

Analysis of disinfectant decay in a water supply system based on mathematical model

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ABSTRACT

The purpose of the water supply system (WSS) is to provide best quality water to consumers. Water composition changes throughout whole WSS, including water production subsystem and water distribution subsystem (WDS) and is caused by variety of factors, that is, quality of raw water, efficiency of treatment method, and quality of the treated water feeding the pipe network. Additionally, water quality in the WDS depends on the following factors: way of storage and transport and technical condition of pipeline and domestic water installations. To ensure good microbiological water quality at every point of the system, water has to be disinfected. Changes in tap water quality should be monitored to undertake an effective precaution to minimize a risk of secondary microbial water contamination. However it is not possible to perform a continuous control of tap water parameters at WDS due to the size and structure of the water pipe network. For this reason, it is necessary to use mathematical models to simulate changes to quality parameters of water in WDS. In this work, three simulations of chlorine decay in the WDS were carried out. Collected data on chlorine decay were used in a special analysis to define areas of risk for secondary water contamination. Simulations were carried out using EPANET for Silesian region WSS.

Keywords: Water distribution network; Free chlorine residual; Chlorine decay; Model simulation; EPANET

1. Introduction

Before using water disinfection, many people died of waterborne diseases, such as typhoid, dysentery, cholera and Legionnaires' disease. In 1880–1900, cholera was widespread both in continental Europe and the United States resulting in thousands of deaths [1]. The reasons for the spread of this disease were poor living conditions and use of raw or poorly treated water in households. Therefore, in 1900, over 23,000 people in United States died of typhoid fever and more than 100,000 died of diarrhea–enteritis and dysenteries. In 1944, the deaths caused by typhoid fever dropped below 600 and in 1960 below 20 [2,3]. According to data from 2006 [4], waterborne diseases in Europe were reported only in five

countries, with total of 3,952 patients, who were affected by many causative agents, including *Campylobacter*, calicivirus, giardia, and *Cryptosporidium*. The cause of these waterborne outbreaks was weather anomalies as droughts or extraneous rainfall that lead to *Cryptosporidium* outbreaks by infiltrating oocysts into drinking water reservoirs from springs and lakes and persisting in the water distribution subsystem (WDS). The number of waterborne diseases decreases after 1900 as a result of the use of drinking water chlorination. The first continuous use of chlorine in water supply system (WSS) was in 1902 in Belgium, as a stage of providing biological safety to water. After that, chlorination was used in North America, first in 1908 in Jersey City, then in whole country [3,5]. Despite the chlorination of water, there is still a risk associated with

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waterborne disease. Recent data indicate numerous cases of illness such as botulism, cholera, cryptosporidiosis, leptospirosis, vero/Shiga toxin-producing *Escherichia coli* infection, Giardiasis, Shigellosis, Typhoid/paratyphoid fever [6,7]. The biggest threats are Cryptosporidiosis, Giardiasis and diseases associated with coli forms, which reach several thousand cases per year (Fig. 1).

The presented literature review shows that threats related to waterborne diseases still exist. The number of their occurrence is much smaller than it was 100 years ago, but they still pose a serious threat to people. The occurrence of threat of waterborne diseases may be caused by some ignorance about the operational work of WSS, that is, water flow directions, water flow velocity, as well as bad water disinfection management.

The first method of water disinfection was chlorination, which brought good results in microbiological stability and is still used today. At first, chlorination was supposed to deactivate the "problematic" microorganisms, but it turned out that it neutralizes all known bacteria and bacterial spores as well as viruses, protozoa and protozoan cysts, worms, and larvae. This is the first aspect of disinfection; the second is to retain the microbiological stability of water to guarantee its safety during transport by the distribution subsystem to customers [8,9]. The effectiveness of disinfection depends on factors such as dose of disinfectant, disinfection time, the physical and chemical water quality, and the number and type of microorganism in treated water. However, the use of chemicals in water disinfection causes creation of disinfection by-product (DBP). The first mention of DBPs was recorded in early 1970s. Rook discovered the reaction of chlorine with natural organic matter resulting in the formation of DBP with toxic properties, for example, trihalomethanes (THM) [10-13]. In the literature, approximately 500 DBPs have been reported, and only a small number has been included in quantitative research or health impact studies. In 1976, the US Environmental Protection Agency presented results of a national survey that showed that chloroform and other THMs were often in chlorinated drinking water. In the same year, US National Cancer Institute published results of close link between chloroform in water and increase of cancer in population [14,15].

