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MODELING THE CHLORINE-CONVEYING PROCESS WITHIN A DRINKING WATER DISTRIBUTION NETWORK

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Abstract

The distribution network is the last component of a water supply system in which potable water must be provided to the consumer. The presence of chlorine in drinking water is a necessity and a guarantee that water is microbiologically compliant. The study was carried out by means of the Epanet 2.0 program on a future distribution network in the hilly area, in which a simulation period of 4 days was considered. The water quality analysis was performed using the flow rates resulting from the hydraulic simulation. To track the propagation of the contaminant through network pipelines, a maximum permissible value of 0.5 mg/L, entered during the entire simulation period, was considered. The reactions that occur in the bulk flow, were modeled by means of a 1st and 2nd order a decomposition law. The obtained values of the free residual chlorine concentration showed that during the 96 h of simulation, there were certain pipelines in which the chlorine concentration did not meet the minimum allowable limit of 0.1 mg/L. Modeling water quality offers the opportunity to view the decreasing of chlorine concentration, so that the free residual chlorine dosage can be optimized.

Key words: chlorine concentration decay, drinking water, EPANET, water distribution network

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1. Introduction

Water is a limited and vulnerable resource, and globally, water sources are scarce: less than 1% of the world's water is proper for human consumption. Promoting human health and well-being is closely linked to drinking water supply (Omar and Aziz, 2019). The main condition that a water supply system must fulfill is to permanently and safely supply water to consumers. A water supply system is a complex of engineering works that ensures the abstraction of water from the natural environment, its quality correction, its storage, and its transportation and distribution at a pressure, quality and all requirements demanded by users. Based on the treatability studies, a treatment scheme will be adopted, to ensure, for the treated water, its final full compliance with the mandatory conditions required by the drinking water legislation in force (Ahmad et al., 2020).

An adequate water quality can be ensured on the water treatment plant's outlet, but this quality can be altered as water flows through the distribution system (that is, the water undergoes transformations) (Tutuianu, 2013). The transformations that appear in the distribution network can lead to the degradation of water quality, by changing its main characteristics: taste, smell, color, iron content, manganese, number of germs and/or streptococci, turbidity, number of biological organisms. The number of bacteria tends to increase as the water passes through the distribution network and is influenced by temperature, stagnation time, presence or absence of residual disinfectant,

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pipes materials and their affinity for the formation of the biofilm.

In drinking water treatment plants, chlorine is used both as a primary disinfectant and as well to prevent the development of micro-organisms inside water distribution networks (Georgescu and Georgescu, 2014). Design standard NP 133–2013 recommends the use of chlorine doses between 0.1 mg/L and 0.5 mg/L. According to Law no. 458/2002, the free residual chlorine concentration must have a minimum value of 0.5 mg/L at the treatment plant's outlet. Also, according to the same law, the free residual chlorine concentration must have a minimum value of 0.25 mg/L at the distribution network's end. Law 311/2004 provides for a maximum permissible value of free residual chlorine concentration in drinking water of 0.5 mg/L.

In other countries around the world, to confirm the safety of drinking water, laws provide for much higher chlorine concentrations. According to the recommendations of the World Health Organization (WHO), chlorine can be present in the range of 0.2 mg/L and up to 1.0 mg/L.

While chlorine is the most common disinfectant (He et al., 2019; Monteiro et al., 2014; Wang et al., 2019; Xu et al., 2018), the reaction of disinfectants with organic matter in water leads to the formation of disinfection byproducts (DBPs). Fig. 1a shows the control volume and the processes controlling the decay of free chlorine inside the pipe. Free chlorine in the bulk water is consumed by the biofilm at the pipe wall, releasing biofilm clusters and the formation of DBPs (Xu et al., 2018). Increasing water temperature also accelerates the formation of DBPs, including THMs, haloacetic acids (HAAs) etc. For example, a sudden boost in THMs and HAAs formation has been reported when tap water was heated (35–50°C) (Li et al., 2019).

