APPLICATION OF MATHEMATICAL MODELING AND COMPUTER SIMULATION FOR SOLVING WATER QUALITY PROBLEMS

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Abstract

Deteriorated water resources in Central and Eastern Europe call for actions that should be undertaken to improve current conditions and to protect human and environmental health. Mathematical modeling and computer simulation is often an integral part of the decision-making process. Models and simulations allow rapid and varied evaluation of causes and effects and the principal advantage is that they enable an analysis of even long-term actions with limited investment costs. This paper provides an overview of popular models used for simulation of major elements of a water quality system: surface water quality (QUAL2E), wastewater treatment (Activated Sludge Model No.1), sewer network (SWMM), and water distribution network (EPANET). Model uses are illustrated by specific examples both in the U.S. or in Central and Eastern Europe.

Introduction

For over 40 years after the World War II, Poland experienced gradual deterioration of the environment including water resources. Although the new political and economical situation, as well as new regulations (e.g., [1]) encourage seeking solutions to water quality issues, the fundamental question: “What actions should be undertaken to protect human and environmental health, and how long would it take to restore contaminated water resources?” [2] still remains valid. Currently, only less than 5% of the monitored river kilometers meets the highest standards suitable for human consumption and over 20% of wastewater generated is discharged without any treatment [3]. High contamination of surface waters cause water shortage problems in over 40% of all Polish towns and cities [4].

Two principal concerns that arise in such situations are the mean fixed level of water quality and the impact of temporal variability of types and levels of pollution on water quality. One of the major factors of effective control is the ability to relate causes (inputs) to effects (outputs) and to predict the effects of control actions and changes to pollution sources. In this context, mathematical modeling and computer simulation may become an integral part of the decision-making process. Models and simulations allow rapid and varied evaluation of causes and effects, and their principal advantage is that they enable an analysis of even long-term actions over a short time with limited investment costs.

In many countries, computer software for simulation of major elements of the water quality system have became an inherent tool for experts involved in designing, operation and control of that system. In Poland, the benefits resulting from application of such programs are still unknown or are not appreciated enough [5,6,7,8]. There are at least two reasons for this situation [6]:

- reluctance of management staff to introduce new tools that require training for future users,
- too few examples of a successful application of such programs causing a lack of confidence among potential users.

Another barrier is the cost dealing with the purchase of commercial simulation programs. Fortunately, it is possible to avoid this by using “public-domain” programs.

The aim of this paper is to present an overview (illustrated by specific examples) of such programs for the major elements of a water quality system (Figure 1):

- QUAL2E – surface water quality and hydrodynamics,
- Activated Sludge Models No.1 and No.2 – wastewater treatment systems with activated sludge,
- SWMM – storm and combined sewer quality and quantity,
- EPANET – water distribution network.

Three of them (QUAL2E, SWMM, EPANET) may be downloaded via internet from the U.S.EPA web page (http://www.epa.gov/epahome/datatool.htm).

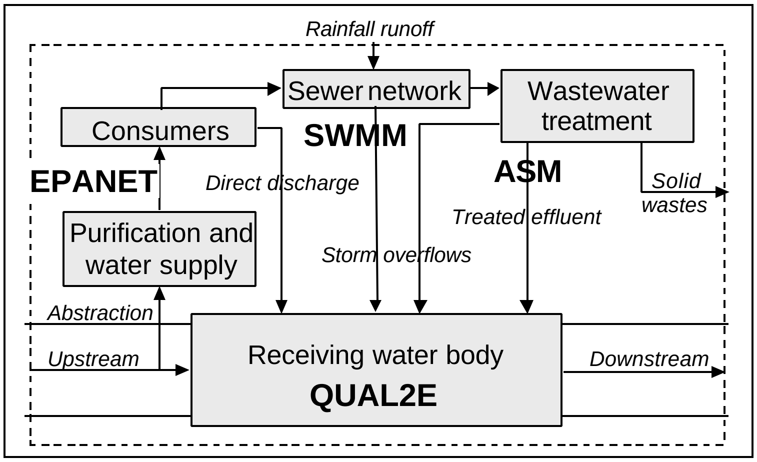

Figure 1. Major elements of the water quality system (adopted from [9]) along with location of the computer models for simulation of these elements

