *k*. The mass flow for the scenario with implemented measures *LOk* may be expressed via present mass flow, expected impact of all improvements upstream of given reach and difference in constitutional change along the reach due to the change of total mass load:

$$
L_{Ok} = L_{Sk} + K \cdot \Delta t \cdot (L_{Sj} - L_{Oj}) - \sum_{p=1}^{n} (L_{Si}^{p} - L_{Oi}^{p}),
$$
 (5.13)

where *n* is number of pollution sources upstream of given reach (node *k*). The effect of weir pools and reservoirs may be estimated using data from monitoring and based on direct proportion with present state based on mass flow entering and leaving the reservoir:

$$
L_{OP} = \frac{L_{SP}}{\sum_{p=1}^{n} L_{SN}^{p}} \cdot \sum_{p=1}^{n} L_{ON}^{p}
$$
 (5.14)

where L_{OP} and L_{SP} are mass flows downstream of the reservoir after and before adopting remedial measures on pollution sources, $\sum_{p=1}^{n} L_{ON}^p$ and $\sum_{p=1}^{n} L_{SN}^p$ are total mass inflows to the reservoir by *n* tributaries after and before adopting remedial measures.

The algorithm is straightforward to be compiled using a spreadsheet where individual streams are configured at separate sheets. The calculation proceeds from the upstream river reaches and follows the river network topology. At river junctions,

Fig. 5.4 The scheme of the Dyje river network. Black—monitoring profiles, colours—clusters of improvements

the mixing law is applied (Fig. [5.7\)](#page-14-0). The present averaged mass flow is derived from available discharge and concentration measurements in the monitoring network (see Figs. [5.1](#page-1-0) and [5.4\)](#page-10-0). The scenarios of pollution reduction from individual sources are introduced to the model.

In the study [\[6\]](#page-23-21), the effect of improvements on sewer and wastewater treatment facilities aggregated into eight "clusters" according to sub-catchments was modelled. The objective of the simulations of 11 scenarios was to assess the effect on water quality in the Dyje river at the boundary profile in the city of Bˇreclav close to the Czech-Austrian boundary (Fig. [5.2\)](#page-3-0) for four water quality indicators, namely BOD, COD, ammonia nitrogen (N-NH4) and phosphorus (P). In Fig. [5.4,](#page-10-0) black dots indicate the profiles with hydrological and water quality monitoring, and coloured dots show improvements on pollution sources.

Figure [5.5](#page-11-0) shows the water quality map according to [\[26\]](#page-24-0) for the BOD indicator. The light and dark blue depict streams with very good and good water quality; further classes are marked by green, yellow and red colour indicating the worst stream water quality. Two lines along the streams show water quality classes before and after expected improvements. Another analysis was done via longitudinal sections of concentration and mass flow of individual water quality indicators. In Fig. [5.6,](#page-11-1)

Fig. 5.5 Water quality map for scenario "all improvements" (scenario 11) showing improvement of water quality for BOD along individual streams

the longitudinal section of the total mass flow in (t/year) along the principal stream the Dyje river is shown for present state and for all realized improvements (scenario 11).

The results of the modelling showed that measures at all 8 groups of pollution sources at scenario 11 resulted in water quality improvement at the Dyje river boundary profile by 12% for BOD, 5.5% for COD_{CR} , 10% for N-NH₄ and about 10% for P. The water quality class usually improves only at the upper part of the catchment where the improvements represent higher portion of total load spilled to the stream.

5.6 Basic Models

Basic models serve as the long-term balance solutions in middle-sized catchments in more details than global screening models. Due to the inadequate monitoring frequency (usually once in a month) and no information about the time course of pollution sources, it is not possible to reliably model short-term fluctuations of concentrations of individual pollutants. Similar to global models discharges, velocities, pollution sources and water quality characteristics are averaged over time. Thus, the model is formulated as quasi-steady state with varying punctuality of input data. However, more realistic values of all model parameters are input and resulting water quality variables obtained, so the model provides not only qualitative but also quantitative information about the pollution sources and their impact on stream water quality.

