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REVIEW OF MATHEMATICAL MODELS OF WATER QUALITY

PRZEGLĄD MODELI MATEMATYCZNYCH JAKOŚCI WÓD

Abstract: Water is one of the main elements of the environment which determine the existence of life on the Earth, affect the climate and limit the development of civilization. Water resources management requires constant monitoring in terms of its qualitative-quantitative values. Proper assessment of the degree of water pollution is the basis for conservation and rational utilization of water resources. Water quality in lakes and dams is undergoing continuous degradation caused by natural processes resulting from eutrophication and due to anthropogenic reasons. One of the tools that are used to solve problems of surface water pollution is modelling of changes which take place in lake waters and associated water quality changes. In the last thirty years a rapid development of mathematical modelling of water resources quality has been observed. A number of computer models have been designed which are successfully applied in practice in many countries, including Poland. This paper presents an overview of mathematical models for assessment of water quality in dam reservoirs. Description of the WASP program which will be used for modelling water quality in the Sulejow Reservoir was the focal point.

Keywords: mathematical models, eutrophication, WASP, quality of surface water

Introduction of mathematical modelling of surface water

In addition to the influence of human economic activity, the current state of surface water quality depends also on natural phenomena. Water quality in lakes and dams is undergoing continuous degradation caused by natural processes resulting from eutrophication and due to anthropogenic reasons. On the other hand, the diversity of needs and priorities by which surface waters are assessed is remarkable. Activity zones that are taken into account include household water supply, agriculture, transport, hydropower, fisheries, recreation and flood wave control. Therefore, the amount of water in rivers, lakes and reservoirs should be assessed strictly depending on the priority needs of a specific case being considered. Treating water conservation as a whole, it should be emphasized that only about 50% of biogenic pollution load originates from point sources (N, P). The remaining 50% comes from dispersed sources. Therefore, even an excellent sewerage may fail to prevent degradation of sensitive receivers. The scale of the problem is reflected by eg cyanosis water blooming. This problem affects primarily the eutrophised (rich in nutrients)

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lakes and reservoirs. Multifaceted usage of reservoirs is possible only if ecological values of their geosystems, especially good quality of water, are retained. This quality is derived from environmental conditions and the way in which maintenance drainage areas are developed. Identification of relationships and interactions in the drainage basin-reservoir system helps indicate optimal forms of land use, triggering protection of accumulated water resources.

One of the tools that are used to solve problems of surface water pollution is modelling of changes which take place in lake waters and associated water quality changes. Such a model can be used to predict water quality, taking into account changes that affect water quality factors or changes in their intensity. The accuracy of environmental assessment using models depends on the understanding of processes which occur in the environment and on appropriate choice of mathematical equations that describe them. On the other hand, it depends on available data sets, namely results of the measurement of water quality indicators, on which the estimation of parameters and coefficients of the model is based [1]. In recent years, computer simulation methods are becoming popular in scientific research, particularly as far as the research on the aquatic environment quality is concerned. Methods of computer analysis have become an independent branch of research, which substantially increases the research capabilities of modern eco-engineers [2].

The aim of mathematical modelling

The aim of modelling of surface water quality is to construct a mathematical model of a stream (flowing water) or water tank (standing water) making it possible to track changes in water quality which depend on varying initial and boundary conditions of the simulation. The application of modelling to solve problems related to water quality allows us to analyse the occurring phenomena and to find dependencies between them as well as to attempt to predict and quantify effects of the changes in the aquatic environment. The most common uses of surface water quality models include [2, 3]:

a) location of area sources of pollution, setting limits (daily, monthly, annual) of pollutant loads for the existing point sources of pollution,
b) planning the location of water intakes and outfalls discharging pre-treated effluent from sewage treatment plants,
c) location of the stream segments or reservoir water depth in which there are adverse or even dangerous environmental conditions for living organisms, due to water pollution, that prevent proper functioning of aquatic and water-land ecosystems,
d) protection of watercourses designed for the location of drinking water sources,
e) establishing the causes of water quality deterioration on a given segment of a stream,
f) forecasting changes in water quality by simulating development of different versions of drainage basin,
g) selecting an optimal strategy for sustainable development of the drainage basin.

Of the above-mentioned issues these are most often subjected to the analysis, which leads to the definition of environmental threats of water resources of the area related to such phenomena as oxygen deficit, eutrophication, acidification, pollution with toxic substances (synthetic organic compounds, heavy metals), salinity and deterioration of sanitary conditions. Mathematical modelling is a relatively young branch of science, therefore, not so long ago a specific mathematical model for each stream was prepared individually to achieve environmental objectives of this type, which was very labour-intensive and expensive. Currently, this practice is discontinued, and existing mathematical modules are used instead, which, depending on the needs and characteristics of the watercourse, undergo necessary modifications [4].

