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MODELLING STUDIES OF WATER CHLORINATION EFFICIENCY IN MUNICIPAL WATER SUPPLY NETWORK

ANALIZA MODELOWA EFEKTYWNOŚCI CHLOROWANIA WODY W MIEJSKIEJ SIECI WODOCIĄGOWEJ

Abstract: Chlorination of water belongs to the basic methods of its disinfection and is commonly used, permanently or periodically, as the final stage of water treatment in many water treatment stations in Poland. Although, the chlorination process is a well-known phenomenon, the selection of an appropriate dose of disinfectant is still a difficult task. The lack of chlorine in the water or its excessively low content (below 0.2 mg · dm^{-3}) may result in the lack of microbiological protection of water flowing through the pipes. A reverse situation is also unfavourable. The use of too high doses of chlorine at the entrance to the network, on the one hand, ensures adequate disinfectant concentration even in the fittings of the network, on the other hand, it can lead to dangerous for health disinfection by-products (DBPs) including trihalomethanes (THMs). The selection of the proper dose of chlorine should take into account factors affecting its consumption, chemical parameters of water as well as hydraulic parameters of water transport. Such possibilities are available due to application of numerical modelling to study the transport of chlorine in water.

The aim of the presented research is to analyse the effectiveness of chlorination of water in a selected water supply network. Simulation tests were carried out for the various doses of disinfectant supplied to the network for the assumed duration of the simulation – 168 hours. The qualitative model was developed in the Epanet 2.0 software using a hydraulic model of the tested network. The first order chlorine decay reaction was assumed to modelling studies, with applied literature values of decay rate of chlorine in water.

The results of simulation tests of chlorine transport in the network revealed difficulties in choosing the right dose of chlorine necessary to ensure microbiological protection of water in the network. The forced flow allowed effective disinfection of water.

Keywords: chlorine decay, chlorination of water, chlorine distribution in water, Epanet

Introduction

The main objective of water supply companies is to deliver water save, meeting all binding physical, chemical and microbiological requirements, to the consumers [1, 2].

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Accomplishment of these requirements is related to the necessary application of various technologies of water purification, including disinfection. According to World Health Organization (WHO) [3] the process of disinfection utilizing reactive chemical compounds, including chlorine, poses the crucial role in delivery of safe water to the consumers due to developed barrier for several pathogens. The properly designed system of water disinfection by chlorine allows effective disposal of bacteria, viruses or other pathogens as well as protection of water inside the whole system of drinking water distribution, preventing its secondary pollution.

During water treatment process, chlorine is usually being supplied as compressed gas, solution of sodium hypochlorite or solid calcium hypochlorite. All used forms of chlorine are generally chemically equivalent due to quick equilibrium between dissolved chlorine and products of dissociation of hypochlorite compounds. In relation to the form of chlorine application, the following reactions occur in water [4, 5]:

Gaseous chlorine: $Cl_2 + H_2O \leftrightarrow H^+ + Cl^- + HOCl$ (1)

Sodium hypochlorite: $NaOCl + H_2O \leftrightarrow H_2O + Na^+ + OCl^-$ (2)

Calcium hypochlorite: $Ca(OCl)_2 + 2H_2O \leftrightarrow Ca^+ + 2OH^- + 2HOCl$ (3)

HOCl will dissociate to give hydrogen ions (H+) and hypochlorite ions:

$$HOCl + H_2O \leftrightarrow H_3O^+ + OCl^- \quad (4)$$

Dissociation of hypochlorous acid HOCl is reversible and depends to both, temperature and pH of water. Along with the increase in pH value, at the same temperature, there is observed the increase in hypochlorite ion content in water, but at lower concentrations, free chlorine remains as HOCl (see Fig. 1).