The problem has to be treated as the combination of hydrodynamic river analysis and transport-dispersion solution. The mathematical model for the individual problem solution must issue from the catchment, stream and pollution data available and from the anticipated accuracy of results. In case of basic models, the hydrodynamics and also pollution transport is usually approximated by steady-state approach. The mathematical model of water quality consists of 1D advection-dispersion mass balance Eq. [\(5.1\)](#page-6-0) expressed for given pollution parameter and corresponding boundary conditions. When solving the long-term pollution balance problem, following additional simplifications have to be assumed:

- the river flow is quasi-steady, the pollution modelling is carried out for selected average and low discharge scenarios,
- the description of the modelled domain is performed with regard to the time delay of water in streams, reservoirs, weir pools and ponds,
- the pollution transport is assumed to be steady and time-independent due to poor data about time variations of the pollution sources; the sampling is performed in relatively long-time intervals (once in the month); seasonal concentration variations are analysed using the mass flow approach and appropriately "smoothed",
- \bullet it can be proved [\[25\]](#page-23-23) that the longitudinal dispersion can be neglected at the steadystate approximation; the error in results does not usually exceed 5%. This error is negligible when compared with sampling error and inaccuracy in determining the pollution sources.

Applying mentioned above simplifications on Eq. [\(5.1\)](#page-6-0), i.e. $\partial c(x, t)/\partial t = 0$, omitting the second member on the right side and assuming steady-state conditions $R(x, \cdot)$ t) = $R(x)$, $c(x, t) = c(x)$, $S(x, t) = S(x)$, $A(x, t) = A(x)$, substituting $Q = A u$ and after some manipulations it reads:

$$
\frac{1}{A}\frac{d(Qc)}{dx} = R + \frac{S}{A},\tag{5.15}
$$

Only the headwater boundary condition [\(5.2\)](#page-6-1) is applied, at the steady-state model, the condition in the node $x = L$ is not specified and is determined during the computation (free parameter).

For the solution of Eq. (5.15) , the explicit finite difference scheme may be used. When denoting the sum of all pollution sources, S_i at the river reach *i* with the length Δx , Eq. [\(5.1\)](#page-6-0) can be written as follows (Fig. [5.3\)](#page-8-0):

$$
\frac{Q_k \cdot c_k - Q_j \cdot c_j}{\Delta x} = R_i \cdot A_i + S_i. \tag{5.16}
$$

An example of numerical solution deals with the modelling of BOD. In accordance with [\[24\]](#page-23-22) the first-order kinetic model may be rewritten:

$$
R^{\text{BOD}} = -K_{\text{BOD}} \cdot c^{\text{BOD}}.\tag{5.17}
$$

After substituting Eq. (5.17) to (5.16) , the BOD concentration in the node k is expressed:

$$
c_k^{\text{BOD}} = \frac{c_j^{\text{BOD}} \cdot Q_j + \Delta x \cdot S_{\text{BOD}}}{Q_k + A_i \cdot K_{\text{BOD}} \cdot \Delta x},\tag{5.18}
$$

where $K_{\text{BOD}}(T)$ is the rate coefficient of BOD change due to sedimentation, scouring, biochemical oxidation, c^{BOD} is BOD concentration, *T* is the temperature, R^{BOD} is the rate of BOD change, S_{BOD} is the BOD pollution source along the reach k . The mass flow L_i and L_k in nodes *j* and *k* is expressed as follows:

$$
L_k^{\text{BOD}} = \frac{L_j^{\text{BOD}} + \Delta x. S_{\text{BOD}}}{Q_k + A_i \cdot K_{\text{BOD}} \cdot \Delta x} \cdot Q_k \tag{5.19}
$$

Substituting the average cross-section *Ai* on the reach *i*

$$
A_i = \frac{Q_k \cdot v_j + Q_j \cdot v_k}{2 \cdot v_k \cdot v_j} \tag{5.20}
$$

the Eq. (5.19) is expressed as follows:

$$
L_k^{\text{BOD}} = \frac{L_j^{\text{BOD}} + \Delta x. S_{\text{BOD}}}{Q_k + \frac{Q_k \cdot v_j + Q_j \cdot v_k}{2 \cdot v_k \cdot v_j} \cdot K_{\text{BOD}} \cdot \Delta x} \cdot Q_k \tag{5.21}
$$

At the stream junction, the mixing equation is applied (Fig. [5.7\)](#page-14-0):

$$
c_k^{\text{BOD}} = \frac{c_j^{\text{BOD}} \cdot Q_j + c_p^{\text{BOD}} \cdot Q_p + \Delta x. S_{\text{BOD}}}{Q_k + A_i \cdot K_{\text{BOD}} \cdot \Delta x}
$$
(5.22)

The influence of the temperature on the biological processes can be expressed by the change of temperature dependent rate coefficients K in Eq [\(5.17\)](#page-13-0) according to the Arrhenius formula [\[24\]](#page-23-22):

$$
K(T) = K_{20} \cdot \Theta^{(T-20)} \tag{5.23}
$$

where $K(T)$ is temperature dependent rate coefficient, *T* is temperature, K_{20} is rate coefficient at temperature 20 $^{\circ}C$, Θ is empirical temperature coefficient differing for typical reactions [\[24\]](#page-23-22). Temperature field has to be input in the individual river network nodes. It is derived from measured or modelled temperatures for given scenario, e.g. season.

