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Use of disinfection by-products (DBPs) generation simulation models in the risk analysis of secondary water contamination

Izabela Zimoch*, Ewelina Bartkiewicz

Silesian University of Technology, Institute of Water and Wastewater Engineering, Konarskiego 18, 44-100 Gliwice, Poland, emails: izabela.zimoch@polsl.pl (I. Zimoch), ewelina.bartkiewicz@polsl.pl (E. Bartkiewicz)

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ABSTRACT

Despite the high efficiency of water treatment and disinfection, waterworks struggle with secondary water pollution. A major threat to human health are the so-called disinfection by-products (DBP), which have carcinogenic properties. Currently, the water quality supervision associated with the DBPs includes water quality control tests at critical points in the water supply system (WSS). However, such a solution only provides information about current water conditions, which makes it more difficult to choose effective countermeasures. In this case, a water quality forecasting system should be developed to support decision-making. Such a system can be a mathematical model that enables analysis of distribution systems' operation in terms of hydraulics and water quality. This model would also generate a forecast of the WSS operation and information about the effects of future changes. In this paper, an analysis of water quality was carried out for the selected area of the main WSS of the Silesian agglomeration. Numerical simulations conducted in the Epanet software was used to assess risks related to secondary water contamination in the water distribution network.

Keywords: Secondary water contamination; Disinfection by-products (DBPs); Water quality model; Epanet 2; Risk assessment; Theory of fuzzy set

1. Introduction

The water supply network is an important part of the urban/regional infrastructure, which is responsible for water supply at sufficient pressure and proper quality. An important parameter is water quality, as it determines water usability. Deterioration of water quality, during delivery to the consumer, may affect the level of services provided, limit water production or cause a stoppage in delivery and may cause epidemics of waterborne diseases [1–3]. In Poland, water quality parameters together with their monitoring rules are strictly defined in the Regulation of the Minister of Health on the quality of water intended for human consumption of 7 December 2017 (J. Laws 2017, Item 2294, 2017.12.11). An important aspect of water quality is the presence of disinfection by-products (DBPs) [4–7]. DBPs are formed when their precursors, mainly natural organic substances, react with the disinfectant. The type and content of precursors depend on the quality of the raw water and treatment efficiency [8–12]. DBPs have become a serious health threat due to their teratogenicity, carcinogenicity and mutagenicity [13–18]. DBPs also affect the reproductive system and the course of pregnancy [19,20]. Therefore, the spatial variability of DBPs in the distribution system is an important topic for study. In the literature, only a few works are devoted to this task. The problems with determining the spatial variability of DBPs in the water supply system (WSS) are related to the structure, water age and hydraulic conditions [21–24]. Water supplied to consumers should meet

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* Corresponding author.

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the conditions of drinking water at every point of the water distribution system. Therefore, a well-functioning tool is necessary to support decision making in water supply management to develop reliable Water Safety Plans. It is therefore justified to use the mathematical model as an element of a decision support system. These simulation models enable an analysis of hydraulic parameters of distribution systems and water quality changes in the water pipe, in the various variants of the WSS operation. Water Utility managers are increasingly reaching out for risk assessment in order to priorities water quality towards effective water supply management. Risk assessment is also proposed in the European Union Directive on the quality of water intended for human consumption [25]. There, a European Norm is referenced, in which concepts of hazard and risk are defined and an indication of what hazard assessment and risk management in water supply companies should use. The risk assessment identifies critical areas of WSS based on scenarios of selected states of water distribution systems operation and their consequences.

Risk is mathematically defined as a product of the probability of an undesirable event and the effects it could cause. Risk analysis is based on a study of the interdependence between probability and the consequences of a negative event. Determination of the probability and consequences of an undesirable event is very complex, as it depends on many uncertain factors. The uncertainties associated with the data may lead to false results. The lack of general rules to determine the implications of an event, applicable to all WSS or the randomness of consequences, may cause errors in determining the risk value. In such cases, an effective tool for estimating risk is an analysis method based on the theory of fuzzy sets [26–29]. Fuzzy logic enables the conversion of language descriptions into a number format, introduces values between the standard 0 and 1 and "blurs" the boundaries between them, giving the possibility of occurrence of values in this range (e.g. almost false, half-true) [30]. Thanks to fuzzy logic, it is possible to determine values close to the expected ones, thus giving information on how much a given parameter meets the given conditions.