Overview of the models

Surface water quality. There are many different public domain water quality models as shown in Table 1 for rivers, lakes, estuaries and reservoirs. There are also near-field mixing models such as the EPA plume models and CORMIX (http://www.epa.gov/CEAM/) that are used to evaluate mixing zones for pollutants from point source discharges.

Table 1. Water quality models for river, lake, reservoir, and estuary systems.

Model name	Temporal Domain	Spatial Domain**	Simulation		Sediment compartment	Hydraulics	Web address
			Eutro-phication	Toxics			
QUAL2E/QUAL2EU	Steady-state*	1-D longitudinal	yes	no	0-order SOD	Steady-state 1-D	http://www.epa.gov/CEAM/
WASP/ DYNHYD	Unsteady	1-D hydraulics; 1-2-3D water quality	yes	yes	0-order SOD	Unsteady 1-D	http://www.epa.gov/CEAM/
HSPF	Unsteady	1-D longitudinal	yes	no	0-order SOD	Unsteady 1-D	http://www.epa.gov/CEAM/
CE-QUAL-RIV1	Unsteady	1-D longitudinal	yes	no	0-order SOD	Unsteady 1-D	http://www.wes.army.mil/el/elmodels/
CE-QUAL-R1	Unsteady	1-D vertical	yes	no	1st order organic, N, P sediment	0-D based on flow balance in reservoir	http://www.wes.army.mil/el/elmodels/
CE-QUAL-W2	Unsteady	2-D longitudinal and vertical	yes	no	0-order SOD, 1st order organic sediment	Unsteady 2-D	ftp://cole.wes.army.mil
HEC-5Q/WQRRS	Unsteady	1-D longitudinal in river; 1-D vertical in reservoir	yes	no	0-order	1-D unsteady for river, 0-D for reservoir	http://wrc-hec.usace.army.mil/software/software.html

*QUAL2E does allow a dynamic dissolved oxygen diurnal simulation but with steady boundary conditions for flow and quality

** 1-D is one-dimensional either vertical or longitudinal, 2-D is two-dimensional (longitudinal-vertical)

The receiving water quality model chosen is dependent on the objectives of the water quality study. For example, a steady-state model such as QUAL2E is appropriate to use for a system that has steady-state inputs. In Poland, the QUAL2E and QUAL2E-UNCAS models have been applied for prediction of water quality in about 30 major rivers from the upper, mid, and lower part of the Vistula River Basin [10]. Another example of the use of QUAL2E evaluating summer eutrophication in the Dnieper River (the Ukraine) as presented in this paper.

The Dnieper River is the largest river in Ukraine with a drainage basin that includes about 47% of Ukrainian territory (drainage basin within Ukraine is 286,000 km^2 of a total for Ukraine of 600,000 km^2). At least 30,000,000 people (about 70% of the population) is supplied by Dnieper River, and most of the industries of Ukraine are dependent on its water. Mean annual runoff is 53 billion m^3 (between 18-73 billion m^3/yr is variance), and the river falls 220 m along its course from Russia, through Belarus, and Ukraine to the Black Sea. Also, the Dnieper River has 6 large reservoirs with total storage of 55.1 km^3.