Classification of mathematical models

The most general division of software modules used to model the processes occurring in the environment includes [2]:

a) physical models (laboratory),
b) mathematical models, including:
   - analytical models - based on exact solutions of the equations of mathematical physics,
   - numerical models - using approximate solutions.

Depending on the complexity of computer simulation models of surface water quality, they can be divided into three groups:

- One-dimensional models (1D), the simplest and most commonly used models in the analysis of river water quality, which assumes that significant changes in the parameters determining water quality occur only along the longitudinal profile of the watercourse. One-dimensional inflow-outflow models are based on measuring the concentration loads of water parameters flowing in and out. On this basis changes in the concentrations of all parameters are calculated. One-dimensional models are not designed to calculate the variation of concentration at the time, so one cannot get information on the specific hourly, daily and monthly water quality parameters. These programs do not describe the complex chemical, physical and biological reactions in water reservoirs which are an essential factor regulating changes in the water quality parameters. An advantage of these programs is that they can be applied quickly to any other water reservoir without pre-calibration and with small available database of measurements [5].
- Two-dimensional models (2D), which assume that significant changes in water quality occur not only along but also in the longitudinal profile of the watercourse, and therefore it is necessary to analyse water quality at various depths. Two-dimensional models are used most often in the case of lakes, reservoirs or deep rivers and require more data and more analytical experience of the user than the one-dimensional models. They require careful calibration and are sensitive to changes of many parameters of water quality. The end result of these programs is a forecast of water quality parameters close to measurements of actual concentrations. Assessment of individual parameters can be performed for given time intervals, ie hour, day, week, month and year [5].
- Three-dimensional models (3D), which examine the spatial distribution of concentrations of simulated water-quality parameters. Three-dimensional models are used to simulate changes in water quality in the sea bays, lakes, dams and deep rivers; they require huge amounts of data and extensive analytical experience from the user. They are most rarely used because of high complexity of the analysed issues.

As with other areas of the environment, computer modelling of surface water quality issues requires a multidisciplinary approach in which mathematical methods and modern computer technologies are applied simultaneously with the basic techniques in the field of environmental engineering. This applies to the description of physical phenomena associated with the formation of pollutants, their distribution and the changes which take place in the aquatic environment, as well as the application of computational methods and models for hazard analysis or control of water quality in specific cases [2]. From the standpoint of applications, the ultimate goal of the model is to use it as a supportive tool in monitoring and forecasting surface water quality, as well as while taking planning decisions. Due to the extent and spatial scale, several categories of models are considered:

a) Operational models - typically related to short-term forecasting and used to real-time control of water reservoirs or flow rate in order to maintain established parameters. Such models require automatic entering of current input data.
b) Tactical models - associated with the use of operational decision-making in taking tactical actions in which relationships of the "input-output" type between the key parameters of the system are vital. The time horizon of this type of analysis covers a period of couple of days, weeks or even a season in the case of control of water quality in a river. In terms of tools used in the tactical model, steady-state analysis and quantitative economic and environmental instruments are used most frequently.
c) Strategic models - refer to a longer time horizon, where one can analyse, predict, or plan the state of the environment as a projection of the current state, taking into account all the relevant trends. This type of modelling is based on an analysis of the results of computer simulation of various scenarios and analysis of its efficiency.
d) Directional models - concern long-term forecasts related to structural changes, testing the possibility of sustainable development and the evolution of the whole system.

Properly chosen calculation programs are the tool that is used to model changes in the aquatic environment. They simulate the behaviour of the aquatic environment and the way its parameters change. These parameters include water temperature, wind strength and direction, the concentration of dissolved oxygen, salinity of water, the amount of biogenic compounds and other parameters depending on the complexity of a program [4].

The world's first surface water quality model was created in 1925 in the United States of America, by Streeter and Phelps in order to layout the location of drainage sewage outfalls on the Ohio River [3]. It was a one-dimensional model, based on the balance of oxygen and simple linear equations. Although since then more than 80 years have passed, basic approach to modelling of surface water quality has not changed, since the construction of all models is founded on three basic principles, ie the conservation of mass, momentum and energy. Ordinary and partial differential equations are used to describe the dynamics of phenomena occurring in the surface waters associated with the spread of various pollutants. For each physical quantity (in the considered control volume and time interval) the general law of conservation is as follows [2]:

Inflow outflow + source of change = accumulation

It is estimated that currently there are at least several thousand surface water quality models derived from public or commercial basic modules and then adapted to the modelled stream or water reservoir [3].