The paper presents a risk assessment of secondary water contamination associated with chloroform and its effects, using a mathematical water quality model and fuzzy logic. Simulations of the spatial distribution of chloroform concentration in water were carried out using Epanet software for developing a Silesian region WSS hydraulic model.

2. Research subject

2.1. Structure of Silesian WSS

The case study system is the selected subsystem of the biggest collective WSS in Poland, which supplies water to recipients in the southern-west of the Silesian region. The average water demand for the selected area is about 17,000 m^3/d, supplying around 115,000 people. This subsystem includes water treatment plant A (WTP A), pumping station B (PS B) and storage tanks C (ST C) and D (ST D). WTP operation bases on surface water captured from the water reservoir located in the east part of Beskid mountains. The water treatment system includes such technological processes as coagulation, filtration and disinfection. The process of coagulation is performed in filters with aluminum sulfate (contact coagulation). Water disinfection is carried out using chlorine gas. PS B is located over 30 km away from WTP A, where water is subjected to another disinfection (with sodium hypochlorite). PS B transports a water volume of 45,000 m^3/d. ST C has located about 12 km from the PS B. In ST C, the water is also being disinfected with sodium hypochlorite. From the ST C water is being routed to three directions, one of them leading to ST D. These tanks are located about 16 km from ST C and their water is being routed to cities E and F. In ST D, water is also being disinfected with sodium hypochlorite.

The subsystem is divided into four sections: S1 – section; WTP A – pumping station PS B; S2 – pumping station; PS B – storage tanks ST C; S3 – storage tanks; ST C – storage tanks ST D and last one S4 – storage tanks; ST D – cities E and F (Fig. 1).

The analyzed main network is build:

- *Section S1*: reinforced concrete pipeline with a diameter of 1,500 mm;
- *Section S2*: steel pipeline with a diameter of 1,400 mm;
- *Section S3*: steel pipeline of 1,200 mm;
- *Section S4*: steel pipeline with a diameter of 1,000 and 600 mm.

The study used data from the period 2015–2017 containing hydraulic parameters of the WSS (i.e. water flow and pressure), as well as the quality parameters of raw and drinking water at monitoring points. Based on the results coming from the hydraulic simulation model the water flow rate was set to within a range of 0.30–0.32 m/s for section S1 and for other sections (S2, S3 and S4) changes from 0.28 to 0.34 m/s.

2.2. Water quality

The subsystem is based on surface water, therefore, it is characterized by a seasonal variability of water composition throughout the year. During the study period, the water

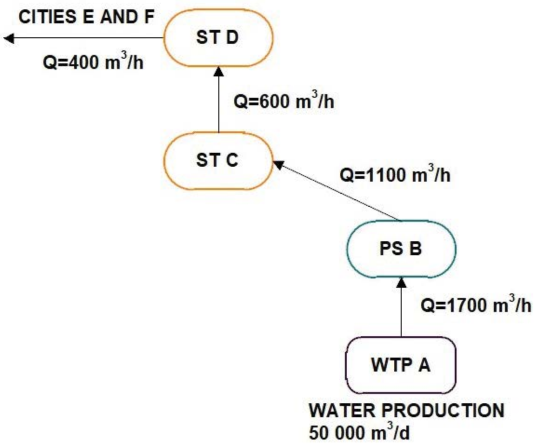

Fig. 1. Scheme of analyzed WSS.

temperature at WTP A has varied from 2°C to 20°C. The potable watercolor at the outlet of WTP A took values from 0.0 to 5.0 mg Pt/l (average 3.1 mg Pt/l) and turbidity ranged from 0.05 to 0.4 NTU (average 0.2 NTU). However, the highest turbidity values occurred in ST C and ST D, ranging from 0.1–0.52 NTU. At all disinfection points, chlorine concentration levels were kept constant, however, concentration levels varied depending on the season. Fig. 2 presents changes in free chlorine concentrations for the years 2015–2017, revealing that the lowest chlorine concentrations occurred in the second half of 2015 (fall/winter). In the case of trihalomethanes (THMs), the lowest values were in winter and the highest in summer (Fig. 3). No exceedances of THMs concentrations were reported during this period. Fig. 4 shows the variation in chloroform concentration between 2015 and 2017. A continuous red line indicates the maximum limit value, defined by the Polish Regulation (J. Laws 2017, Item 2294, 2017.12.11). The highest concentrations occurred in the summer months. Exceedances of the limit value occurred in tanks D in 2015 and 2016.