There are large water diversions to the water-deprived areas of Donbass and Krivbass and large industrial and agricultural areas of Crimea. Diversions from the Kakhivka Channel and the North Crimean Channel each 400 km long are each able to divert 400 m^3/s [11]. Considerable eutrophication in the reservoirs is observed because of seasonal blue-green algae blooms. The QUAL2E model of the Dneiper system comprises 780 km from Kiev Sea to the Black Sea. The boundary conditions for the 17 river and point source discharges were developed from data between 1980 and 1991. This model was used to evaluate the overall factors of eutrophication, not dynamic algal blooms. For example, Figure 2a and Figure 2b show model predictions compared to summer 1986 field data for dissolved oxygen and ammonia. Model predictions for dissolved oxygen and ammonia, as well as other water quality variables, seemed to reasonably agree with the scatter in the field data for 1986, but the model accuracy was difficult to determine because of coarse boundary condition data and dynamic water quality field data. Hence, QUAL2E may be used for a general tool for evaluating simple cause-effect relationships of steady-state water quality problems, but should not be used for evaluating systems that require more refined scientific tools.

For dynamic inflows, such as storm water, or highly dynamic point loads, an unsteady receiving water model is required. One model, HSPF, also models the drainage basin runoff into the receiving water, similar to the SWMM model, discussed below.

For river systems, the QUAL2E model uses a steady-state Manning's equation or user-defined stage-discharge and flow-velocity power curve functions. For the more complex dynamic river models, the 1-D form of the cross-sectionally integrated Navier-Stokes equations for turbulent flow are used. 1-D Reservoir models are typically termed zero-dimensional in the sense that a simple volume balance is performed on each model vertical cell to determine the vertical velocity field. More complex models like CE-QUAL-W2, utilize a two-dimensional solution of the laterally averaged Navier-Stokes equations for turbulent flow. The CE-QUAL-W2 model accurately accounts for stratification impacts in river and reservoir systems and is the preferred model for long, narrow reservoir systems.

All of the models listed in Table 1 include modeling eutrophication processes, i.e., the dissolved oxygen-temperature-nutrient-algae cycling. Even though techniques for modeling these processes differ somewhat between models, in general they all can be used with adequate calibration data to model a river system. Only the WASP model includes the fate-and-transport of toxic organics or metals. None of the models shown in Table 1 included realistic sediment diagenesis models except the CE-QUAL-R1 reservoir model which had a simplified sediment model.

The process of modeling a surface water system should follow these steps:

- Determination of goals and objectives of the modeling effort
- Determination of dominant physical processes and dominant spatial and temporal scales
- Selection of model that accurately reflects the physical processes, spatial and temporal scales of the problem
- Model calibration/verification
- Use of model to forecast management strategies

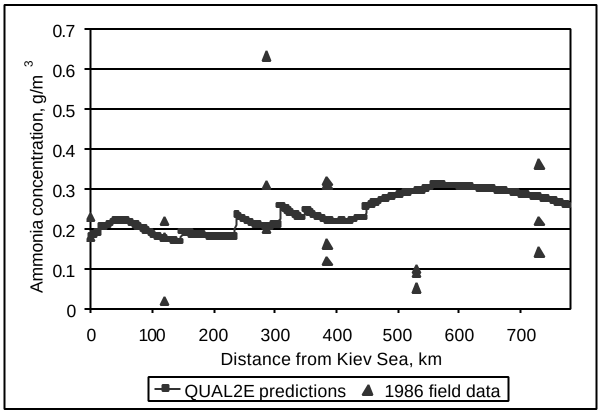

Figure 2a. Dnieper River model predictions of ammonia compared to 1986 field data.

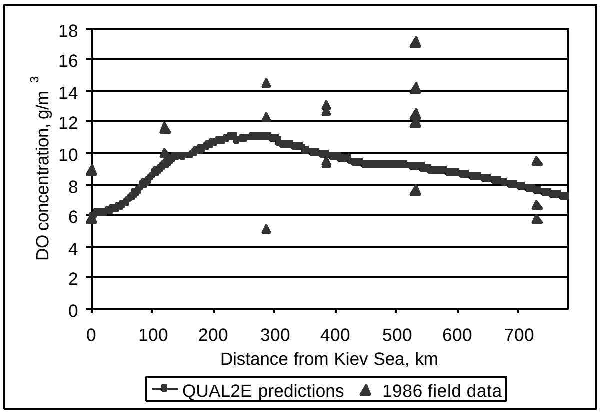

Figure 2b. Dnieper River model predictions of Dissolved oxygen compared to 1986 field data.