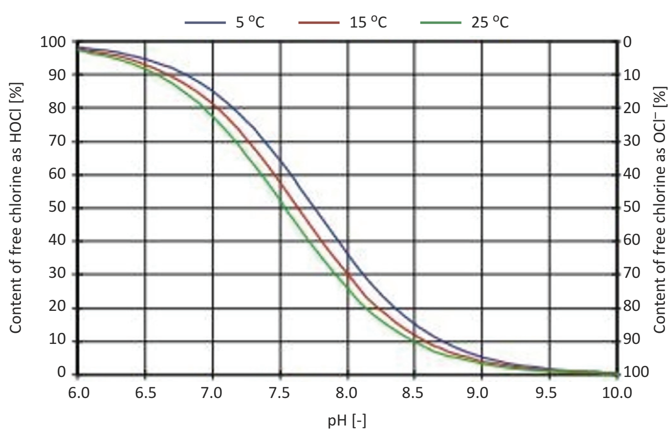

Fig. 1. Distribution of hypochlorous acid and hypochlorite ion in water at different pH values and temperatures [6]

Taking into account the stronger disinfectant capabilities of HOCl in relation to hypochlorite ion, the predominance of HOCl in water should be sustained during the disinfection process. Besides pH and temperature of water, the efficiency of disinfection is significantly related to type and content of microorganisms in water, characteristics of treated water, initial chlorine dose, upkeeping the required chlorine concentration during the time duration necessary to disposal the microorganisms.

Chlorine added to water decomposes in different ways, four types of reactions may be noted: (1) oxidation, (4) addition, (5) substitution, and (6) catalysed or light decomposition:

$$HOCl + 2Fe^{2+} \rightarrow 2Fe^{3+} + Cl^{-} + OH^{-} \quad (5)$$

$$HOCl + Mn^{2+} \rightarrow Mn^{4+} + Cl^{-} + OH^{-} \quad (6)$$

$$4HOCl + S^{2-} \rightarrow SO4^{2-} + 4Cl^{-} + 4H^{+} \quad (7)$$

$$HOCl + Br^{-} \rightarrow HOBr + Cl^{-} \quad (8)$$

$$3HOCl + 2NH_3 \rightarrow N_2 + 3Cl^{-} + 3H_2O + 3H^{+} \quad (9)$$

$$R\text{-}CHO + HOCl \rightarrow R\text{-}COOH + Cl^{-} + H^{+} \quad (10)$$

Equations (5) to (9) are reactions of hypochlorous acid with inorganic substances, leading to the immediate use of residual chlorine. Reaction described by equation (10) occurres between HOCl and functional groups in particles of natural organic matter (NOM) available in water. All equations presented above result in the consumption of chlorine in water.

The wrongly selected dose of chlorine, both to low and too high, unfavourably affects characteristics of water quality. Decrease in free chlorine content below the minimal level may trigger the secondary development of microorganisms [7–12]. Sustaining the minimal concentration of chlorine inside the whole water distribution system prevents water against growth of bacteria and deterioration of qualitative characteristics of water.

On the other hand, application of too high dose of chlorine disinfectant during water purification may result in occurrence of dangerous water disinfection by-products (DPBs) including trihalomethanes (THMs) as well as change of water smell and taste [3, 13–19].

Thus, the proper determination of chlorine dose required for water disinfection is crucial. According to WHO guidelines, concentration of free chlorine in points of water delivery should be in range 0.2–0.5 mg $\cdot$ dm^{-3} [3]. Polish standards [2] determine the acceptable concentration of chlorine in drinking water as 0.3 mg $\cdot$ dm^{-3}.

Chlorine, added to water during its disinfection process decomposes, as it was mentioned before, as a result of chemical reaction with inorganic and organic compounds available in transported water. Chlorine, as a strong oxidant is being used during interaction with sediments, product of corrosion as well as biomass, deposited on the inner walls of pipes. Thus, its constant decomposition in time is being observed, irrespectively to availability of other factors affecting its usage [20–22]. The total sum of all processes occurring in water body and in the boundary layer is known as the chlorine demand by water.

Taking into account the large number of factors influencing chlorine decomposition and complexity of processes occurring inside the water supply system, it is hard to correctly predict the final chlorine content in water, especially inside large piping systems, operating under unfavourable technical and hydraulic conditions. Thus, the new tools supporting this process are still researched. Nowadays, the numerical models, allowing to reflect the variable hydraulic conditions inside water supply network as well as the individual factors affecting decomposition of chlorine, are commonly used in the studies of chlorine transport.

The key factor related to application of different equations of chlorine decomposition is determination of its decay constants, which, in turn, are related to quality of source water, its temperature, Reynolds number and properties of pipes materials. Therefore, the total constant of chlorine decay, k, is expressed and sum of two factors: decay in water constant, k_b, and decay in boundary layer k_w [23].