Chloroform concentration was the only THMs compound, which recorded exceedance of permissible levels. Moreover, other constituents of THMs sum (bromodichloromethane, dibromochloromethane, bromoform) contributed only marginally to the THMs sum (not more than 15%), therefore they were not included in the analysis of DBPs in drinking water delivered to customers.

3. Methodology and results

3.1. Water quality model

The presented study uses a hydraulic model of the WSS built in the Epanet 2.0 software. The model was built for the average values of water demand in 2017. The model was subjected to calibration and validation processes, during which the following correlation values of control parameters were obtained: flow rate of 98.7% and pressure 98.6%. The simulated values were also verified using the determination factor R^2 (flow rate 97.3% and pressure 97.1%).

The subject hydraulic model was used to build the water quality model (chloroform formation and chlorine decay models). For the purposes of building the subsystem qualitative model, water tests were conducted to determine a constant rate of chloroform formation/chlorine decay rate in bulk zone-k_b (bulk reaction rate coefficient). The tests were performed through in-field sampling using a bottle method. Water samples were taken at places of water disinfection. In the conducted study, DBPs concentration was determined by the gas chromatography method with super surface phase analysis and electron capture detection in accordance with EN ISO 10301: 2002. Chlorine concentration was determined by the spectrophotometric method based on standard EN ISO 7393-2:2018-04.

The values of k_b coefficient were determined based on the first-order reaction Eq. (1):

$$\ln \frac{C_t}{C_0} = \pm kt \tag{1}$$

where C_t is the chloroform/chlorine concentration at time t (mg/L), C_0 is the initial chloroform/chlorine concentration (mg/L), k is the constant rate of compound formation/decay (mg/L/d) and t is the time (d).

The values of the wall coefficient for chloroform formation/chlorine decay were determined by trial and error, adjusting simulation results to measurements of chloroform as well as chlorine concentration at checkpoints. Table 1 presents the obtained values of both coefficients.

The water quality models were also subjected to calibration and validation processes, during which the following correlation values of water parameters were obtained: chloroform concentration 96.8% and chlorine concentration 98.1%.

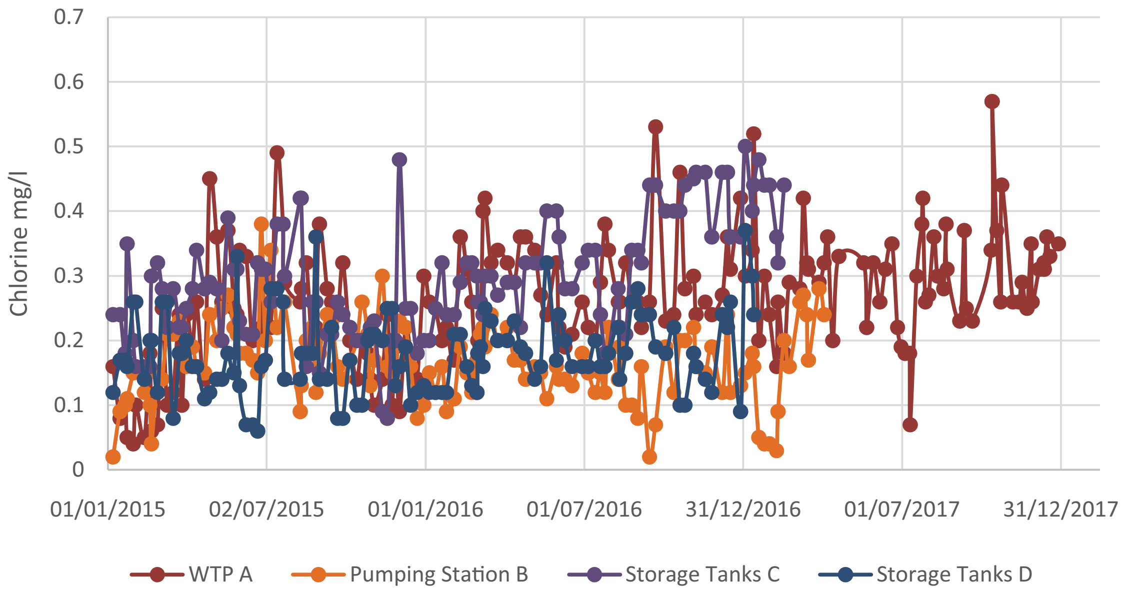

Fig. 2. Chlorine concentrations for the period 2015–2017.