Nowadays, several models allowing simulations of water quality inside the water supply systems are available (Zimoch and Bartkiewicz, 2018). One of the most popular is EPANET, allowing calculations of chlorine transport, studies of increase in DBPs and trihalomethanes (THMs) concentrations (Musz-Pomorska et al., 2019; Zhao et al., 2018) as well as determination of water age.

2. Materials and method

2.1. EPANET program

The EPANET 2.0 application, developed by the US-EPA Environmental Protection Agency, is a computing software that allows users to simulate pressure networks in real time, by focusing on hydraulic and water quality parameters. With the aid of the software can be monitored the flow variations in each pipe, the pressures in each node, the amount of water in each tank, and the concentrations of chemical substances in the network, during the simulation process. This software provides an integrated environment for pre-processing, via a network editor, simulation running, and, as well, for post-processing of computed data, via color-coded network maps, tables with parameter values (initially entered and/or computed), and different types of variation graphs for computed parameters.

The EPANET 2.0 program offers many facilities for modeling water quality:

- provides the tracking of flow rate in a node that reaches the other nodes;
- the modeling of actual flow inside pipe sections and the flows in the vicinity of pipe walls;
- the motion modeling for non-reactive materials inside the network, over time unit;
- the motion and evolution modeling of a reactive material, by showing the increase or decrease of concentration, in time;
- the modeling of the network's water quality, in terms of its age;
- allows the decrease or increase of reactions up to an imposed concentration limit;
- allows the concentration to be changed over time at any location of a network.

EPANET is a critical research tool used in the development of water quality analysis models in distribution networks. The hydraulic model for calculating a distribution network is the basic component, from which water quality modeling is started (Dineț, 2010).

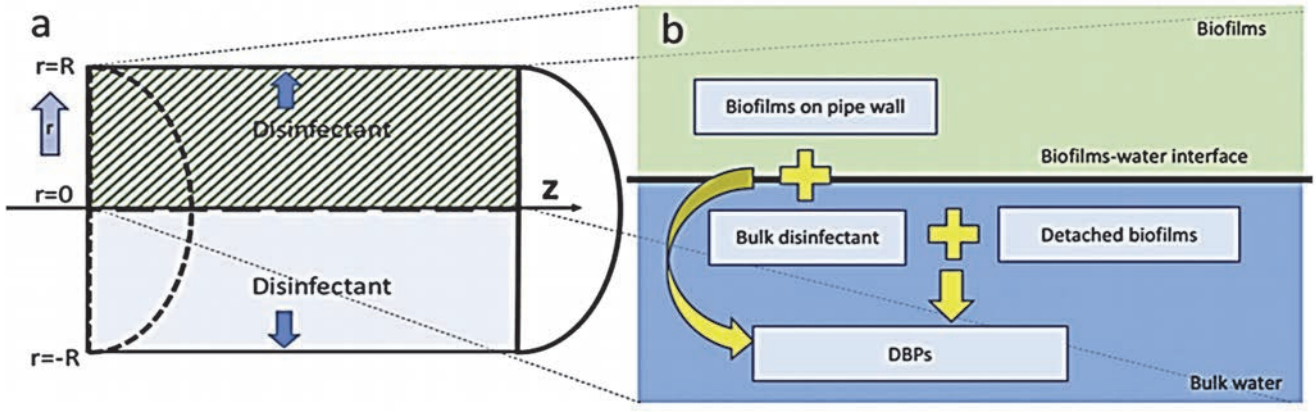

Fig. 1. a - Selected control volume marked by dash lines; b - Schematic of the biofilm covered pipes (adapted upon Xu et al., 2018)

The software offers the possibility to choose the hydraulic relationship, which will be the basis of the performed simulation (Hazen-Williams, Darcy-Weisbach, Chézy-Manning), to determine the linear head losses on sections. Also, it is possible to monitor the variation of the substance concentration next to the reactions that occur during flowing inside the distribution system. To accomplish this, it is necessary to know the rate at which the substance reacts and how it depends on the concentration (Peirovi Minaee et al., 2019; Țuțuianu, 2013). For example, the hypochlorous acid reacts with natural organic matters and it is conveyed through the boundary layer on the pipe wall, where it enters oxidation reactions with iron generated by corrosion. Hence, mass reactions may also occur at the pipe wall.