The simplest and popular model of chlorine decay assumes that chlorine concentration is proportional to its initial content, according to equation:

$$c = c_0 e^{-kt} \tag{11}$$

where: c – chlorine concentration in time t [mg · dm^{-3}], c_0 – initial chlorine concentration [mg · dm^{-3}], k – constant of chlorine decay rate [min^{-1}], t – time [min].

The value of constant of chlorine decay in mass of water, in relation to temperature and pH of water, initial dose of chlorine as well as hydraulic conditions (velocity of flow and Reynolds number) may be equal 0.07–0.74 h^{-1}. This constant may be determined under the laboratory conditions by the bottle test. The research performed by Hua et al. [24] indicated the empirical relations between the initial concertation of chlorine and its decay constant in mas of water:

$$k_b = \frac{0.018}{c_0} - 0.024 \tag{12}$$

The studies performed under the laboratory conditions by Hallam et al. [25] showed the significant influence of pipe material on k_w value. The determined values of k_w varied in range 0.03–1.64 h^{-1} for various materials.

Recent development of numerical techniques and software for water distribution networks and sewerage system modelling allows increased application of modelling studies in water and swerage supply companies [26, 27]. Available pieces of computer software, e.g. Epanet 2.0 [28], Aquis [29] or Mike Urban [30], based on reported kinetic model of chlorine decay, allows high-accuracy prediction of applied disinfectant in nodes of the tested networks [7, 31–33].

The Epanet modelling software, due to its free access, gained huge popularity. The kinetics of chlorine decomposition in this software was described by the first order model [28]. The research reported by Ozdemir and Ucak [34] covering comparison of numerical modelling results obtained in Epanet and DYNAQU computational algorithm to the results of chlorine concentration measured in nodes of water supply system showed the satisfactory agreement between modelled and measured values.

The aim of this paper was variant analysis of water chlorination efficiency for selected municipal water supply network. The performed analyses of chlorine transport and decay was supplemented by studies over water age. The qualitative numerical calculations were performed in Epanet model, basing on the calibrated hydraulic model of the network.

Materials and methods

Object of study

Our studies were performed for municipal water supply network delivering drinking water to approx. 8600 residents. The studied network has mixed structure and is supplied with water by three water supply stations, but station WSS III works as support and is unable to provide required water demand during emergency situation. The length of whole network is 57.3 km and consists of asbestos-cement, polyvinyl chloride (PVC) and polyethylene (PE) pipes. Diameters of pipelines in the network vary in range 500–90 mm, while connection pipes 63–25 mm. The pressure head at the beginning of the network is being sustained at the constant level of approx. 0.4 MPa.

Hydraulic model

The hydraulic model of studied network was developed in Epanet 2.0 computational software. This model consists of 444 lines, 410 nodes and three reservoirs combined with pumping stations (described in Fig. 2 as WSS-I, WSS-II and WSS-III). Calculations of pressure loss were performed according to Darcy-Weisbach formula. Diameters, lengths and elevations of pipelines introduced to our model were obtained from the situation map. The computable water demands were based on the real readings

Fig. 2. Network scheme with marked characteristic nodes and pipelines

from domestic watermeters (0.003–0.97 $dm^3 \cdot s^{-1}$) while the applied water demand patterns were based on network watermeters readings from water supply stations (Fig. 3).