The United States of America leads the way in the field of modelling of surface water quality using its own, world's best-developed network of continuous monitoring of surface waters. One- and two-dimensional models are used on a large scale, both by research centres and federal or state institutions. The biggest role is played by three state institutions: EPA (*United States Environmental Protection Agency*), United States Geological Survey and Waterways Experiment Station, belonging to the United States Army Corps of Engineers. European achievements in this area are also significant, however free access to the U.S. models and their documentation, programming language and numerous examples of practical application promotes the choice of models generated in the United States [4]. A brief description of selected models of surface water is given below.

- **AQUATOX 2.2**, is a PC-based ecosystem model that predicts the fate of nutrients, sediments, and organic chemicals in water bodies, as well as their direct and indirect effects on the resident organisms. AQUATOX simulates the transfer of biomass and chemicals from one compartment of the ecosystem to another. It does this by simultaneously computing important chemical and biological processes over time. AQUATOX simulates multiple environmental stressors (including nutrients, organic loadings, sediments, toxic chemicals, and temperature) and their effects on the algal, macrophyte, invertebrate, and fish communities. AQUATOX can help identify and understand the cause and effect relationships between chemical water quality, the physical environment, and aquatic life. It can represent a variety of aquatic ecosystems, including vertically stratified lakes, reservoirs and ponds, rivers and streams, and now estuaries.
- **CE-QUAL-ICM** has evolved from a 3D water quality model developed for Chesapeake Bay to evaluate the effectiveness of nutrient reduction proposals on Bay eutrophication. This model contains a bottom sediment chemistry submodel that interacts with the water column for simulating sediment oxygen demand and nutrient fluxes. The CE-QUAL-ICM modelling approach involves first applying a 2D or 3D hydrodynamic model and coupling the output to CE-QUAL-ICM for driving the transport terms. The water quality model can then be applied for a variety of conditions without having to rerun the hydrodynamic model. The CE-QUAL-ICM model has been used on a number of systems, including Chesapeake Bay, the New York Bight, Lower Green Bay, Los Angeles - Long Beach Harbor, and Indian River - Rehoboth Bay.
- **CE-QUAL-RIV1 1D** is a one-dimensional (cross-sectionally averaged) hydrodynamic and water quality model, meaning that the model resolves longitudinal variations in hydraulic and quality characteristics and is applicable where lateral and vertical variations are small. CE-QUAL-RIV1 consists of two parts, a hydrodynamic code (RIV1H) and a water quality code (RIV1Q). The hydrodynamic code is applied first to predict water transport and its results are written to a file, which is then read by the quality model. It can be used to predict one-dimensional hydraulic and water quality variations in streams and rivers with highly unsteady flows, although it can also be used for prediction under steady flow conditions. RIV1H predicts flows, depths, velocities, water surface elevations, and other hydraulic characteristics. The hydrodynamic model solves the St. Venant equations as the governing flow equations using the widely accepted four-point implicit finite difference numerical scheme. RIV1Q can predict variations in each of 12 state variables: temperature, *carbonaceous biochemical oxygen demand* (CBOD), organic nitrogen, ammonia nitrogen, nitrate(V) + nitrate(III) nitrogen, dissolved oxygen, organic phosphorus, dissolved phosphates, algae, dissolved iron, dissolved manganese, and coliform bacteria. In addition, the impacts of macrophytes can be simulated.
- **CE-QUAL-W2 2D** is a water quality and hydrodynamic model in 2D (longitudinal-vertical) for rivers, estuaries, lakes, reservoirs and river basin systems.

It is a two-dimensional water quality and hydrodynamic code supported by the USACE Waterways Experiments Station [6]. The model has been widely applied to stratified surface water systems such as lakes, reservoirs, and estuaries and computes water levels, horizontal and vertical velocities, temperature, and 21 other water quality parameters (such as dissolved oxygen, nutrients, organic matter, algae, pH, the carbonate cycle, bacteria, and dissolved and suspended solids).