An algorithm is based on explicit procedure when the mass flow for particular pollution parameter (analogically to BOD) is modelled. The calculation is carried out from headwater nodes of individual stream branches in the downstream direction. Input data are dealing with stream network topology, geometric and hydraulic properties, pollution sources and calibration data. The results are saved in appropriate formats to be transferred to graphical applications (GIS), various types of graphical outputs are available—pollution sources, calibration results, mass flow, and concentration.

Practical application using basic model was carried out at four catchments of Czech rivers the Jihlava, Želetavka, Oslava, and Svratka (Fig. [5.2\)](#page-3-0). The total length of modelled streams at all rivers was about 600 km. Following examples are referred to the study of Jihlava river catchment [\[27\]](#page-24-1).

For the calibration, the extensive set of observation data has to be collected and analysed. The data from sampling are usually obtained in the form of concentration of given water quality indicator. For the processing, this should be completed with the discharge data and finally, the mass flow values for each profile and sampling time has to be calculated. Assuming that the stream mass flow is generally higher during the wet periods (rainwash, street pollution, sewer separators), it is advisable to classify mass flow results according to stream discharges and arrange them into two calibration sets for "wet period" characterized by approximately annual average discharge *Q*^a and "dry period" characterized e.g. by *Q*³⁵⁵ days discharge or rather higher.

Fig. 5.8 The Jihlava river—sampling data analysis—BOD mass flow, dry spell

Example of such analysis at the Jihlava river for the dry period is shown in Fig. [5.8.](#page-15-0) In such a way the numerical model was calibrated for two scenarios mentioned using analysed and smoothed sampling data. The calibration proceeded from headwater nodes of individual stream branches in the downstream direction. During the calibration, coefficient K_{BOD} in Eq. [\(5.21\)](#page-13-3) was determined along the streams by the trial-and-error method. Characteristic values of coefficients were set for modelled flow and pollution conditions.

Verification of the model was performed for the set of independent observation data obtained from various NGO's. Results of model calibration are shown in Fig. [5.9](#page-16-0) for the dry period, and BOD mass flow in the Jihlava river. The simulations of selected scenarios were based on calibrated and verified model. Quite an extensive number of variants dealing with improvements of various pollution sources was evaluated and analysed.

The graphical outputs enabled the assessment of individual pollution sources, their significance and impact on water quality along water courses. The outputs were expressed in the form of mass flow and concentration of individual pollution parameters in tabular and graphical form. An example of the results is shown in Fig. [5.10](#page-16-1) where the proportion of inputs from municipal, industrial and agricultural pollution sources in terms of COD_{CR} can be seen along the Želetavka river.

In Fig. [5.11](#page-17-1) another presentation of results is shown where individual water quality indicators at selected profile are compared with their division according the pollution sources in the catchment upstream.

The balance models may serve as powerful and efficient decision support tool when allocating financial sources at stream water quality improvement. The results of modelling may indicate the most significant pollution sources considerably affecting

Fig. 5.9 The Jihlava river model calibration—BOD mass flow in (g/s), dry period. Results of model \longrightarrow calibration data ,verification data •

Fig. 5.10 The Želetavka river—COD mass flow (g/s) with the division to agricultural, industrial and municipal pollution origin

water quality. For example, it can be seen from Fig. 5.11 that BOD, N-NH₄ and phosphorus pollution come mostly from the municipalities, on contrary nitrates N-NO3 come dominantly from agriculture.

Experience shows that more sophisticated transient models may not give more accurate results. The most crucial is to collect all relevant information, namely those about all important pollution sources, to be included into the model and relevant data from water quality sampling.

5.7 Detailed Models

Detailed models deal with local water quality solutions. They focus mostly on the limited part of the catchment or river reach. The objectives of the solution may be the impact of the interaction of sewer network on stream water quality via sewer overflows, detailed modelling of the progression of spills due to accidents, development of emergency plans and others.