Organic compounds in water and biofilm on the inner surface of pipes react with chlorine, decreasing its concentration. The rate of decrease in chlorine concentration will be modeled by a 1st order reaction law or by a 2nd order reaction law.

2.2. Calculation methods and fundamental equations

The equations that control water quality analysis are based on mass conservation principles and reaction kinetics. When a reagent (chlorine) is conveyed via a water-filled pipe, certain reactions occur between the pipe and the organic compounds carried by the fluid. These reactions are called bulk flow reactions. As regards a flow inside a pipe, the dissolved compounds can be conveyed toward the pipe wall where they enter the reaction with the corrosion products and/or with the wall biofilm. The surface area of the wall that gets involved in the reaction, and the mass transfer rate between the bulk flow and the pipe wall also provide an influence on the global reaction rate at the pipe wall (Georgescu and Georgescu, 2014).

The water quality analysis is imposed by the following phenomena: the conveying of the substance inside pipes, fluid volume reactions (inside bulk flow) and reactions at the pipe wall. The studies by Georgescu and Georgescu (2014) showed that the dissolved chlorine transits a pipe j, of length L_j and diameter D_j at the same average velocity v_j as water, where the velocity is expressed according to the flow rate Q_j, reacting at the same time (decreasing its concentration) at a certain reaction rate r_j. The mass transportation of a single substance (chlorine decay) is described by the advection-dispersion-reaction equation, which for a circular pipe j is to be written as (Eq. 1):

$$\frac{\partial C_j}{\partial t} = d_l \frac{\partial^2 C_j}{\partial x^2} - v_j \frac{\partial C_j}{\partial x} - r_j, \tag{1}$$

where: $C_j=C_j(x,t)$ is the free residual chlorine concentration, in mg/L, which depends on the curvilinear abscissa $x\in[0;L_j]$ measured along the pipe and the time $t>0$ (greater than the initial moment $t=0$); d_l is the longitudinal dispersion coefficient (m^2/s); v_j - velocity (m/s); $r_j=r_j(C_j)$ is the reaction rate inside the pipe j, in mg/(L·s), depending on concentration. In the advection-dispersion-reaction equation, the reaction rate r_j has positive values for the decreasing reaction, respectively negative values for the increasing reaction.

In hydraulic systems with turbulent flow (Zhao et al., 2018), such as water distribution networks where flow characteristics are considered permanent and uniform, the main transportation mechanism is advection, the coefficient of longitudinal dispersion is considered null ($d_l=0$), and, hence, the equation becomes (Eq. 2):

$$\frac{\partial C_j}{\partial t} = -v_j \frac{\partial C_j}{\partial x} - r_j \tag{2}$$

According to Georgescu and Georgescu (2014), the reaction rate on pipe j is the sum between the reaction rate inside the bulk flow in the pipe j and the reaction rate at pipe wall (Eq. 3):

$$r_j = k_b C_j^n + k_{gw_j} \frac{4}{D_j} C_j, \tag{3}$$

where: n is the reaction order ($n=0$, for a 0 order reaction; $n=1$, for 1st order reaction, respectively $n=2$ for a 2nd order reaction); k_b is the reaction constant in the fluid volume (in the bulk flow) in the pipe, measured in s^{-1} and k_{gw_j} is the reaction coefficient at pipe wall, measured in m/s. As travel time increases and pipe diameter and bulk reaction rate decrease downward the distribution system, wall decay should eventually become a quantifiable component of the overall chlorine decay (Fisher et al., 2017). The first term of the sum in (Eq. 3) represents the reaction rate in the bulk flow in the pipeline (Georgescu et al., 2006) and it is considered that the instantaneous reaction rate depends on the concentration (Eq. 4):

$$r_j = k_b C_j^n \tag{4}$$

As highlighted by Musz-Pomorska et al. (2019), the kinetics of chlorine decay in Epanet is described by the first-order reaction, in relation to which, the final concentration is dependent only to the initial concentration of one component. In case of chlorine transport, its final concentration is related only to its initial concentration (Eq. 5):

$$C_j = C_0 e^{-k_b t} \tag{5}$$

where: C_0 is initial chlorine concentration (mg·L); t - time (s).