By the development of industry and continual cities expansion, WDSs have increased their spatial reach over the last few decades, resulting in an extended flow time of water to people living in the suburbs. Unfortunately, the

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Fig. 1. Reported number of cases of waterborne disease in EU, data from 2008 to 2012 [7].

global water policy focused on reducing water losses has significantly reduced water consumption over the last three decades. These efforts have contributed to oversizing the current WDS causing water flow velocity to drastically decrease. The decrease in flow velocity in pipes affects both the biofilm formation and corrosion processes. The technical condition of water pipes, age, as well as a type of material influence the processes that take place in the network, for example, corrosion, cracks, and sediment formation. Abovementioned conditions of WDS operation increase the chlorine consumption in the WSS and the need to implement additional water disinfection points in water pipe network to ensure microbiological safety of tap water. Placing appropriate disinfection points requires many analyzes of the chlorine decay in WSD, which will finally provide the basis for decision support.

Considering the presented conditions, a rational approach in WSS managing is using various analytical tools, which in a quick and simple way will give the answer whether a given situation there is a threat. The basic tools used in all science fields are mathematical models. In the management of WSS, these models contain a full water network graph together with technical and operational data that carry out hydraulic and water quality simulations. Since 1960s, mathematical models have been used as a tool to simulate the work of the water supply network. The development of the information technique allowed creation of computer programs that significantly speeded up calculations. At the beginning, the mathematical models were used only for hydraulic simulation [16], but now they are used to predict water quality based on water age, chlorine decay, and THM growth [13,17,18]. A lot of software tools allow simulating the chlorine decay in WDS, including EPANET, WaterGEMS, PICCOLO, and MikeUrban. These software tools use chemical equations of the first and higher order to solve the problem of water quality changes. The basis for the modeling of chlorine decay or THM growth is to determine the reaction rate. Many chlorine decay models use first-order kinetics and relate chlorine concentrations between two points, according to the equation [19-22]:

$$C_t = C_0 \exp\left(-k_t\right) \tag{1}$$

where C_t is chlorine concentration at time t (mg/L), C_0 is initial chlorine concentration (mg/L), t is residence time of water in the pipe (h), and k is a first-order reaction rate coefficient (h⁻¹). Chlorine depletion models are commonly used in network management [22–26], but many studies confirm that the kinetics of the reactions occurring during water transport is not fully understood [17,21,27–31] Chlorine decay models can be used for both the optimization of disinfectant dosage and prediction of locations of the hazard areas with total chlorine decay. They are very useful to create water safety plans because of given possibility to determine the part of WDS exposed to microbiological contamination.

The purpose of this work is to determine the chlorine concentration in WSS during normal system operation and during emergency situations using a water quality model and determining the risk associated with chlorine deficiency, as a part of WSS risk management. The presented simulations were used to identify problematic areas of WSS and suggest solving a given problem. This paper presents scientific research results from analysis of spatial residual chlorine distribution in water pipe network of a large WSS located in the southern-west of Poland.

2. Chlorine decay models

Water quality models used to predict changes in the water composition in WSS are mostly used to the estimation of the chlorine content in water and the amount of produced THM (Fig. 2).

In one well-known model change in the amount of reactive substance (*C*), for example, chlorine, both in the bulk fluid and in the boundary layer, proceeds in accordance with the first-order reaction [17]:

$$R_{c}(c_{c},K,t) = \frac{dc_{c}}{dt} = \pm / -k_{b}c_{c} + \frac{k_{f}}{r_{H}}(c_{c} - c_{c,w}) = / -Kc_{c}$$
(2)

where $R_c(c_{C'}K, t)$ is function of first-order reaction (mg·L⁻¹h⁻¹), c_c is the reactive substance content (*C*) in the water stream at time *t* (mg/L), $c_{C,w}$ is the content of the reactive substance (*C*) in the boundary layer at time *t* (mg/L), k_b is bulk first-order chlorine decay constant (h⁻¹), k_f is mass transfer coefficient between the bulk and boundary layer (m/h), $r_H = C/V$ is hydraulic radius (m), and *K* is total first-order reaction rate constant (h⁻¹), determined according to the formula [28,32]:

$$K = k_b + k_w \tag{3}$$

The $k_{\rm h}$ value depends on kind of raw waters (source), treatment technology and seasons [22]. The k_w values depend on type of pipe material and on the amount and type of deposits. The wall demand coefficient mainly occurs in metallic pipes and in pipes with significant biofilm. The first-order model is a simple tool that describes reactions taking place in the system. However, it is assumed that chlorine reacts at a constant rate with an excess of reagent requiring chlorine. This tends to work well when the initial rapid demand for chlorine is ignored, when the initial chlorine concentration is not varied and there is no re-chlorination. To overcome these deficiencies, a number of alternative models have been proposed; for example, a two-reactant second-order model. This model assumes that chlorine reacts with two groups of water compounds, with one rapidly and with one slowly, according to the following formulae [20,22,25]:



Fig. 2. Diagram of the disinfection effect in the pipe [30].

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -k_f c_c C_f - k_s c_c C_s \tag{4}$$

$$\frac{\mathrm{d}C_f}{\mathrm{d}t} = -k_f C_{cl} C_f \tag{5}$$

$$\frac{\mathrm{d}C_s}{\mathrm{d}t} = -k_s C_{cl} C_s \tag{6}$$

where C_f and C_s are, respectively, the concentrations of fast and slow reducing agents (*C*) in the water that react with chlorine (mg/L), C_d is concentration of chlorine, c_c is instantaneous chlorine concentration (mg/L), and k_f and k_s are decay rate coefficients for fast and slow reactions (L·mg⁻¹h⁻¹). Using this model requires estimation of four parameters: reaction rate coefficients and initial concentrations of C_f and C_s .

The paper proposes a simple model of chlorine decay (Eq. (1)), used by EPANET 2.0. This model has been chosen due to the lack of chlorine decay rate data as well as the quality of the input data.

3. Research object

The subject of the study is the selected subsystem of the biggest collective WSS in Poland and also in Europe. It is located in the southern-west of Poland in Silesian region. The study was conducted in 2016. This distribution subsystem (Fig. 3) is composed of four local water treatment plants (WTP; A, B, C, and D) with a total average daily production of 72,577 m³ (variability range 65,759–82,830 m³/d). The highest share in water production is played by WTP A, which during conducted study changed from 58% to 80% (mean 71%). The average daily water production of WTP A is 51,391 m³/day and changed from 43,253 to 63,348 m³/d (Fig. 4).

The integral elements of the DWS are four complexes of storage tanks (E, F, G, and H) with the total capacity of $155,200 \text{ m}^3$ (Table 1).

The study area is characterized by high altitude variability from 240 to 364 m above sea level. The central point of the subsystem (Fig. 3) is the storage tank E (345 m above sea level), which are supplied from two directions (WTP A and Pump Station I) and delivers water to the largest number of



Fig. 3. Scheme of the water distribution subsystem.





Fig. 4. The water production of water treatment plants in 2016.

Table 1 Characteristics of water tanks

Storage	Number of	Minimum	Maximum	Diameter	Volume
tanks	chamber	level (m)	level (m)	(m)	(m ³)
F	12	2.5	8	35	100,000
Е	6	2.5	8	33	30,000
G	3	2	7.5	33	20,000
Н	2	1	3.67	30	5,200

customers in north area. The storage tanks F are water receivers (330 m above sea level) and cooperate with Pump Station I, whereas tanks G (315 m above sea level) and H (364 m above sea level) keep the pressure on the water pipe network. WTP C and B supply the smallest part of this area, while WTP D works occasionally in a case of higher water demands.

Considered WDS is a wide system with a total length of 256 km with pipe diameters from 55 to 1,600 mm. Analyzed network is made mainly of steel, as well as polyethylene (PE), cast iron, and ductile cast iron (Fig. 5). The oldest pipes that build this subsystem come from 1929 (steel) and the latest ones from 2016 (PE).