- **COASTOX**, this model was developed at the Cybernetics Center, Kiev [7] to simulate the transport and the dispersion of pollutants in the Dnieper reservoirs and in the Pripyat River. It contains the radionuclide transport submodels similar to those used in FETRA. The model includes the sediment transport, the transport by the advection-diffusion, and the radionuclide-sediment interactions. It considers the dynamics of the bottom depositions and describes the rate of the sedimentation and the resuspension as a function of the difference between the actual and equilibrium concentration of the suspended matter depending on the transport capacity of the flow.
- **DELFT 3D** is a complete coastal hydrodynamic modelling system, capable of simulating hydrodynamic processes due to waves, tides, rivers, winds and coastal currents. It is a system of three-dimensional calculation programs developed by Delft Hydraulics. Delft 3D is a software package that was designed primarily as an application focused on water flow and quality. The package consists of several modules coupled together to provide a complete picture of three-dimensional flow, surface waves, water quality, ecology, sediment transport and bottom morphology in complicated, coastal areas. The modelling system includes hydrodynamic module-FLOW, water quality module WAQ, wave module-WAVE, particle tracking module-PART, morphodynamic MOR module, sediment transport module-SED, ecological module-ECO.
- **DUFLOW 1D** is a computer package for simulating 1D unsteady flow and water quality in open watercourses. Simulates both water flow and its quality, suitable for modelling the transport of substances *via* free movement of surface; phasing out of bottom substances enables analysis of phenomena and processes which take place between the substances dissolved in water and contained in the sediments. DUFLOW has been applied with great success to several river systems [8]. DUFLOW is compatible with geographical information systems, which facilitate representation and display of the open water system.
- **DYRESM 1D** (*DYnamic REServoir Simulation Model*) is a one-dimensional hydrodynamics model for predicting the vertical distribution of temperature, salinity and density in lakes and reservoirs satisfying the one-dimensional approximation. This model study was conducted by the Flow Science Inc. DYRESM provides quantifiably verifiable predictions of the thermal characteristics in such systems over time scales ranging from several weeks to tens of years. The model thus provides a means of predicting seasonal and inter-annual variability of lakes and reservoirs as well as sensitivity testing to long-term changes in environmental factors or watershed properties. DYRESM can be run either in isolation for purely hydrodynamic studies or coupled to CAEDYM (*Computational Aquatic Ecosystem DYnamics Model*) for investigations involving biological and/or chemical processes. The computational demands of DYRESM are quite modest and multi-year simulations can be carried out on PC platforms under Windows or Linux.

- **ECOM** (*Estuarine, Coastal and Ocean Model*) it is a three-dimensional, time-dependent model developed by Blumberg and Mellor [9] for shallow water environments such as rivers, lakes, estuaries and coastal oceans. Since the last few years it is the most popular model used for simulation calculations of flows in coastal waters and lakes.
- **FLESCOT** it is an unsteady, three-dimensional, finite difference model [10]. It consists of sub-models of hydrodynamics, turbulence, water temperature, salinity, sediments (both cohesive and non-cohesive) and contaminants (both dissolved and sediment-sorbed). The FLESCOT model also simulates the behaviour of sediments and contaminants in the riverbed, affected by erosion/deposition, direct adsorption/desorption between water and bottom sediments, and bioturbation. It can calculate wind-induced flow and wave-induced sediment transport, thus affecting contaminants transport in shallow water. The model has been applied to the Hudson River estuary in New York for Cs-137 migration and accumulation, to Buzzards Bay/new Bedford Harbour in Massachusetts for PCBs and heavy metals assessing their transport and potential remediation activities, and to hypothetical 3000 m deep ocean for low-level radioactive waste disposal assessment. FLESCOT uses multiple bed layers.
- **HSPF** (*Hydrological Simulation Program - FORTRAN*), is a US EPA analytical tool designed to allow the engineer to simulate hydrology and water quality in natural and man-made systems. HSPF is used to apply mathematical models to simulate the movement of pollutants through watersheds. It is a set of computer codes that can simulate the hydrologic, and associated water quality, processes on pervious and impervious land surfaces and in streams and well-mixed impoundments.
- **MIKE-3**, a three-dimensional model/software system that is implemented in the form of computational programs by the Danish Institute of Hydrodynamics. This enables modelling of any system of surface water, takes into account both water flow and its quality, enables modelling of the transport and metabolism of nutrients, heavy metals, the phenomenon of drying troughs, floods, and the processes occurring in bottom sediments. Mike-3 is designed in a modular structure with the three main components: estuarine and costal hydraulics and oceanography environmental hydraulics sediment processes. The group of environmental modules includes the *Advection-Dispersion Module* (AD) and three process modules: the *Water Quality Module* (WQ), the *Eutrophication Module* (EU) and the *Heavy Metal Module* (ME).
- **MIKE 11**, a program developed by the Danish Hydraulic Institute [11] is a one-dimensional modelling system for the simulation of flows, sediment transport and water quality i estuaries, rivers, irrigation systems and other water bodies. Mike 11 has been designed to have an integrated modular structure with basic computational modules for hydrology, hydrodynamics, advection-dispersion, water quality and cohesive and non-cohesive sediment transport. The system also includes a module for the calculation of runoff rainwater. The program enables analysis of flood phenomena, design of prevention and flood forecasting in real time. MIKE 11 enables also analysis of dam breaks and optimization of reservoirs and hydraulic equipment. It is also a helpful tool in estimating the effect of water on the environment that surrounds us.