2.3. Case study description

A simplified scheme of the water supply system of a hilly area locality was considered, with a population of less than 4.000 inhabitants, and namely a scheme consisting of a storage tank (volume 450 m^3), and where the water is conveyed to consumers by gravity. The network was sized for a flow rate of 8.92 L/s, this being the average hourly flow. A constant pressure of at least 1.5 bar (pressure required at connection) needs to be provided in the network for groundfloor +2 storeys housing units.

The diagram of the water supply system (Fig. 2) is drafted using the graphical interface of EPANET 2.0, a program designed to perform hydraulic calculations and water quality analysis in distribution networks. The geometrical characteristics of the branched network are introduced directly into EPANET application (we considered HDPE PN10 pipes with diameters between 63 and 140 mm), with initial hydraulic parameters (the absolute roughness for the new high density polyethylene pipes is 0.007 mm). The program performs hydraulic simulation for water temperature at 20°C, which corresponds to a kinematic viscosity coefficient of 1.0110^{-6} m^2/s.

Chlorine decay rate increases with elevated temperature, which could be influenced by the change in microbial activities. Furthermore, even in the absence of microbes, chlorine undergoes self-decay, which is a temperature-dependent reaction. The tank (located in the locality's urban area) ensures the storage of the required water amount, water needed for providing the hourly offset of consumption and supply flows. The distribution network is composed of pipes, which are needed to convey water from the tank to the farthest consumption point, providing in the same time the water flows at the required service pressure.

The variation of hourly flow during a day is regulated according to the number of inhabitants (size of the urban agglomeration). With the help of the hourly variation coefficients for the daily water consumption graph corresponding to a rural locality, the schedule of hourly variation of flow consumed in each node was implemented in the EPANET software (Fig. 3), according to the Romanian standard 1343-1/2006 - Annex 2.

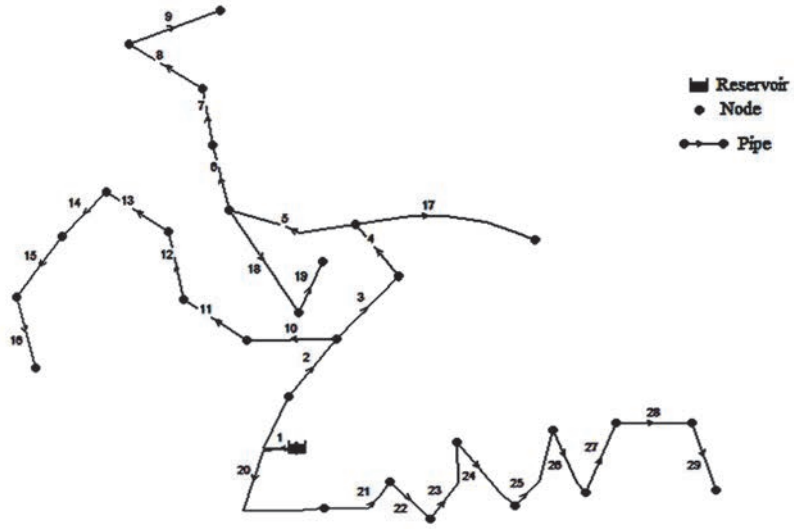

Fig. 2. Diagram: the water supply network (pipes numbering)