In 2016, average daily water demand in this area was 102,000 m³. Minimum water demand of 87,000 m³/d was recorded on January 1, 2016, and the maximum water consumption of 104,000 m³/d was recorded on June 26, 2016. In recent years, the amount of water consumption in this region has decreased by about 30%, which has contributed to a significant reduction in water production and water flow velocity (Table 2). Low flow velocity affects disinfection contact time and disinfection efficiency.

WTP A, B, and D are based on surface water and WTP C on groundwater. Water disinfection in this subsystem is carried out in five facilities: WTP A, WTP B, WTP C, WTP D, and storage tanks E, using chlorine in WTP A and sodium hypochlorite in other objects, with small differences in disinfectant dose between seasons (Fig. 6). Storage tanks E are dispensing disinfectant in two directions—east and west. During the study period, concentration of chlorine residual was measured at 21 control points (Fig. 3), which were the basis for the chlorine decay model.



Fig. 5. Materials structure of water pipe network.

Table 2

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Velocity value for maximum and minimum daily water demand

Level of water	Velocity (m/s)				
demand	Maximum	Minimum	Average	Modal	
Maximum	1.01	0.01	0.16	0.09	
Minimum	0.71	0.01	0.08	0.04	



Fig. 6. Average value of residual chlorine concentration for each disinfection point.

4. Research methodology

4.1. Hydraulic and quality simulation model

The model was developed within research framework financed by National Centre for Research and Development (project no. POIG.01.03.01-14-034/12). In study, the EPANET software for hydraulic calculations was used. Topography and topology data were exported from an updated Geographic Information System database while water demand from the Supervisory Control and Data Acquisition (SCADA) telemetry system and the available billing databases.

Operational data from one month (October 2016) included information about water flow rate, pressure, and chlorine concentration at representative points of WSS. Validation files were created from the period of 17–19 October 2016. The correlation was carried out for average values of water demands, for which a high correlation coefficient was obtained, for pressure 99.4% and for flow 99.0% (Fig. 7). For the obtained results (pressures and flows), the residual analysis was carried out using Statistica 12 (Figs. 8 and 9). The analysis of the residuals distribution for both flow and pressure showed that at the predefined significance level $\alpha = 0.01$ the null hypothesis of normal distribution was not rejected.



Fig. 7. Correlation plot for (a) pressure and (b) flow.



Fig. 8. Residual analysis for the pressure correlation results.



Fig. 9. Residual analysis for the flow correlation results.

The measurements of residual chlorine were conducted during the research study from January 1 to December 31, 2016. Water samples were collected once a month from 21 control points located in the whole analyzed area, as part of periodic water tests conducted in water distribution company (Fig. 3). Water samples were taken in accordance with direction and time of water flow. These data were basis for the creation of chlorine decay simulation model within EPANET software. Chlorine concentrations at the dosing locations are included into the SCADA system and are measured at an equal time interval of 15 min. The values of free chlorine in the model were taken as mean values from October. Initial values of chlorine concentration for each object are as follows:

- WTP A 0.49 mg/L,
- Tanks E—east direction 0.18 mg/L and west direction 0.31 mg/L,
- WTP B-0.25 mg/L,
- WTP C-0.12 mg/L, and
- ▶ WTP D−0.12 mg/L.

In this water pipe network more than 70% pipes are made of steel, therefore in quality simulation model the wall decay coefficient was taken into account.

The first-order reaction rate coefficient k (Table 3) was preliminarily based on the literature data [18,25,28,33]. Model compliance was checked by the least squares method. Quality model calibration was carried out by trial and error in three steps (Table 4). After each step, the sum of squared deviations (MSE) was calculated and after third stage, a rectilinear regression was determined. Fig. 10 illustrates the matching of simulation results to actual measurements.