Wastewater treatment. In spite of the substantial interest in modeling the unit processes of wastewater treatment, the activated sludge alone has attracted most of this attention [9]. This may be easily explained by the fact that the operation of the activated sludge reactor is crucial for the treatment efficiency of the entire wastewater treatment plant (WWTP) and incurs the greatest cost.

Activated Sludge Models No.1 (ASM1) and No.2 (ASM2) were developed by the task groups of IAWQ (formerly IAWPRC). The ASM1 [12] predicts the performance of biological processes in suspended growth systems including carbon oxidation, nitrification and denitrification. The ASM2 [13] was extended with the phosphorus removal reactions.

Since the first release of the ASM1 in 1987, application of the original or modified versions of the model to a number of pilot and full-scale activated sludge systems with various process configurations has confirmed its ability to predict performance under stead-state and dynamic conditions. The ASM2, however, has had a limited verification at full-scale plants so far.

Several computer programs have been developed based on the mathematical models mentioned above. The most commonly used ones are SSSP, ASIM, EFOR and GSP-X [14]. Except for the first one (SSSP), the other programs posses capabilities to simulate phosphorus removal. However, the SSSP program is of special interest because it is in the public domain. The program was developed by Bistrup and Grady [15] and is available from prof. C.P.L. Grady of Clemson University (USA). Several applications of the SSSP program in the U.S. were given by Daigger and Nolasco [16]. The applications included the plant upgrading, estimating oxygen requirements, optimizing process configurations, sizing reactor volumes, and operator training.

In this paper, an example of modeling studies performed at the Rock Creek WWTP is presented. The plant, operated by the Unified Sewerage Agency of Washington County, is located in Hillsboro in the Portland metropolitan area, OR (USA) and treats over 26,000 m^3/d of wastewater under normal summer conditions. The plant provides one of the best treatment levels in the whole country with the summer effluent limits equal 7.5 g/m^3 for BOD_5, 4.0 g N/m^3 for $N\text{-}NH_4^+$ and 0.17 g P/m^3 for total P. A modified Ludzack-Ettinger (pre-denitrification) configuration has been applied for the activated sludge process. The process has been controlled by maintaining the dissolved oxygen (DO) concentration, recorded on-line, at a set point in Zone 3 of the reactor. Since 1995, the set point was gradually reduced from 6.0 g O_2/m^3 to 4.0 g O_2/m^3 in 1997.