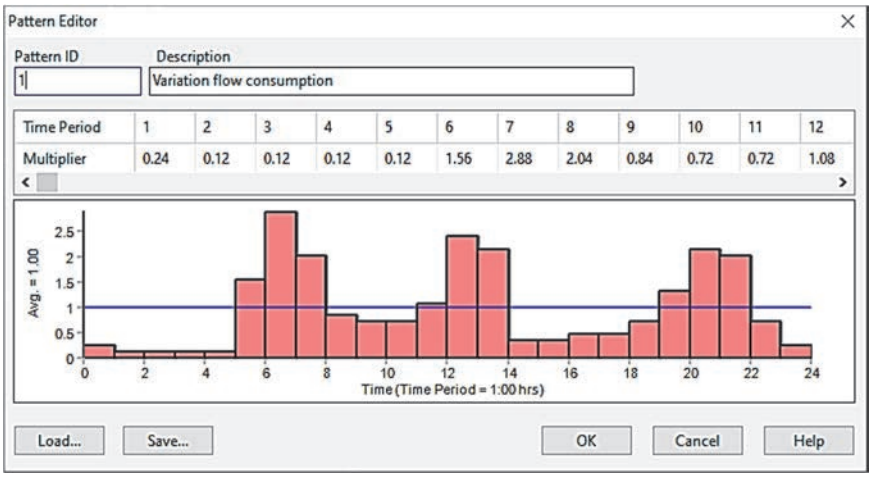

Fig. 3. Graph: hourly variation of flows consumed in each node

2.4. Water quality analysis

To track the free residual chlorine propagation through the distribution network, the hydraulic calculation can be performed first because the water quality analysis will be conducted using the hydraulic simulation flow rates. The output data for pipes in the case of hydraulic simulation are: flow (L/s), water velocity (m/s), head loss (m/km), the Darcy coefficient λ and for the nodes: pressure (mH2O), the piezometric head (m), the terrain level (m) and the water flow demanded (L/s). The first results obtained after running of software for the chosen system are shown in Table 1 (values were calculated by presuming that the hourly consumed flow has an average value).

When studying the behavior of drinking water networks serving the population, an important role is played by the study of water quality variation during the network transit, from the tank down to consumer. To study the variation in chlorine concentration in a water distribution network, the most commonly used equation is the transport and diffusion equation. This equation allows the modeling of processes that occur inside a distribution network: the change of chlorine concentration while water flows through the network (transportation process) and the change of chlorine concentration in pipeline section (diffusion process).

To perform the simulation of the free residual chlorine conveying in the branched network, with a time varying water consumption, the value of 0.50 mg/L was introduced at network entry (injection node - Tank), value that continuously enters the network.

To study the 1st and 2nd order decrease of chlorine concentration (a 1st order reaction in the fluid volume and at the pipe wall and a 2nd order reaction in the fluid volume), this modeling was conducted over a period of 4 days (96 h). For the modeling of the chlorine-conveying process the selected time increment was 5 min, and the bulk flow decay constant was selected as 1 day^{-1}, a figure proposed by Rossman (2000), this being a negatively entered value. The modeling was performed according to the variation of water flow in the network.

In the case of the reaction rate on pipe wall, the following factors were determined: the Reynolds number (*Re*), the mass transfer coefficient on pipe (k_{f_j}) and the reaction coefficient on pipe wall (k_{gw_j}), all these corresponding to the geometrical features and flows values for an average consumption rate (from Table 1).

Table 1. Geometric and hydraulic pipe features

Pipe	*Length (m)*	*Diameter (mm)*	*Flow (L/s)*	*Velocity (m/s)*	*Unit Headloss (m/km)*
1	588	140	4.46	0.29	0.6751
2	397	140	4.32	0.28	0.6377
3	250	140	2.29	0.15	0.2079
4	560	140	2.00	0.13	0.1642
5	340	110	1.16	0.12	0.1998
6	115	110	0.73	0.08	0.0890
7	430	90	0.53	0.08	0.1351
8	355	90	0.25	0.04	0.0353
9	180	75	0.06	0.01	0.0087
10	380	125	1.67	0.14	0.2044
11	570	125	1.33	0.11	0.1377
12	155	110	1.07	0.11	0.1733
13	170	110	0.95	0.10	0.1423
14	320	110	0.78	0.08	0.1003
15	580	90	0.46	0.07	0.1043
16	355	90	0.13	0.02	0.0081
17	730	110	0.26	0.03	0.0113
18	240	110	0.19	0.02	0.0053
19	140	90	0.05	0.01	0.0035
20	635	140	4.46	0.29	0.6728
21	920	140	4.13	0.27	0.5875
22	880	140	3.49	0.23	0.4358
23	605	125	2.96	0.24	0.5598
24	793	125	2.46	0.20	0.4045
25	197	110	2.11	0.22	0.5666
26	570	110	1.83	0.19	0.4439
27	780	90	1.35	0.21	0.6771
28	495	75	0.90	0.20	0.7885
29	1015	63	0.36	0.12	0.3720

The k_{f_j} coefficient was defined by Rossman (2000). For the calculation of k_{gw_j}, the wall decay constant was considered, a constant noted as k_w and considered by Georgescu and Georgescu (2013) to be equal to 0.3 m/day. The values of reaction coefficients in pipe wall were entered in the pipes editing menu, in section "Wall Reaction Coefficient", the obtained values being negative (expressed in m/day).