In the first stage, coefficients k_b and k_w assumed on the basis of the most common value in the literature. After this stage, an MSE value of 0.0957 and R^2 value of 0.640 were obtained (Table 4); therefore, in the second stage the value of the k_b coefficient was reduced by 20%, which contributed to increase the accuracy of the simulation by 27%. Despite increased accuracy of the model after the second stage, areas with large differences between simulation results and actual

Table 3

Minimum and maximum values of chlorine decay coefficient *k* (18, 25, 28, 31)

Decay coefficient (h ⁻¹)	Minimum	Maximum
Wall	0.03	5.00
Bulk	0.08	1.32

Table 4

Values of k_b and k_w coefficients and MSE for three stages

Stage	k _b	k _w	MSE	R^2
Stage I	-1.0	-0.03	0.0957	0.640
Stage II	-0.8	-0.03	0.0707	0.530
Stage III	-0.6	-0.03	0.0331	0.776
	-1.0	-0.03		
	-0.4	-0.03		
	-1.0	-0.10		

values were obtained. In the third stage, based on pipes age, local values of k_v and k_w coefficients were adjusted in the following areas:

- west direction from storage tanks E: k_h = -0.6 h⁻¹
- east direction form storage tanks E: $k_{\mu} = -1.0 \text{ h}^{-1}$,
- north direction from WTP A: $k_b = -0.4$ h⁻¹, and
- area between control points 20 and 19: $k_b = -1.0 \text{ h}^{-1}$, $k_m = -0.1 \text{ h}^{-1}$.

For the quality model with different local values of k_v and k_w coefficients w, the MSE was obtained at the level MSE = 0.0331 and R^2 = 0.776 (Table 4). After the third step, residual analysis of the predictive chlorine concentration and actual chlorine concentrations were also performed. The analysis of the residuals distribution for chlorine concentration WDS showed that at the significance level α = 0.01 the null hypothesis of normal distribution was not rejected (Fig. 11).

4.2. Spatial analysis of chlorine decay

The task of the research procedure is to identify areas potentially threatened by bacteriological contamination to determine additional water disinfection points at WDS.



Fig. 10. Graph of compliance of simulation results with actual measurements, after third stage.



Fig. 11. Residual analysis for the chlorine concentration correlation results.

Analysis of spatial distribution of chlorine concentration in water pipe network was carried out for variable operating conditions of WDS caused by different random events. Typical random events that characterize WSSs include failures of water intakes, water treatment stations (individual elements), loss of electricity in the mentioned facilities, overflow of water turbidity, and pipeline failures. There were several emergency events in the analyzed subsystem; therefore, the following simulations were carried out:

- Scenario I: normal operational work (the conditions for which the model was calibrated)—WTP A and Pumping Station I are working simultaneously, supplying water to the northeast area,
- Scenario II: shutdown of Pumping Station I—increasing the water production in WTP A to 4,800 m3/h, and
- Scenario III: shutdown of WTP A—increasing the water flow in the Pumping Station I to 4,200 m³/h.

In spatial analysis of changes in quality of transported water, concentration of residual chlorine was treated as an identifying parameter of a risk of microbiological safety loss of tap water. Analysis of chlorine decay from water was made to allow evaluation of loss of microbiological safety of water in the studied model. The minimum concentration of chlorine in water, at the end of distribution pipe network, was set up at 0.05 mg/L what was based on literature data. This makes it necessary to keep chlorine concentration at main water pipes at a minimum level of 0.1 mg/L. To ensure such level is kept all the time, a 0.15 mg/L level was set up followed from a study of chlorine decomposition from water in Silesian WTP. Chlorine concentration of 0.25 mg/L was defined as a maximum acceptable concentration in the studied model. This was based on Silesian WSS exploitation principles which say that concentrations greater than 0.25 mg/L may lead to undesired side effects of water disinfection. To determine the spatial localization of hazard zones of water safety loss, five categories of chlorine concentration were established, for which a procedure for operational risk management was designed (Table 5).

5. Results and discussion

The simulation results are shown in Fig. 12, in the form of contour graphs created by EPANET software. Table 6 presents the percentages of areas belonging to the individual residual chlorine concentrations for all simulations.