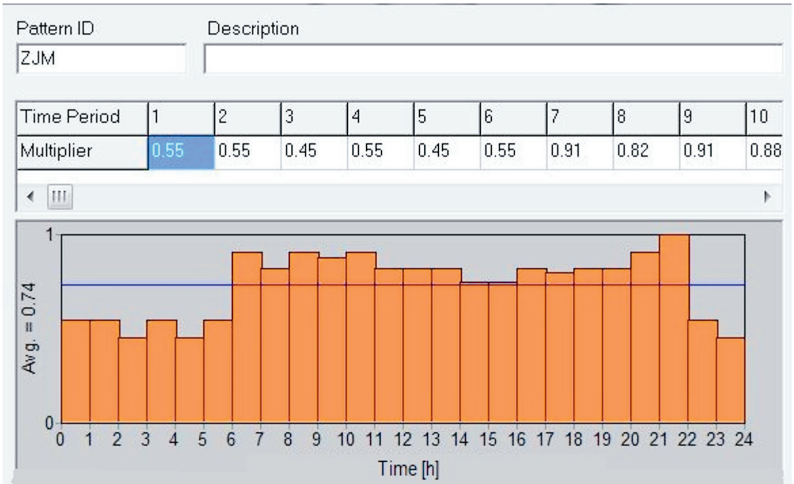

Fig. 3. Assumed water demand pattern

The maximal water flow rate inside the studied network occurs at 21.00 and reaches the level 32.6 $dm^3 \cdot s^{-1}$, while the lowest water demand equaled 14.33 $dm^3 \cdot s^{-1}$ and appears at 02.00. The Manning's roughness coefficient values for materials of studied pipelines were accepted after literature reports as k = 1.5 mm for cast iron pipes, k = 0.6 mm for asbestos-cement pipelines and k = 0.025 mm for plastic pipelines.

Qualitative model

The variant analyses of water chlorination efficiency inside the tested water supply network were performed in Epanet 2.0 software, developed and published by EPA, USA, with usage of the hydraulic model of the network. The applied hydraulic model was previously calibrated in relation to pressure and volumetric water flow distributions.

Due to lacking in situ measurements, values of chlorine decay constants were assumed after literature. Value of chlorine decay constant in water was assumed as k_b = 0.012 h^{-1}, after Hua et al. (1999) [24]. The assumed value is similar to the k_b = 0.0182 h^{-1} determined empirically and reported by Musz-Pomorska et al. [35] for the similar network. The value of chlorine decay constant in the boundary layer, k_w = 0.16 h^{-1}, was assumed as average of values proposed by Hallama et al. [25] for different pipeline materials.

Water inside the studied network is chlorinated periodically, in cases of water pollution danger or after repair works. According to information obtained from the local water supply company, water delivered to the networks belongs to the semi-hard (of medium hardness) with alkaline pH. Iron content in water reaches level of 60 μg · dm^{-3}, while compounds of chlorites, ammonium and nitrites are available in trace quantities.

In order to determine the water chlorination efficiency inside the studied water distribution network, six variants of modelling calculations of chlorine transport and decomposition were performed, with different assumed dose of disinfectant during operation of all water supply stations as well as during failure of one of them. All accepted variants of calculations are presented in Table 1.

Table 1

Variants of chlorine simulation

Variant	Working of Water Supply Station	Initial concentration of chlorine c_0 [mg · dm^{-3}]	Chlorine dose [mg · dm^{-3}]
I	WSS-I, WSS-II, WSS-III	0	0.3
II		0	0.5
III		0	1.0
IV	WSS-II, WSS-III	0	0.3
V		0	0.5
VI		0	1.0

The applied modelled dose of chlorine was accepted after available literature [33, 36], including WHO guidelines (2011) [3], according to which concentration of free chlorine in water delivered to the customers should be in range 0.2–0.5 mg · dm^{-3}. Thus, meeting such value of free chlorine inside the distant pipelines, the initial dose in WSSs should be respectively greater. Variants IV–VI assume failure of water supply station WSS-I. Taking into account similar amount of water supplied by stations WSS-I and WSS-II as well as similar hydraulic conditions occurring in the network during failure of WSS-I and WSS-II, variants of sole WSS-II failure were skipped in our studies. Similarly, variants of simultaneous failure of WSS-I and WSS-II was not introduced to our simulations due to impossibility of providing the required water demand by station WSS-III.

Additionally, simulations of water age inside the pipelines were also performed. The assumed time of simulation was equal 168 h. The accepted time duration of simulation is with agreement witch "long" time of water detention inside the pipes, according to literature equal 3 days [37].

Results

In order to present chlorine decomposition and water age inside pipelines of the studied municipal water distribution system, 10 nodes and 10 pipelines, assumed as representative, were selected. The choice was influenced by distance to water pumping station, daily change of hydraulic characteristics and range of the network. The selected localizations of reference nodes and lines are presented in Fig. 1.

Table 2 presents time-related changes of modelled free chlorine concentration in selected nodes of the tested network.