The models are usually conceived as transient, time series of the discharge and pollution sources have to be provided as input data. When the duration of events is short, and the transport of the solids is fast, constitutive changes may often be neglected and the pollutants are considered to be conservative. On the other hand concentration gradients are considerable so dispersion together with advection are the prevailing and the most important processes influencing the time and spatial course of concentration.

For the solution, full shape of Eq. (5.1) is used. To realistically describe the dispersion processes, the dispersion coefficient has to be reliably estimated. For this purpose tracing experiments are executed and evaluated [\[1\]](#page-23-0). Another, less reliable method is to derive the dispersion coefficient using empirical formulae, e.g. by Eqs. [\(5.5\)](#page-7-0) and $(5.6).$ $(5.6).$

River	Reach length (km)	Average width of the river bed (m)	Number of sewer overflows
Velká Haná	0.7		3
Malá Haná	0.4	4	
Drnůvka	2.0		13
Roštěnický potok	1.0	4	5
Haná	5.0	Q	31

Table 5.1 Summary of the streams in the Vyškov city

One example is the use of the simulation models for the optimization of the management of sewer systems and sewer overflows releasing sewage waters to the receivers during extensive storm events. The municipalities have been traditionally provided with combined sewer systems. Newly built urban areas have been appended to the existing sewer mains, causing their frequent overloading. To release water and avoid sewer overloading sewer overflows (SO) are proposed along the sewer mains usually following local rivers [\[28\]](#page-24-2). The appropriate tool for the assessment of the impacts of sewer overflow effluent discharges into surface streams is the pollution transport modelling [\[5\]](#page-23-24). In practice, both single models of sewer and open channel networks and coupled models including both systems may be used [\[29\]](#page-24-3). It is true that the single stream water quality models often enable easier, faster and more transparent data handling.

The input data consist in the detailed topology and geometry of the streams, including local arrangements like water diversions, intakes, headraces, etc. The stream topology has to be completed by the locations of pollution sources. These are frequently storm sewer overflows, both present and proposed to be built. Hydrological conditions in streams have to be described both for the no-rain period and for the design storm event. Usually, the storm event and its impact on sewer system is the subject of the modelling of sewer network response in terms both water amount and its quality. In this case outflow hydrographs from sewer overflows and water quality resulting from the sewer model are inputs to the open channel water quality model.

This kind of model is demonstrated in the following example where the impact of effluents from sewer overflows in the city of Vyškov and their superposition is modelled by 1D transient water quality model. The purpose of the modelling was to assess the changes over time in the concentration of six water quality indicators, namely BOD, COD, Ammonia nitrogen (N-NH4), total Nitrogen (N), total Phosphorus (P), and suspended solids (SS) in the principal rivers in Vyškov. Assessed rivers represent small- and middle-sized streams. The study was the part of General Water Management Plan as a part of the urban plan of the city of Vyškov in the South Moravian Region of the Czech Republic (Fig. [5.2\)](#page-3-0). The scheme of local streams and sewer overflows along the receivers are marked in Fig. [5.12.](#page-19-0) The summary of local streams is shown in Table [5.1.](#page-18-0)

In Vyškov, the revision and improvements of existing sewer overflows have been planned together with the eventual design of new ones. The rehabilitation of sewerage

Fig. 5.12 River network in the Vyškov city with marked sewer overflows: red—existing remaining, blue—existing, blank—proposed

also involves the design of storm water retention tanks, which attenuate the peak discharges in the sewers and so decrease the released amount of polluted water to receiving streams via storm water overflows. In urban areas, the common problem is spatial constraints which limit wider application of large storm tanks. Certain problems are also maintenance and keeping tanks clean from sediments after each storm event. An assessment of above mentioned arrangements for water quality improvement was also an objective of the modelling.

In Figs. [5.13](#page-20-0) and [5.14](#page-20-1) modelling results for BOD concentrations in (mg/l) during the design storm event in the Vyškov city are plotted along the Haná river (see Fig. [5.12\)](#page-19-0). The graphs depict the envelopes of maximum concentrations reached at given channel profile during the transient propagation of pollution gradually spilled from sewer outflows and the superposition of pollution "cloud" along the Haná river during the storm event. In the figures, both present state and state corresponding to proposed arrangements at the sewer network are shown.

Figure [5.13](#page-20-0) shows the conditions along the Haná river during the average discharge *Q*a, Fig. [5.14](#page-20-1) the conditions at the low discharge*Q*²⁷⁰ with the exceedance of 270 days.