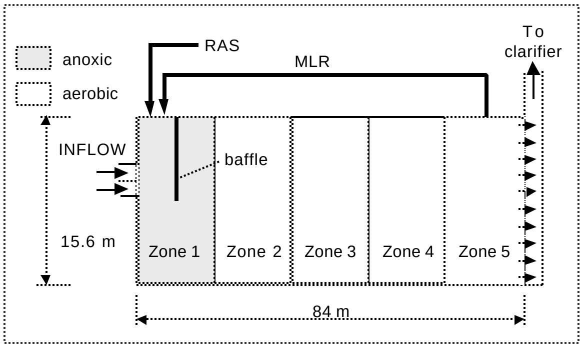

Figure 3a. Scheme of the aeration basin at the Rock Creek WWTP in Hillsboro, OR

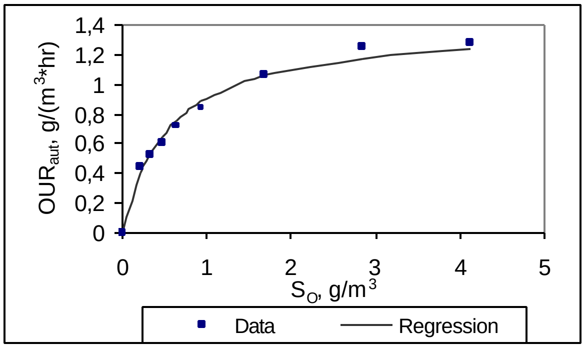

Figure 3b. Relationship between the oxygen concentration and autotrophic OUR

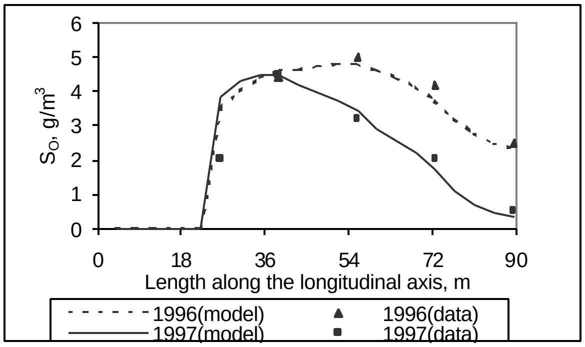

Figure 3c. Typical oxygen profiles in the aeration basin in 1996 and 1997

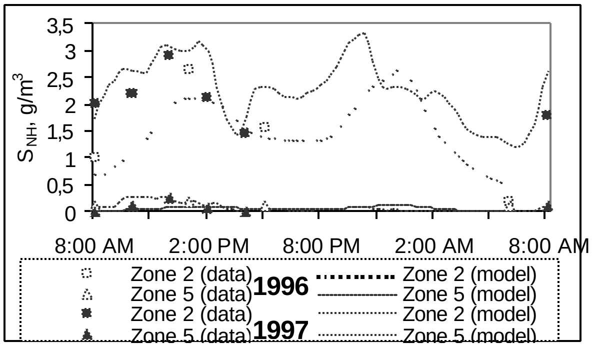

Figure 3d. Observed and calculated ammonia concentrations in the aeration basin

A modified version of the ASM1 with the transport equation described by the one-dimensional advection-dispersion equation was used to evaluate this strategy [17]. A series of batch tests indicated that the impact of oxygen on nitrification is minimal at such high DO concentrations (Figure 3b). Next, the simulation program was run for two 24-hour data sets obtained in October, 1996 and June, 1997. Typical DO concentration profiles (observed and modeled) are illustrated in Figure 3c. The average air input to the reactor was reduced by approximately 20% from 8500 m^3/hr (1996) to 6800 m^3/hr (1997).

Simultaneously, the TKN loads were relatively constant, i.e., 595 kg N/d (1996) and 630 kg N/d (1997). Effluent concentrations of some pollutants remained almost unchanged, as presented for ammonia in Figure 3d, and some were even lower, e.g., nitrates due to favorable conditions for denitrification.

A steady-state version of the program was further used to evaluate a configuration alternative (i.e., 4-stage Bardenpho) for the reactor and estimate the maximum capacity of the reactor without violating established standards [18].

Sewer network. An overview of comprehensive urban models with respect to both water quantity and quality was given by Marshalek et al.[19]. Among them the United States Environmental Protection Agency (EPA) program Storm Water Management Model (SWMM) is probably the most used model in the world [20]. An extensive bibliography of SWMM usage and useful case studies is available [21].

SWMM originated from a consortium of United States consultants, Universities and government agencies. The first SWMM component was produced in 1969-71 [22-25] and was capable of simulating urban stormwater runoff and combined sewer overflows. The SWMM model is comprised of a series of blocks that allow investigation of water quantity and quality problems and control options with associated cost estimates for storage, treatment or storage/treatment controls. The effectiveness of controls can be evaluated by review of model results including flow hydrographs, pollutant hydrographs and the modeled changes in receiving water quality. Receiving water quality models can obtain pollutant-loading estimates (for existing and control alternative scenarios) from the SWMM model. In 1974 EPA obtained another block of the system called EXTRAN (Extended Transport Model) to distinguish it from the Transport Block developed for the original package. Over the past 25 years SWMM has had numerous refinements and custom adaptations including commercialization. For example, XPSWMM is a complete Microsoft Windows based system of interfaces and solutions, and PCSWMM is a useful set of pollution and storm water management tools. Most of the SWMM blocks are written in Fortran.