Table 2

Chlorine concentration on selected nodes of the network

Variant	Time[h] / Number of node	Chlorine concentration [mg · dm^{-3}]									
		1	2	3	4	5	6	7	8	9	10
I	12	0.25	0.00	0.22	0.18	0.00	0.00	0.00	0.00	0.00	0.00
	24	0.25	0.08	0.20	0.19	0.00	0.00	0.00	0.03	0.07	0.00
	48	0.25	0.09	0.20	0.19	0.00	0.11	0.05	0.03	0.07	0.00
	72	0.25	0.09	0.20	0.19	0.06	0.11	0.05	0.03	0.07	0.07
	168	0.25	0.09	0.20	0.19	0.06	0.11	0.05	0.03	0.07	0.07
II	12	0.42	0.00	0.37	0.31	0.00	0.00	0.00	0.00	0.00	0.00
	24	0.41	0.11	0.34	0.30	0.00	0.00	0.00	0.05	0.11	0.00
	48	0.41	0.11	0.34	0.30	0.00	0.19	0.07	0.05	0.11	0.11
	72	0.41	0.11	0.34	0.30	0.11	0.19	0.07	0.05	0.11	0.14
	168	0.41	0.11	0.34	0.30	0.11	0.19	0.07	0.05	0.11	0.14
III	12	0.83	0.00	0.74	0.61	0.00	0.00	0.00	0.00	0.00	0.00
	24	0.82	0.23	0.68	0.61	0.00	0.00	0.00	0.11	0.23	0.00
	48	0.82	0.24	0.68	0.60	0.00	0.39	0.15	0.12	0.23	0.00
	72	0.82	0.24	0.68	0.60	0.22	0.38	0.16	0.11	0.23	0.23
	168	0.82	0.24	0.68	0.60	0.21	0.38	0.16	0.11	0.23	0.23
IV	12	0.24	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	24	0.24	0.16	0.23	0.17	0.00	0.00	0.00	0.03	0.00	0.00
	48	0.24	0.16	0.23	0.17	0.00	0.11	0.04	0.03	0.00	0.00
	72	0.24	0.16	0.23	0.17	0.05	0.11	0.04	0.03	0.00	0.05
	168	0.24	0.16	0.23	0.17	0.05	0.11	0.04	0.03	0.01	0.05
V	12	0.41	0.00	0.41	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	24	0.39	0.11	0.37	0.27	0.00	0.00	0.00	0.00	0.00	0.00
	48	0.41	0.12	0.37	0.27	0.00	0.17	0.06	0.01	0.04	0.00
	72	0.39	0.11	0.37	0.27	0.09	0.17	0.06	0.01	0.04	0.09
	168	0.39	0.11	0.37	0.27	0.09	0.17	0.06	0.01	0.04	0.09
VI	12	0.82	0.00	0.81	0.00	0.00	0.00	0.00	0.01	0.01	0.00
	24	0.78	0.24	0.75	0.53	0.00	0.00	0.00	0.01	0.01	0.00
	48	0.78	0.24	0.75	0.53	0.00	0.35	0.13	0.02	0.09	0.00
	72	0.78	0.24	0.75	0.53	0.17	0.35	0.13	0.01	0.09	0.17
	168	0.78	0.24	0.75	0.53	0.18	0.35	0.13	0.01	0.09	0.17

* Grey color indicates values equal or higher 0.2 mg · dm^{-3}, required by WHO [3] as the minimal concentration of chlorine in drinking water.

The results of selected hydraulic characteristics of water flow inside the tested pipelines during the hour of maximum water demand are presented in Table 3.

Table 3

Parameters of flow in selected pipes at 168 hours of modelling

Description	Pipe	Diameter of pipe [mm]	Flow [$dm^3 \cdot s^{-1}$]	Velocity [$m \cdot s^{-1}$]	Flow [$dm^3 \cdot s^{-1}$]	Velocity [$m \cdot s^{-1}$]
			Variants I–III		Variants IV–VI	
1	41	250	4.12	0.08	4.12	0.08
2	86	100	1.04	0.13	1.04	0.13
3	228	150	2.65	0.15	6.24	0.35
4	M17	250	3.99	0.08	2.00	0.04
5	424	100	0.06	0.01	0.06	0.01
6	159	100	0.07	0.01	0.07	0.01
7	402	150	0.26	0.01	0.26	0.01
8	250	65	0.70	0.21	0.35	0.11
9	427	150	1.95	0.11	0.04	0.00
10	20	100	0.05	0.01	0.05	0.01

Figure 4 shows scheme of isolines differentiating free chlorine concentration for selected variants of water supply.