- **MINLAKE 1D** models water quality of lakes and reservoirs. It is designed to calculate water quality parameters such as temperature, dissolved oxygen concentration, the concentration of phosphorus, nitrogen and dissolved substances.
- **TELEMAC** is an advanced system utilizing the finite element method to calculate the transport of contaminants and water quality in two and three dimensions. This system was developed by HR Wallingford in collaboration with Electricite de France/SOGREAH. TELEMAC together with MIKE-3 and Delft3D are the most common software systems which are available on a commercial basis for the calculation of three-dimensional flow, transport and water quality.
- **WASP** (*Water Analysis Simulation Program*) - the WASP modelling system is a generalized modelling framework for contaminant fate and transport in surface waters. Based on flexible compartment modelling, WASP can be applied in one, two, or three dimensions. WASP is designed to permit easy substitution of user-written routines into the program structure. Problems that have been studied using WASP include biochemical oxygen demand, dissolved oxygen dynamics, nutrients/eutrophication, bacterial contamination, and toxic chemical movement. WASP is a dynamic compartment model that can be used to analyze a variety of water quality problems in such diverse water bodies as ponds, streams, lakes, reservoirs, rivers, estuaries, and coastal waters.

Modelling procedure

There is no universal and generally applicable procedure for mathematical modelling of water resources quality. But there are many conditions that may help formulate a general procedure for the test model. The first step in the modelling procedure is to define the goal and scope of mathematical modelling of water quality of the receiver, although it does not make up the same procedure. The procedure should begin with a general concept, which will present how the receiver - and thus physical system, will be represented in a three-dimensional space. The test model of the environment is “an area of modelling”. Description of the area of modelling involves both the definition of its borders, ie separating it from its surroundings, and description of the existing relationships, and relationships characterizing the impact of the environment outside the borders of the chosen system [12]. Definition of the area of modelling has to include the terms of time and space as well as the selection and characterization of the processes occurring in the system. An overall approach is closely connected with the division of the receiver into segments and layers and construction or selection of the model itself. Pre-assessment of the selected model can be made using sensitivity analysis. Proper writing of mathematical equations and their numerical solutions, using the chosen method is vital in this step.

The purpose of calibration of the model is to establish to what extent the results of obtained calculations are consistent with the results of field measurements. The calibration is usually done by successive approximations for different sets of parameters. It is performed on one or more data sets for both inputs and outputs. The parameters of models and the model itself are adjusted or modified in order to get a result that is closest to the currently observed water quality. Model calibration is burdened with an error due to uncertainty and errors in spatial mapping and temporal distribution of the parameters in the tested area as well as because of inaccuracy of boundary conditions. Model sensitivity is analysed to determine the impact of these errors on the solution, using special methods and algorithms.

Model verification is aimed at increasing its credibility by performing calculations for a number of sets of parameter values to determine one optimal set which will characterize the modelled object. Verification of the model requires an independent set of data inputs and outputs that can be used to test the calibrated model. The data used for the verification must be independent of the data used to calibrate the models. A model is considered verified if the model forecasts, for the range of results other than the calibration data, coincide with those observed in the field [2]. In view of the multidisciplinary nature and generally high complexity of computer models of the environment, one should pay attention to several conditions to be met in the process of the models' creation, calibration and verification, which will allow us to expect usefulness of the model in practice. The following items are especially noteworthy:

- Models based on the best available theoretical results should be used to describe the processes, for example, using full description of the present three-dimensional spatial phenomena, avoid approximation in steady-state dynamic processes, changing over time.
- Adopted description should be fully documented (basic assumptions, equations and parameters should refer to reviewed publications).
- Computer code should be fully tested, both as a whole and at the level of its individual modules.
- The model should be tested not only by its creators, but also by other independent teams.
- Input data must be reliable. Applied time and spatial discretization should be consistent with the scale of simulated physical phenomena.
- Computer code should be numerically correct. All the iterative processes should be consistent, providing adequate accuracy of the solutions and their results should not depend (within the assumed accuracy) on the length of temporal and spatial discretization steps.
- The model should be fully verified on real data.
- Attention should be paid to the proper calibration parameters, including their range of uncertainty.
- Applications of the model should be fully documented in such a way that individual projects can be repeated for the same values and input data.

Surface water quality model may have practical applications, and once calibrated (and subsequently verified) becomes a powerful analytical tool which enables wide-range engineering and environmental protection of the given watercourse, in particular while preparing forecasts of quality. Verified functioning of a surface water quality model provides a scientific basis for the subtraction of specific actions which can be either to maintain the existing state of the aquatic environment as well as to improve it in a given time horizon, depending on the changing human pressure on the environment [4].