3. Results and discussion

If a water quality simulation is considered, the computed output data included number of the free residual chlorine loads for both pipelines and nodes. Table 2 shows the changes that occur in the chlorine concentration (mg/L) for some sections of network being studied, at the 5 time reference points chosen for the simulation. The decreasing rate of residual chlorine was modeled with the help of a first-order reaction, where the reaction rate is influenced by the concentration in the fluid mass, but also by the reactions at pipe wall. Chlorine needs a time to transit the network, and in time, it reacts in water with organic and inorganic compounds, decreasing its concentration (Georgescu and Georgescu, 2014).

In the 96 h of simulation, it can be observed that only one section did not meet the permissible limit of 0.1 mg/L for water quality compliance, namely section 29. The process of decreasing the chlorine concentration is more intense since it implies a low water consumption and, when water consumption is high, the water velocity gets higher. Hence, the water passes faster through the network and chlorine has no time to react. Therefore, if the consumer demand rates would be constant, the chlorine concentration would no longer have visible variations (being stabilized).

To study the water quality in the case of a 2nd order decrease of chlorine concentration, a single working model change was conducted. Specifically, in the "Bulk Reaction Order" editor a value of 2 was entered. Table 3 presents the chlorine concentration figures, simulation that was performed using a 2nd order reaction, in which the reaction rate is influenced only by the reactions in the fluid mass.

The results obtained for the 2nd order reaction show that these values of chlorine concentration are higher than those of the 1st order reaction. In this case, a slower decrease of chlorine concentration occurs in the second-order chlorine reaction, compared to the 1st order reaction case.

Table 2. Variation of chlorine concentration inside the network (1st order reaction)

Number of pipe	*Chlorine concentration (mg/L)*				
	Day 1, (7:00 AM) 7h	***Day 2, (1:00 AM) 25h***	***Day 2, (8:00 PM) 44h***	***Day 3, (3:00 PM) 63h***	***Day 4, (11:00 PM) 95h***
1	0.4855	0.3971	0.4710	0.4263	0.4523
2	0.4631	0.2995	0.4253	0.3778	0.3840
3	0.4430	0.2711	0.3898	0.3654	0.3655
4	0.4124	0.2626	0.3005	0.3413	0.3393
5	0.3709	0.2288	0.1939	0.2994	0.2971
6	0.3345	0.2261	0.1416	0.2819	0.2737
7	0.2299	0.2270	0.1267	0.2486	0.2418
8	0	0.1672	0.1058	0.1801	0.1680
9	0	0.0771	0.1216	0.1046	0.0812
10	0.4361	0.2663	0.3721	0.3583	0.3581
11	0.3924	0.2473	0.2480	0.3212	0.3181
12	0.3463	0.2201	0.1559	0.2882	0.2842
13	0.3193	0.2062	0.1292	0.2727	0.2663
14	0.2298	0.2183	0.1277	0.2536	0.2450
15	0.0018	0.1743	0.1077	0.1910	0.1730
16	0	0.0744	0.0924	0.1008	0.0771
17	0.1069	0.2146	0.1969	0.2373	0.2268
18	0.1417	0.2481	0.1576	0.2716	0.2714
19	0	0.1268	0.1754	0.1733	0.1350
20	0.4847	0.3914	0.4693	0.4241	0.4484
21	0.4470	0.2721	0.3951	0.3612	0.3661
22	0.4293	0.2481	0.3454	0.3371	0.3456
23	0.4092	0.2293	0.3006	0.3204	0.3230
24	0.3669	0.2027	0.1940	0.2847	0.2824
25	0.3254	0.1811	0.1273	0.2576	0.2550
26	0.2935	0.1638	0.1042	0.2375	0.2321
27	0.1192	0.1278	0.0878	0.1930	0.1898
28	0	0.0944	0.0704	0.1430	0.1452
29	0	0.0776	0.0425	0.0780	0.0753