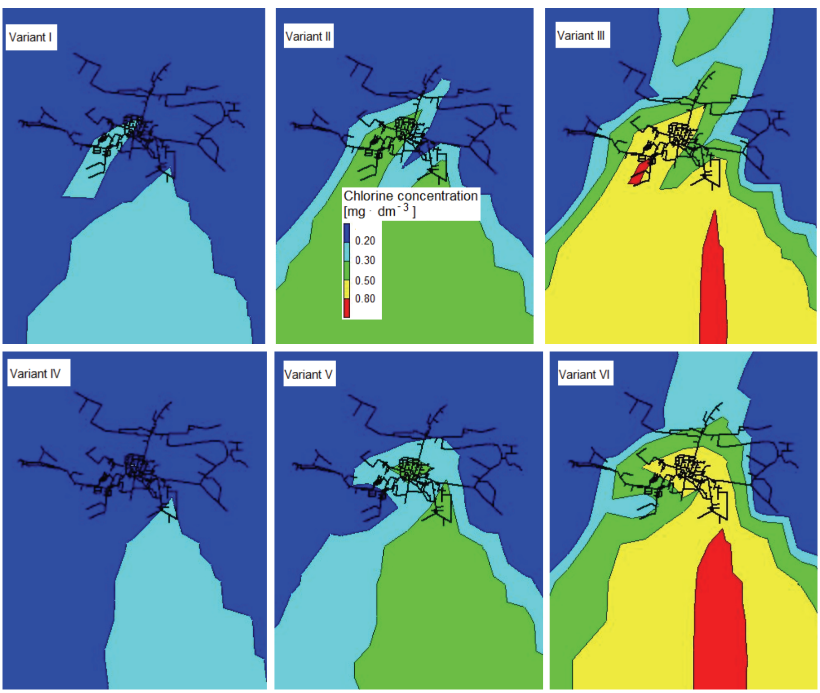

Fig. 4. Scheme of counter lines dividing the chlorine concentration in pipelines

The obtained results of modelled chlorine transport inside the pipelines of studied network, with assumed variable initial doses of disinfectant, shows that in none of tested computational variants the required satisfactory level of water protection was achieved due to failure to achieve required by WHO minimal concentration of free chlorine (min. 0.2 mg · dm^{-3}) [3].

In case of the modelled lowest doses of chlorine applied during drinking water treatment (Variants I and IV) the minimal chlorine concentration was noted only in the nodes very close to water supply station (nodes 1 and 3), characterized by the highest velocity and volumetric flow rate of water (Table 3).

The obtained results of calculations showed similar situation for chlorine dose equal 0.5 mg · dm^{-3}. The concentration of free chlorine higher than threshold value of 0.2 mg · dm^{-3} was observed only in three selected representative nodes. The slight increase in free chlorine, in relation to Variant I, was observed in the remaining points, however, below the required minimal value. In case of disinfectant dose equal 1.0 mg · dm^{-3} (Variants III and VI) the best results of chlorination were observed. The minimal threshold vale of free chlorine concentration was exceeded in 8 from 10 representative nodes at Variant III, with all water supply station operational.

The slightly worse situation was observed in Variant VI assuming failure of water supply station WSS-I. For both tested initial doses of chlorine, 0.5 mg · dm^{-3} and 1.0 mg · dm^{-3}, the concentration of free chlorine exceeding the maximum allowed by Polish regulations [2] 0.3 mg · dm^{-3} was observed in several nodes of the network.

Taking into account WHO's guidelines and maximum allowed concentration of free chlorine in water equal 0.5 mg · dm^{-3} the exceeding of this threshold value was observed only for the 1.0 mg · dm^{-3} initial dose of disinfectant. The nodes with determined increased free chlorine concentration are located on the main pipeline (diameters 250 mm and 150 mm) (Table 3), without the direct connections to the households. Distribution of free chlorine concentration inside the water supply network during the hour of maximum water demand, presented in Fig. 5 (Variant III), indicates that for the same initial dose (1.0 mg · dm^{-3}) the maximum allowed threshold value was also exceeded in the distributive benches of pipeline system. Such situation was observed for the nearly whole central part of the city. Too high concentration of free chlorine in water may negatively affect its taste and odor as well as may result in increased content of water disinfection by-products [5, 19].