Specifics of the WASP program

The WASP program was developed under the auspices of the Environmental Protection Agency of the United States [13], as an enhancement of the original WASP [14, 15]. This model helps users interpret and predict water quality responses to natural phenomena and man-made pollution for various pollution management decisions. It is designed for dynamic modelling of transport phenomena and changes occurring in the aquatic environment and in the layer of benthic deposit resulting from sedimentation. It is used to simulate water quality changes which occur in streams, rivers, lakes, artificial reservoirs, estuaries and marine coastal waters. The program reflects the time-varying processes of advection and dispersion, considers both point and aerial tributaries and boundaries of the exchange. WASP is a dynamic program, multipartite suite enabling modelling of one-, two- and three-dimensional structures.

This program consists of two separate computer programs: DYNHYD and WASP, which can work both together and independently. The DYNHYD-5 program is a hydrodynamic model which creates a set of data to determine the flows and other transport values. By contrast, the WASP-6 program enables modelling of the spread and interaction of pollutants in the water. The equations solved by the WASP-6 program are based on the principle of conservation of mass. The input data must be supplied to be able to perform the mass balance; the data describe:

- concentration limits,
- advective transport and dispersion,
- type of simulation, the number of segments, starting time of the simulation, time step,
- geometry of the segments into which the analysed basin was divided,
- advective transport and dispersion,
- concentration limits,
- point and linear sources of pollution,
- function of time: temperature, wind speed, solar radiation, the flow of biogenic compounds load,
- initial concentration.

These data together with the general mass balance equations which are included in WASP-6, enable solving of a set of equations that describe water quality. The WASP model requires high selectivity of input raw data. Entering the input data and initial calibration of the model requires a lot of time and leaves no margin for error in implementation of the initial parameters of the database. Final analysis of the results provides complex two-dimensional dependencies. We get the values of various parameters of water quality in the water reservoir segments in terms of two other parameters. This enables a very accurate prediction of concentrations of various parameters and their variability in response to changes of not one but several parameters with which the modelled parameter is connected [5]. WASP-6 has as well two kinetic subprograms designed for simulation of other issues related to water quality. The EUTRO model enables modelling of phenomena related to water eutrophication by solving problems of the dynamics of dissolved oxygen, BOD (*Biochemical Oxygen Demand*), nutrient concentrations and phytoplankton abundance in the water depths. The TOXI model includes procedures for simulation of toxic pollutants (COD (*Chemical Oxygen Demand*), heavy metals) in the analysed waters [13]. The program in its simplified version was successfully used for modelling the eutrophication of Tampa Bay, inflow of phosphorus to Okeechobee Lake, eutrophication of the Neuse River and its estuary, eutrophication of phenolic contaminants in Grand Lake, eutrophication of the Potomac estuary, Delaware estuary, organic pollutants and heavy metals contamination of the Deep River - WASP-4 [13]. WASP-4 was used in Poland to model changes in water quality in the water reservoir Dobczyce [16], and WAPS-5 was used to model water quality of the Warta River.

Description of the EUTRO model

Eutrophication is a factor severely limiting the use of reservoirs. It is a consequence of the increased supply of organic and mineral matter. The trophic state of reservoir water is determined mainly by phosphorus concentrations which in range of only 20 to 30 μg P/dm^3 can lead to water blooming [14]. The following limit values of indicators of eutrophication of standing water are used in Poland: total phosphorus - more than 0.1 mg/dm^3, total nitrogen - more than 1.5 mg/dm^3, chlorophyll *a* - above 25 μg/dm^3, transparency - less than 2 m. The important manifestations of eutrophication - in addition to water blooming - include also the development of algae epiphytes, deoxidation of the hypolimnion and reduction of biodiversity. The EUTRO model simulates nutrient enrichment, eutrophication and decrease of the concentration of dissolved oxygen. The simulation can be carried out at different levels of complexity and the user can select all available or selected processes in the modelled system. The way of solving the given problem depends on the number of entered data. The EUTRO program enables modelling and simulation of transport and changes of eight water quality parameters (variables of the eutrophication):

- ammonium nitrogen,
- nitrate nitrogen,
- organic nitrogen,
- phosphate,
- organic phosphorus,
- dissolved oxygen,
- BOD,
- phytoplankton (chlorophyll *a*).

Specified state variables are calculated by taking into account many parallel and interrelated processes that are considered in the model as the four basic phenomena:

- kinetics of growth of phytoplankton,
- nitrogen cycle,
- phosphorus cycle,
- dissolved oxygen balance.

Initial parameter values required to calibrate the WASP model need to come from a period longer than one calendar year. Monitoring of water quality parameters enables accurate calibration of the calculation program. With the appropriate calibration, hydraulic coefficients can be determined enabling an accurate account of various parameters. After the calibration, the program proceeds to calculate various parameters of water quality [15].