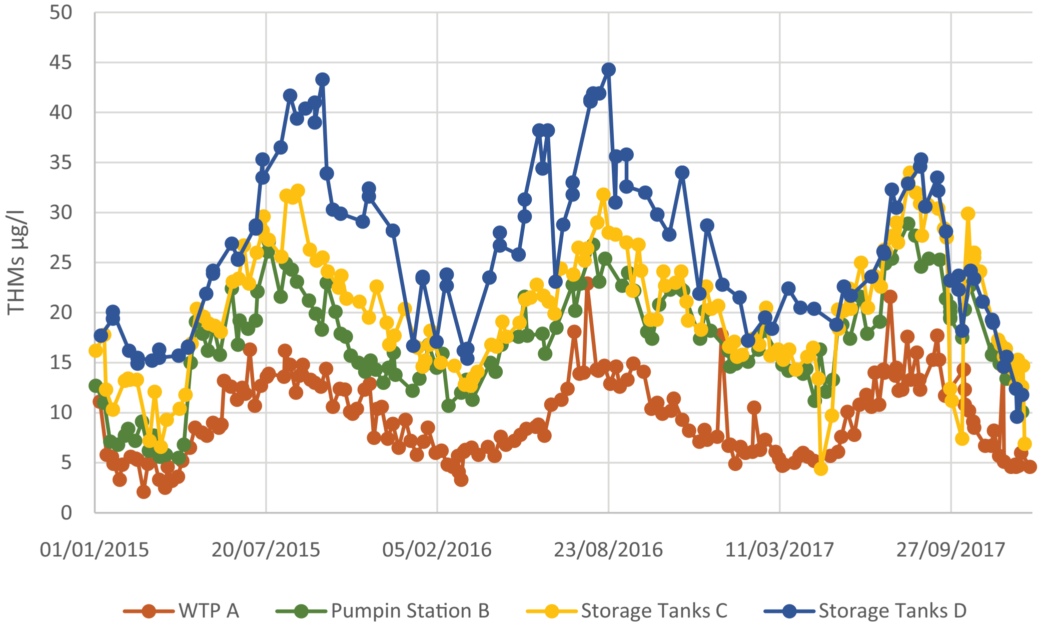

Fig. 3. THMs concentrations for the period 2015–2017.

Table 1
Reaction rate coefficient k_b and k_w values in separate zones of the modeling subsystem

Section	Chloroform formation (h⁻¹)		Chlorine decay (h⁻¹)	
	k_b	k_w	k_b	k_w
S1	0.23	0.22	–0.79	–0.46
S2	0.14	0.02	–0.21	–0.05
S3	0.30	0.02	–0.23	–0.18
S4	0.05	0.02	–0.17	–5.00

3.2. Probability of exceeding the allowable concentration of chloroform

The probability of exceeding the allowable chloroform concentration was determined on the basis of the water quality model. For this purpose, three scenarios of WDS work were carried out. The first analysis scenario (AS-1) assumes normal operation of the WSS for average water demand, the second analysis scenario (AS-2) for maximum water demand and the third one (AS-3) for minimum water demand. Simulations were carried out for time T equal to 30 d. For each scenario exceedances of the limit value of chloroform concentration $E_{\mathrm{CHCl_3}}$ and time of exceedances t, were noted. The probability P for each section is determined using Eq. (2). Table 2 summarizes the results for each scenario.

$$P = \frac{\sum t}{T} \tag{2}$$

where t is the time of exceedances of the limit value of chloroform concentration $E_{\mathrm{CHCl_3}}$ (h) and T is the simulation duration (h).

3.3. Fuzzification of consequences

The paper assumes three consequences levels of secondary water contamination belonging to subsets $A_j^{i,k}$ – low, medium and high. Each level is assumed as a triangular fuzzy number (TFN), shown in Table 3 and Fig. 5. The consequence C^i of an event may belong to subset $A_j^{i,k}$ at a certain degree of membership $\mu_j(C^i)$, in the range 0–1.