Fig. 5.13 BOD concentrations along the Haná River—average discharge *Q*a. Marked sewer overflows: red—existing, blue—proposed including remaining

Fig. 5.14 BOD concentrations along the Haná River—average discharge *Q*270. Marked sewer overflows: red—existing, blue—proposed including remaining

Water quality indicator	The Haná	The Rostěnický potok	The Drnůvka	Imission standard
BOD	164	157	191	
COD_CR	440	423	508	26
$N-NH_4$	15	14	17	0.23
NTOTAL	21	20	24	6
P_{TOTAL}	4.1	3.6	4.6	0.15
Suspended solids	264	253	310	20

Table 5.2 Maximum modelled concentrations at Q_a —perspective, comparison with immission standards

It can be seen that the most influential is the very upstream sewer overflow which increases significantly (more than 15 times) the concentration in the Haná river, another significant worsening of water quality in the Haná may be observed close to the town centre where numerous sewer overflows with significant effluents increase BOD up to the 250 mg/l which practically comply with sewage concentration in the sewer. It can be seen that due to relatively low annual average discharges Q_a $= 0.44-0.64$ m³/s when compared to the outflow from sewer separators (in total about 7.3 m^3 /s) the BOD concentration in the Haná river is not so much influenced by original river discharge in the stream before the storm event. This is true namely downstream of the town centre. However, it can also be seen that the effect of technical arrangements on the sewer network upstream of the town centre is more significant in case of small discharges in the Haná river. This is due to minimal discharge Q_{270} $= 65-84$ l/s.

Downstream of the town centre where the most of improvements concentrated the maximum effect reaches about 35% of the original concentration. All the same even in case of improvements anticipated the effluents from sewer overflow would harm water quality in surface streams for a limited time during the storm which is about 1.5–2 h. As an example, modelled maximum concentrations of individual water quality indicators along individual watercourses in Vyškov for the *Q*^a scenario and proposed improvements are shown in Table [5.2.](#page-21-0) In the last column, the immission water quality standards according to [\[10\]](#page-23-4) are mentioned for simulated water quality indicators. The comparison shows that even if considerable investments into water quality improvement were introduced the temporary exceeding of acceptable concentrations specified for long-term stream water quality was significant.

Experience shows that imission standards should not be employed in case of little incidents like e.g. spills from sewer overflow during extreme storm events with low periodicity. The acceptable concentrations have to be designated at the negotiation of all involved bodies like river agencies, water companies, municipalities, modellers and independent consultants. At the decision the nature of the streams, endangered habitat and also possibilities for technical arrangements on the sewer system and at the urban area have to be taken into account.

5.8 Conclusions

At present water quality, numerical modelling plays a significant role in stream water quality management, in the assessment of present water quality in water courses and predicting impact of individual pollution sources. Modelling techniques are recently frequently used for the optimization of remedial measures adopted on pollution sources at different levels of the river basin extent and input data accuracy. For this purpose models of various classes may be used, like global screening models, basic balance models and detailed transient flow and contaminant transport models answering particular questions about local water quality issues.

In this chapter, the principles of individual model types are mentioned. Their use is demonstrated on case studies carried out by the author during last three decades on the territory of the Czech Republic. Particular problems, results achieved and questions arose at the modelling are briefly discussed together with comments on the of interpretation of typical graphical and tabular outputs.

5.9 Recommendations

When modelling stream water quality in water courses the appropriate model has to be proposed based on conceptual considerations containing set of simplifications and preliminary assumptions. The reasons of these assumptions should be carefully discussed and justified.

The crucial issue are comprehensive, complete, reliable and homogeneous data on catchment and channel characteristics, pollution sources and also water quality in streams obtained by monitoring. For the data assembling sufficient time and adequate financial sources have to be reserved.

The reliability of the model may be significantly improved by its calibration and verification. When the stream water quality data are missing sensitivity study is strongly recommended. Here the data about the parameters influencing water quality should be taken from the literature sources and from the previous studies.

For decision makers the results of the modelling should be properly summarized, depicted and interpreted.

Generally, the last step of the modelling process should be feedback on the compliance between predicted values of water quality indicators by modelling and the real values obtained by monitoring after adopting proposed measures. Unfortunately, this step is mostly omitted. The impact usually manifests itself after numerous years after the initial proposals and modelling. Moreover, there are usually no extra financial sources for additional on-purpose monitoring and for such comparisons and evaluation of possible shortcomings of the forecasts.

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