Modelling of eutrophication

The EUTRO module allows us to predict changes of state variables, taking into account all the dependencies defined in the program and enables selection of certain variables and processes that shape the quality of surface waters. Relationships between variables in the model calculation procedures include three interrelated physical and chemical processes:

- simple kinetics of eutrophication - simulation of the process of growth and decay of phytoplankton, taking into account the impact of this process on the balance of dissolved oxygen and circulation of biogenic compounds,
- complex kinetics of eutrophication - takes into account the impact of phytoplankton on the process of mineralization of nitrogen and organic phosphorus, as well as nitrification and denitrification,
- complex kinetics of eutrophication of the benthic deposit - takes into account the exchange of the analysed parameters with benthos: diffusive exchange of dissolved substances, benthic deposition and leaching.

The level of simulation calculations can be adjusted to specific needs. Reliability of results depends mainly on the accuracy with which the reservoir ecosystem, environmental parameters, the parameters of processes in the environment, and sources of pollution are described.

The simulation of eutrophication is based on solving differential equations of mass balance. These equations are solved using numerical methods of finite elements. After assuming vertical and lateral uniformity within segments, the differential equation takes a simplified form of [16]:

$$\frac{\partial}{\partial t}(Ac) = \frac{\partial}{\partial x}\left(-U_x Ac + E_x A \frac{\partial c}{\partial x \partial t}\right) + A(S_l + S_b) + AS_k \quad (1)$$

where: c - concentration of water quality component [g/m^3], t - simulation time [d], U_x - longitudinal speed of advection [m/d], E_x - coefficient of dispersion in the direction of water flow [m^2/d], S_i - direct and diffusive external contamination load [g/m^{2}d], S_b - load exchanged between segments as a result of longitudinal dispersion [g^3/md], S_k - contamination load due to kinetic transformations [g/m^{2}d], A - transformation area [m^2].

The WASP program models the parameters which affect the process in time and space, from the point of supply to the point of the estuary of the pollution. The model takes into account all possible ways of mass exchange, such as advective transport (macroscopic fluid motion resulting in the shipment of contaminants with no change in its concentration) and dispersive transport (particles are moved from one place to another which is caused by repeated turbulent diffusion along the velocity gradient), inflow and outflow of loads outside of the tested system, physical, chemical and biological transformations. The following kinds of transport of mineral and organic particles are to be indicated in terms of computational procedures [17]:

- transport in a water column (advective flow of water and dispersive mixing between areas of high and low concentration),
- transport in the layer of the sediment, taking into account the flow of water in the pores and diffusion between the sediment and water column,
- transport of pollution as a result of deposition and re-suspending particles in water (transport between the water layer and sediment bed),
- transport by evaporation from the surface waters and deposition on its surface.

The key assumption in defining the model is the division of the modelled environment into segments in a spatial coordinate system, representing its physical configuration [18]. This division depends on the purpose of simulation. In the case of forecasting the overall process of eutrophication of lakes, the division into segments should take into account the characteristics of the aquatic environment which can be distinguished on the basis of variables, and changes in the intensity of the processes which affect water quality in those parts as well as their variability in time. The environment can be divided vertically, along and across. The concentrations of components of the environment (considered variables) are calculated for all segments, while the transport rate of environment components is calculated for the boundary surface between adjacent segments. By dividing the segments of the environment one can distinguish four different kinds of them, ie epilimnion, hypolimnion and upper and lower layers of benthic [19]. Thermal stratification is the basis for differentiating water quality in different parts of the lake at the same time, and different directions of changes in water quality in those parts in time. The presented model of eutrophication of lakes takes into account the following processes [20]:

- transformation cycle of phosphorus compounds, taking into account their dissolved, organic and phytoplanktonic-organic forms. The organic form is divided into dissolved and not dissolved, inorganic phosphorus is divided into dissolved and absorbed on solids suspension;
- transformation cycle of nitrogen compounds, including organic nitrogen, phytoplanktonic-organic, ammonium and nitrate(V) nitrogen;
- dissolved oxygen balance, including the processes of recreation, biochemical oxidation of organic matter in water (BOD), nitrification, denitrification, sedimentation, and phytoplankton growth and decay;
- the interaction of segments with the subsurface benthic deposits. These interactions are defined as a function of time estimated in the calibration of the model, taking into account oxygen consumption and release of ammonium nitrogen and phosphate(V) phosphorus as a result of sediment mineralization.

The growth rate of phytoplankton populations in the environment depends on the species composition of algae, the availability of light and nutrients. Providing such information to the model, which is sufficient to describe the growth kinetics of individual species of phytoplankton, is not possible. Therefore, the EUTRO model describes the population of algae characterized as the total biomass in the form of phytoplankton or chlorophyll. The abundance of phytoplankton is reduced as a result of endogenous respiration, eating algae by zooplankton and because of parasitism.