SWMM works with real storm events (hyetographs) and other meteorological conditions plus description of the physical system (basin characterization, runoff catchment, collection system, and storage/treatment) to simulate the quantity and quality of routed flows arriving at the outfalls of the system. The outfalls become the input locations of the receiving water models. SWMM can produce results tailored to fit a variety of study objectives – both complete temporal and spatial detail as well as gross effects such as total kilograms of pollutant discharged for a given storm. Usual SWMM output consists of time series results (hydrographs, pollutographs) and daily, monthly or annual total loading.

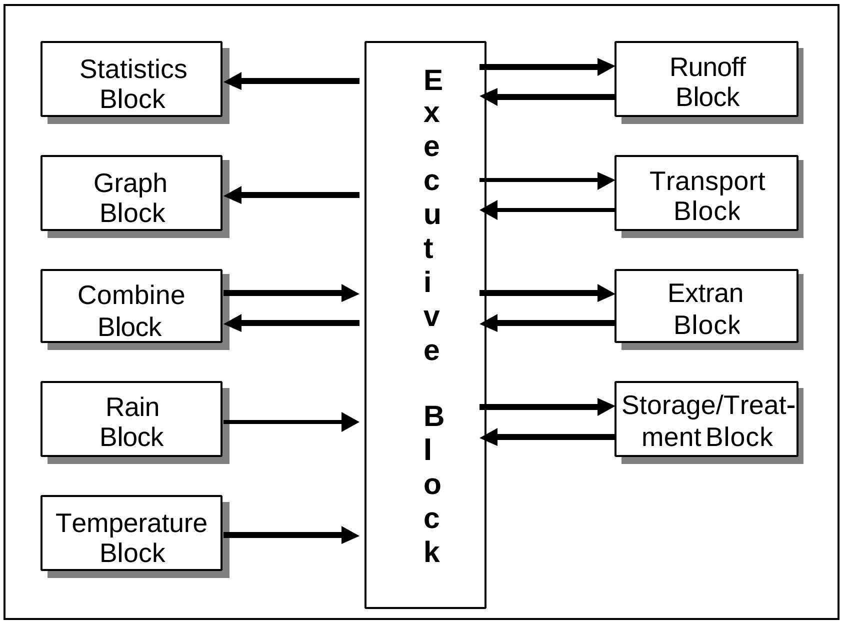

Figure 4. Relationships Among SWMM Blocks (adapted from[26])

SWMM is a combination of service (left side of chart) and computational “blocks” (right side of chart) interconnected through a executive block as shown in Figure 4. Table 2 shows the primary functions of each of the blocks and some interactions (adapted from [27])

Table 2. Summary of SWMM Blocks

Category	Blocks	General Usage/Results
Input sources	**Runoff**	Generation of surface and sub-surface runoff based on rainfall and/or snowmelt hyetographs, antecedent conditions, land use, and topography
	Transport	Generation of dry-weather flow and infiltration
	Interface	External flow generation creates inflow file to Extran or Transport nodes (manholes)
Central Core	**Runoff**	Generation and simple routing of flows and pollutants
	Transport	Routing of flows and pollutants using Kinematic Wave method
	Extran	Routing of flows using full St. Venant Equations. No quality routing available in public domain software
Devices	**Storage/treatment**	Characterizes the effects of control devices upon flow and quality and elementary cost computations
Utilities	**Interface**	Generation of interface files for input between Blocks and other programs such as WASP or DYNHYD. Input files for analysis Blocks/Utilities
	Graph	Plotting of hydrographs, pollutographs, and other time series output. Plots measured and simulated time series
	Rain	Processing and analysis of time series rainfall data. Creates rainfall file for Runoff Block and can perform synoptic statistical analysis on rainfall records
	TEMP	Similar to the Rain block only for temperature records
	Statistics	Utility that helps manage the volumes of output generated by the model. Capable of review the time step output from continuos or event simulation and produce summaries, rank events according to desired criterion (such as peak flow, volume etc.) and assign return periods to the events