The relationship of consequences to membership is given by the equation [31]:

$$\mu_1\left(C^{i,k}\right) = \begin{cases} 1 - 4C^{i,k} 0 \le C^{i,k} \le \dfrac{1}{4} \\ 0, \dfrac{1}{4} \le C^{i,k} \le 1 \end{cases} \tag{3}$$

$$\mu_j\left(C^{i,k}\right) = \begin{cases} 0, 0 \le C^{i,k} \le \dfrac{j-2}{6} \\ 4C^{i,k} - (j-2), \dfrac{j-2}{4} \le C^{i,k} \le \dfrac{j-1}{4} j = 2 \\ j - 4C^{i,k}, \dfrac{j-1}{4} \le C^{i,k} \le \dfrac{j}{4} \\ 0, \dfrac{j}{4} \le C^{i,k} \le 1 \end{cases} \tag{4}$$

$$\mu_3\left(C^{i,k}\right) = \begin{cases} 0, 0 \le C^{i,k} \le \dfrac{3}{4} \\ 4C^{i,k} - 3, \dfrac{3}{4} \le C^{i,k} \le 1 \end{cases} \tag{5}$$

where μ_j is the degree of membership and $C^{i,k}$ is the consequences of ith pipe of a given event, kth relative consequence

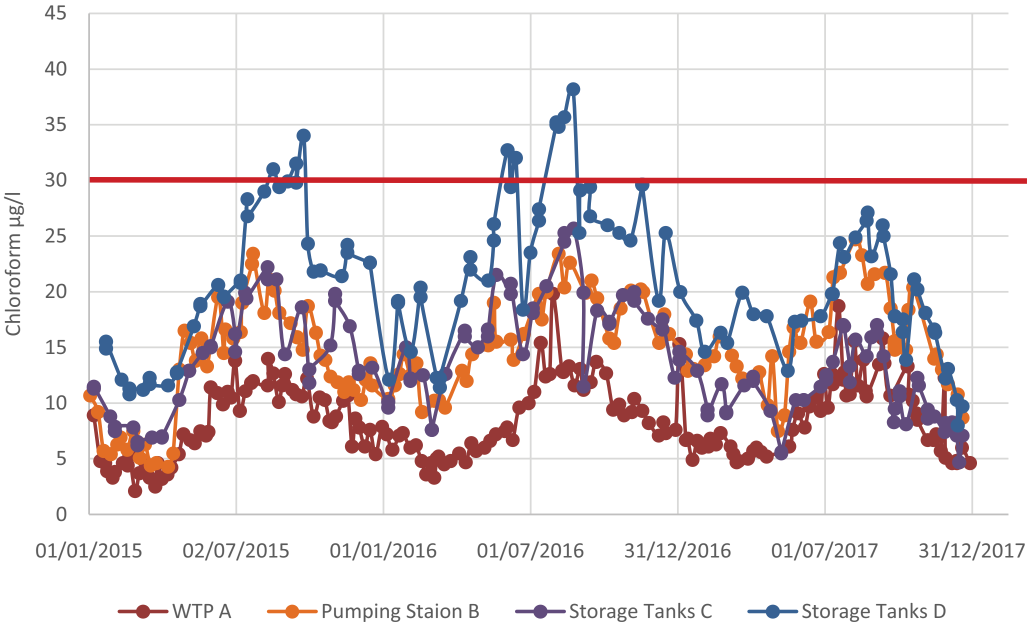

Fig. 4. Chloroform concentrations for the period 2015–2017.

Table 2
Probability of exceeding the allowable chloroform concentration

Section	Analysis scenario		
	AS-1 – Average water demand	AS-2 – Maximum water demand	AS-3 – Minimum water demand
S1	0	0	0
S2	0	0	0.15
S3	0	0	0.25
S4	1	1	1

(*k* corresponds to an excess concentration of DBP or a correction to the disinfectant).

In this paper two types of consequences are considered, the first one is connected with the volume of water in which the maximum concentration of chloroform was exceeded, the second one is connected with the correction (reduction) of the disinfectant dose. The correction of the disinfectant dose was determined on the basis of received water quality data. The obtained value of disinfectant reduction was applied for all used models. The choice of these parameters to determine the consequences was guided by the deterioration of water quality. Exceeding the maximum concentration of chloroform and reducing the dose of disinfectant may cause a risk to human health. If the disinfectant dose is reduced, microbiological contamination of the water can occur.

The paper uses the method of aggregation of consequences by using fuzzy logic. The fuzzy rules were used for this purpose. The fuzzy rule is presented using language expressions and logical operations such as AND or OR, as in the example below (Rule 1). Aggregation of consequences consists of plotting the field under the chart (on the basis of the diagram in Fig. 5) according to the above-mentioned rules and determining the value finding the center of gravity for the plotted figure. The fuzzy rules for the WSS in question are presented in Table 4.

Table 3
Three stages of function fuzziness

Subset	Qualitative scale	TFN
A1	Low	0; 0; 0.4
A2	Medium	0.1; 0.5; 0.9
A3	High	0.6; 1; 1

Rule 1: If consequence (related with water volume) is, low or consequence (related with disinfectant dose) is medium, then (aggregated consequence) is low.