In a series of transformations of phosphorus compounds three variables are modelled: organic phosphorus, inorganic phosphorus, and algae cumulating phosphorus in their cells. Algae consume during their growth dissolved inorganic phosphorus which becomes inbuilt into the biomass. During endogenous respiration and death of phytoplankton phosphorus is released from the cells of algae in the form of soluble organic and inorganic compounds. The last link in the cycle is the mineralization of organic phosphorus compounds.

Transformation of nitrogen compounds features kind of a similarity to the transformation of phosphorus compounds. Ammonia and nitrates are absorbed by phytoplankton and inbuilt into the biomass during the growth of algae cells. The speed of this process depends on the concentration of available inorganic nitrogen. Nitrogen is returned to water in the form of dissolved organic and inorganic compounds during the endogenous respiration and death of algae. Organic compounds are mineralized to form ammonia. Further transformation processes of nitrogen compounds are nitrification and denitrification. The nitrification process occurs in oxygen conditions - the substrate is ammonia and nitrates are the product. Denitrification takes place in oxygen-free conditions and nitrates are the substrates of this process, whereas nitrogen gas is the product [21].

The fact that Poland is a member of the European Union forces Poland to improve the quality of water resources and to protect them. It is necessary to determine the trophic level and impact of the drainage basin on the lakes and their vulnerability to natural degradation, thereby defining the extent of activities in the drainage area (especially if it is susceptible to load release), the protection of individual reservoirs and ways of their rehabilitation.

Protection of water quality in dam reservoirs, particularly for water supply purpose may be implemented in different ways. The basis for selection of a protection method should be a detailed and multifaceted analysis of specific conditions. Among other things, the time of water retention in the reservoir plays an important role. Correct economic use of the area located in the basin of water intake is essential. Among many possibilities of protection and improvement of water quality in the reservoirs, reduction of nutrient loads in the inlet to the reservoir still takes the first place. It is a prerequisite to obtain good results, both for thermal stratification collapse and direct aeration of the reservoir.

Summary

One of the tools that are used to solve problems of surface water pollution is modelling of changes which take place in lake waters and associated water quality changes. Such a model can be used to predict water quality, taking into account changes that affect water quality factors or changes in their intensity. The accuracy of environmental assessment using models depends on the understanding of processes which occur in the environment and on appropriate choice of mathematical equations that describe them. On the other hand, it depends on available data sets, namely results of the measurement of water quality indicators, on which the estimation of parameters and coefficients of the model is based. In recent years, computer simulation methods are becoming popular in scientific research, particularly as far as the research on the aquatic environment quality is concerned. Methods of computer analysis have become an independent branch of research, which substantially increases the research capabilities of modern eco-engineers.

In the last thirty years a rapid development of mathematical modelling of water resources quality has been observed. A number of computer models have been designed which are successfully applied in practice in many countries, including Poland. This paper presents an overview of mathematical models for assessment of water quality in dam reservoirs. Description of the WASP program which will be used for modelling water quality in the Sulejow Reservoir (Lodz Province) was the focal point.

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PRZEGLĄD MODELI MATEMATYCZNYCH JAKOŚCI WÓD

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Abstrakt: Jednym z narzędzi znajdujących zastosowanie w rozwiązywaniu problemów ochrony wód powierzchniowych przed zanieczyszczeniem jest modelowanie matematyczne. Odpowiedni model może zostać wykorzystany do przeprowadzenia prognoz jakości wody, przy uwzględnieniu zmian czynników oddziałujących na jakość wód czy też zmian ich natężenia. O prawidłowości oceny stanu środowiska za pomocą modeli decydują z jednej strony znajomość procesów zachodzących w środowisku i odpowiedni dobór równań matematycznych je opisujących, a z drugiej dostępne zbiory danych, czyli wyników pomiarowych wskaźników jakości wody, które są wykorzystywane do estymacji parametrów i współczynników danego modelu. W ostatnich latach coraz powszechniej w badaniach naukowych wykorzystuje się metody symulacji komputerowych, dotyczy to zwłaszcza badań nad jakością środowiska wodnego. Metody analizy komputerowej stały się samodzielną gałęzią badań naukowych, która w zasadniczy sposób zwiększa możliwości badawcze nowoczesnych inżynierów-ekologów. W ostatnich trzydziestu latach nastąpił dynamiczny rozwój modelowania matematycznego jakości zasobów wodnych. Opracowano wiele skomputeryzowanych modeli, które zostały z powodzeniem zastosowane w praktyce w wielu państwach, w tym w Polsce. W niniejszej pracy przedstawiono przegląd modeli matematycznych, służących ocenie jakości wód w zbiornikach zaporowych. Bardziej szczegółowo skupiono się na omówieniu programu WASP, który posłuży do modelowania jakości wód w Zbiorniku Sulejowskim (woj. łódzkie).

Słowa kluczowe: modele matematyczne, eutrofizacja, WASP, jakość wód powierzchniowych