Input data requirements for SWMM can be extensive depending upon the application and objectives of the study. Collection of data is usually achieved through review of construction drawings or collection of additional data from land and aerial surveys. After data is collected then data reduction in the form necessary to build models is facilitated through databases. Recently more attention and effort is being spent on connecting data stored in Geographical Information Management (GIS) systems and hydraulic models such as SWMM [28]. SWMM is flexible enough to allow a “lumped” approach for preliminary modeling when data is sparse. Preliminary results can be therefore attained with limited data. This is preferable than a wholesale condition of being overwhelmed with the immensity of collecting data from scratch and often leads to a much better program for additional data collection and identification of the key parameters or basin definitions required to refine model results.

Although the SWMM model routines and processes are physically based, the results should be tested against local verification and calibration data sets. Quality of input data and the numerical methods are often not accurate enough for real world applications without rational adjustments based on local data. Many of the computational blocks are based on limited data (some of the code dates back to the 1970s) and are highly empirical, especially surface quality estimations. Some of these drawbacks have or can be fixed through custom adaptation of the SWMM code for local conditions. Fortunately the Fortran code is open and available for downloading with the executable and example data files.

Water distribution network. The EPANET program for simulation of the water distribution networks was developed in the U.S.EPA [29]. The network structure in the program is built by the following elements: reservoirs, water pipes, nodes, pumps and five types of valves. Modeling the water flow in the network may be performed by one of three formulas describing the head loss in the network: Hazen-Williams, Darcy-Weisbach, Chezy-Manning. An additional feature of the program is simulation of the changes of several water quality parameters. Other common programs used in Poland for the water network simulation are OPUS and NET-SIMULA (based on the EPANET program) [6].

The application of computer models such as EPANET would enable agencies operating and maintaining water distribution networks to explore hydraulic conditions of their the network structure. In Poland, a common problem is secondary water contamination as a result of the oversizing of the water distribution networks. Operational experience indicates that sedimentation of the particulate contaminants occur in cases when the flow velocity is below 0.1 m/s. The sediments disturb the flow in water pipes by increasing roughness and by stimulating the growth of biofilms. Due to physio-chemical processes, water quality in the water pipes may worsen (increased turbidity, color, odor) and oxygen depletion zones may occur [6]. To prevent these phenomena, the water distribution network must be rinsed periodically. A common method of rinsing is water bleeding by hydrants without controlling the hydraulic parameters in the network. Often times the water flow in the oversized network is not sufficient to remove the effects of the incrustation. A significant increase in the efficiency of the conventional rinsing may be achieved by planning and applying water bleeding under controlled water flow. In such a case, the computer simulation can be used to estimate the bleeding rate, location, rinsing frequency and the number of opened hydrants.

The effects of excessive retention times in the water pipe networks are the oxygen depletion zones. Elimination of the negative effects is possible by the water oxygenation in result of increasing the circulation frequency. The idea of forcing a directed flow is to generate a faster water flow in those regions of the network that are threatened by stagnation [30]. The increased flowrate can be generated in a natural manner by regulating the valve set point or in an artificial manner by installing additional pumps. Each time, before applying the method in practice, the computer simulation is necessary to estimate the desired water flow conditions by adjusting the optimal valve set point. The efficiency of the method in full-scale has been confirmed for the water distribution network in the city of Lebork (northern Poland) based on the water quality monitoring during six months of the studies [30].

Conclusions

Due to their advantages, mathematical modeling and computer simulation may become a more common tool used in management of the water quality systems in Central and Eastern Europe. To achieve this goal, joint efforts of consultants, universities and government agencies, including also the international level, are necessary. Examples of actions to achieve this goal may be popularization of positive cases studies illustrating the model application, enhancing the access to the “public domain” software, and the organization of training sessions for modeling techniques.

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