The results of the aggregated consequences mentioned above are summarized in Table 5.

3.4. Risk assessment

Based on the probability of an adverse event occurring and the aggregated consequences, the risk in the analyzed WSS is calculated. Due to the fact that simulations were performed for three cases of network operation, the risk is presented for all cases. The results of the calculations are summarized in Table 6.

Since the study uses the probability and consequence values in the range 0–1, the following risk values were assumed: 0–0.25 low, 0.26–0.75 medium and 0.76–1.0 high. This means that low risk prevails in these cases. One exception is the average risk received for Section 4 for the minimum model. Exceedances of the chloroform concentration limit for this water distribution subsystem are sporadic, as shown by the historical water quality data and the quality

Table 4
Fuzzy rules for a consequence

Rule number	Relative consequences		Aggregated consequence
1	A1	A1	A1
2	A2	A1	A1
3	A3	A1	A2
4	A1	A2	A1
5	A2	A2	A2
6	A3	A2	A3
7	A1	A3	A2
8	A2	A3	A3
9	A3	A3	A3

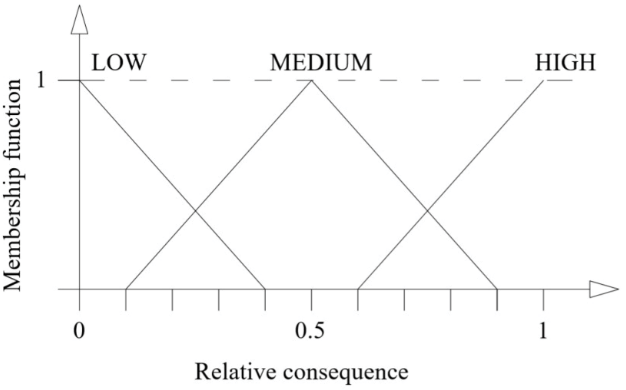

Fig. 5. Fuzzification of consequences.

Table 5
Aggregated consequence

Section	Analysis scenario		
	AS-1 – Average water demand	AS-2 – Maximum water demand	AS-3 – Minimum water demand
S1	0	0	0
S2	0	0	0.58
S3	0	0	0.45
S4	0.13	0.14	0.48

model. Data on disinfectant correction are presented in general terms, which may also underestimate the results obtained. Nevertheless, the methodology presented provides the basis for estimating the water quality risk. These procedures can be used to support decision making by managers.

4. Conclusions

This article presents the methodology for the determination of risks of secondary water pollution. The methodology involves water quality simulation models, which were the basic source of data for risk determination. The probability determination of unwanted event occurrence was calculated using the duration of exceeded DBPs concentration. Results were obtained from numerical simulations of different cases of WSS operation. These can be used to determine the critical areas defined by the heterogeneous vulnerability of secondary water contamination. The novelties of the proposed method are the spatial analysis of conditions of WSS operation where water quality in consumer tap could be harmful to people. The presented method is a useful tool for mapping and assessing (including valuation of consequences) of critical areas to contribute to a priority setting as one criterion of dividing a waterpipe network into district metered areas for both hydraulic and water quality parameters. In the case of determining the consequences, a fuzzy logic method was proposed, which combined different consequences in order to obtain aggregated consequences for the risk calculation. In this paper two types of consequences were chosen, the volume of "polluted" water and the concentration of free chlorine after correction of the disinfectant dose. The first one gives indirect information about the number of people who may be exposed to an increased amount of chloroform water. The second one indicates the extent to which water may be exposed to microbiological contamination by insufficient protection of water by disinfection.

Table 6
Risk value of exceedances of permissible level of chloroform concentration [Inline Equation 1] for three cases of WSS operations

Section	Analysis scenario		
	AS-1 – Average water demand	AS-2 – Maximum water demand	AS-3 – Minimum water demand
S1	0	0	0
S2	0	0	0.09
S3	0	0	0.11
S4	0.13	0.14	0.48

Three scenarios of WSS operation (average, maximum and minimum water demand) were worked out in the paper, thanks to which the full range of operation of this system was obtained. On the basis of the simulation results, the most unfavorable state of operation of the WSS was determined. The most unfavorable conditions (highest risk) were obtained for the case of the minimum water demand for which secondary water contamination occurred in three sections of the WSS under consideration. For the other examples, the risk remains low. The risk identified gives water distribution system operators information on what extreme conditions they can maintain to provide high-quality water to their customers.

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