For Scenario I, the smallest area (0.27%, Table 6) with a residual chlorine concentration less than 0.01 mg/L was obtained. This area (dark blue color) is located near closed valve, where there is no water consumption. For this scenario, a large area (57.21%, Table 6) with a chlorine concentration below 0.1 mg/L was obtained; according to the mentioned procedure, bacteriological test should be carried out in this area and in a case of microbiological excesses, occasional disinfection should be determined. For the fourth class of chlorine concentration (0.15–0.25 mg/L), an area of 21% was obtained (Table 6); therefore, a precise analysis of chlorine concentration should be carried out and, if necessary, the dosage of the disinfectant at the WTP should be reduced. For Scenario II, area with chlorine concentration below 0.01 mg/L is 5.50% of the total area (Table 6), and except the ends of

Table 5	
Classes of risk management for chlorine concentration	

Residual chlorine concentration (mg/L)	Operational procedures in risk management
0.0–0.01	Water samples for microbiological control, chlorination of water and correction of chlorine dose in
	disinfection at water treatment plants
0.01-0.1	Water samples for microbiological control at representative points of the zone, in case of
	identification of exceedances of microbiological parameters-local water chlorination
0.1-0.15	Analysis of spatial distribution of chlorine in the supply zone, if the concentration of chlorine
	residual above 0.15 occurs in an area less than 25% of supplied zone-increasing the chlorine dose in
	the disinfection process at water treatment plant
0.15-0.25	Analysis of spatial distribution of chlorine in the supply zone-possible correction of chlorine dose in
	the disinfection process (decrease) at water treatment plant
>0.25	Analysis of spatial distribution of chlorine in the supply zone, reduction of the chlorine dose in the
	disinfection process if the area with a chlorine concentration above 0.25 mg Cl/L exceeds 20% of the
	area of the supply zone



Fig. 12. Spatial decomposition of residual chlorine concentration.

Table 6

Percentage of the area belonging to particular residual chlorine concentrations

Residual chlorine	Scenario I	Scenario II	Scenario III
concentration (mg/L)			
0.0-0.01	0.27%	5.50%	6.14%
0.01-0.1	57.21%	67.68%	68.31%
0.1-0.15	12.54%	10.49%	9.34%
0.15-0.25	21.06%	8.60%	14.00%
>0.25	8.92%	7.73%	2.21%

the network, it also covers the area around tanks G and small area in north part of subsystem. For this simulation, a large area with chlorine concentration of 0.01–0.1 mg/L was obtained, which is 67.68% of whole area (Table 6). In this case, it is also necessary to carry out microbiological tests and possibly additional chlorination at designated points of disinfection at WDS. For the third simulation (Scenario III), the area at risk of secondary contamination is the largest and amounts to 6.14% (Table 6). The largest area for the second class of chlorine concentration was obtained, which is 68.14% (Table 6).Therefore, the operational procedure undertaken in this area has to be the same as in scenarios I and II. For each

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scenario, the water demand in the area at risk of secondary contamination of water has been determined:

- Scenario I: 0 m³/d,
- Scenario II: 9,200 m³/d, and
- Scenario III: 15,300 m3/d.

Data analysis shows that the current (Scenario I) water disinfection at both WTP and WSD has been carried out correctly and, with assumed water supply failure, may result in secondary contamination of water. In Scenario III, the greatest number of people may be exposed to microbiological contamination of water; however, in both cases (scenarios II and III) additional disinfection points at WDS should be considered.

6. Conclusion

Conducted research showed that mathematical models can be used to model water quality changes in WDS, for example, chlorine decay during water transport to consumers. Simulation results will help with identifying areas with increased risk of microbiological contamination. The results can also be the basis for developing water safety plans.

Chlorine decay simulation model can be helpful to make decisions about the dose of disinfectant at a WTP, which allows reducing the cost of disinfection.

In the case of the simulation of extreme events of operation condition of the WSS, such as WTP shutdown, it is possible to specify points of additional disinfection, such as temporary disinfection stations. Based on the conducted simulations, these stations should be located near control point nos. 8 and 20. These points are located in the areas with the lowest chlorine concentration, as well as at the pipes with the highest water flow. Such location of additional disinfection points will enable securing not only designated areas but also the remaining system area, in which the chlorine concentration is low.

The proposed model of WSS can be the basis for analysis of different scenarios of chlorine decay undertaken in risk management procedures. However, bulk and wall first-order chlorine decay constant $(k_{i} \text{ and } k_{j})$ should be determined experimentally to refine the model. The decay constants should be designated for different types of pipes (steel, iron, and PE).

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