The presented scheme of isolines for chlorine concentration in water (Fig. 4) shows that in all tested variants the highest concentrations of free chlorine are visible in pipelines close to water supply station, while the lowest chlorine content was noted for the perimeter pipelines. These observed low concentrations of free chlorine in the distant parts of the network are related to low water demands, resulting in very low velocities of water flow (Table 3). Additionally, the prolonged time of water retention (long water age) was observed in distant pipelines of the network, which also affects values of free chlorine concentration in water. The nodes in which the lowest values of free chlorine concentration in water were observed, were also characterized by the longest water age, exceeding even 4 days (Table 4). Such prolonged time of water retention in pipelines results in spontaneous chlorine decay as well as the extended

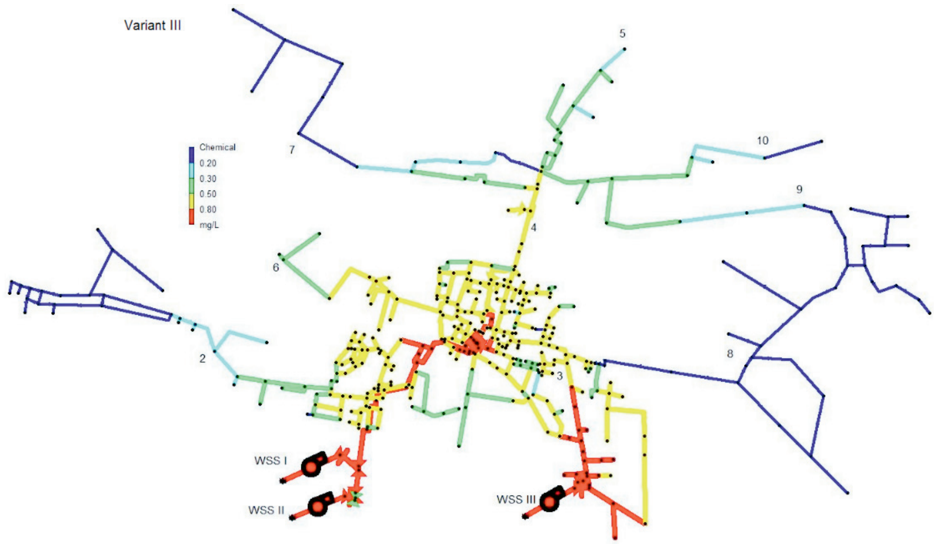

Fig. 5. Chlorine concentration in water – variant III

duration of chlorine contact with organic and inorganic compounds available in water and on inner walls of pipes.

Table 4

Water age on selected nodes of the network

Variant	Water age [h]									
	1	2	3	4	5	6	7	8	9	10
I–III	4.1	15.7	6.1	9.8	55.8	38.6	40.4	21.3	17.4	57.8
IV–VI	6.1	16.5	1.9	13.0	59.8	40.1	46.4	47.9	33.1	63.5

Conclusion

Meeting the minimal required concentration of residual chlorine in water, without exceeding the maximum allowed contents, in all nodes of the water distribution network is a very difficult task, especially in systems operating under unfavourable conditions or suffering technical problems. Low water demands, flow velocities far below the required minimal values and extended water age trigger deteriorated water exchange in the system, thus, constrict chlorine transport to the distant, perimeter parts of the network.

Analysis of the obtained results of chlorine transport modelling in the municipal water supply network, with assumed various initial doses of disinfectant, showed that, regardless the initial dose, there are visible pipelines in the studied system in which concentration of chlorine is below the required minimal value (0.2 mg $\cdot$ dm^{-3}).

These pipelines are located at the perimeter of the network and are characterized by very low values of water flow velocity (below 0.01 m · s^{-1}) and a long water age (above three days). Increased initial disinfectant dose caused increase in its concentration in close vicinity of water supply stations, even above the maximum allowable values described by Polish (0.3 mg · dm^{-3}) and WHO (0.5 mg · dm^{-3}) standards.

Assertion of the required concentration of free chlorine in the whole, vast water supply system with disinfection performed in one or several close locations may be very hard to achieve.

Taking into account assumption of literature values of chlorine decay to modelling and missing calibration of qualitative model the obtained results should be treated as preliminary but providing interesting and useful information concerning chlorine distribution inside the water supply network.

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