Table 3. Variation of chlorine concentration inside the network (2nd order reaction)

Number of pipe	*Chlorine concentration (mg/L)*				
	Day 1, (7:00 AM) 7h	***Day 2, (1:00 AM) 25h***	***Day 2, (8:00 PM) 44h***	***Day 3, (3:00 PM) 63h***	***Day 4, (11:00 PM) 95h***
1	0.4860	0.4073	0.4736	0.4330	0.4558
2	0.4649	0.3177	0.4303	0.3877	0.3943
3	0.4478	0.2927	0.3977	0.3781	0.3753
4	0.4191	0.2872	0.3160	0.3563	0.3530
5	0.3805	0.2547	0.2169	0.3164	0.3136
6	0.3464	0.2536	0.1662	0.3006	0.2913
7	0.2483	0.2582	0.1521	0.2679	0.2604
8	0	0.1989	0.1319	0.2054	0.1904
9	0	0.1094	0.1627	0.1318	0.1092
10	0.4407	0.2886	0.3814	0.3714	0.3691
11	0.4005	0.2722	0.2668	0.3372	0.3330
12	0.3549	0.2473	0.1805	0.3061	0.3001
13	0.3358	0.2310	0.1552	0.2912	0.2832
14	0.2497	0.2498	0.1543	0.2739	0.2648
15	0.0022	0.2058	0.1336	0.2158	0.1944
16	0	0.1042	0.1261	0.1280	0.1028
17	0.1125	0.2537	0.2405	0.2670	0.2555
18	0.1513	0.2843	0.1914	0.2967	0.2957
19	0	0.1714	0.2288	0.2154	0.1748
20	0.4850	0.4018	0.4711	0.4305	0.4526
21	0.4513	0.2921	0.4030	0.3732	0.3762
22	0.4252	0.2659	0.3531	0.3487	0.3509
23	0.4156	0.2518	0.3144	0.3339	0.3360
24	0.3757	0.2250	0.2138	0.3007	0.2972
25	0.3367	0.2054	0.1498	0.2764	0.2708
26	0.3059	0.1856	0.1253	0.2539	0.2488
27	0.1353	0.1477	0.1073	0.2107	0.2066
28	0	0.1105	0.0874	0.1593	0.1611
29	0	0.0966	0.0543	0.0926	0.0890

In the studied 5 time periods, the obtained results showed small values of the water flow velocity inside pipes, from 0.01 m/s to 0.626 m/s. The minimum self-cleaning velocity according to regulation NP 133-1/2013 must be 0.7 m/s, but in this case, in none of the pipes this value was exceeded. Therefore may negatively affect the qualitative characteristics of water and may result in deposition of sediments inside the pipelines and increase in roughness as well as development of bio-film (Musz-Pomorska et al., 2019).

Generally, we could consider that results obtained for the 2nd order reaction in the volume of fluid are closer to reality compared to final results for the 1st order reaction in the fluid volume (Georgescu and Georgescu, 2013). To efficiently and accurately characterize bulk decay as a property only of the source water, bulk decay parameters must be derived from decay-tests on water sampled post treatment and before secondary chlorination (Fisher et al., 2017).

4. Conclusions

The analysis of the drinking water quality in the studied water supply system shows that, on certain sections of distribution network, the chlorine concentration is not maintained at the values required to ensure a proper disinfection process (i.e. minimum 0.1 mg/L according to design regulation NP 133-1/2013 and minimum 0.25 mg/L at the end of the distribution network according to Law no. 458/2002).

Taking into account the input data it can be said that the decrease of free residual chlorine concentration depends directly on the variation of flow consumed over time. It can be seen that in pipes located close to the tank there were much higher residual chlorine concentrations compared to distant extreme pipes.

If we are to comply with regulations in force, each section should have a minimum diameter of 110 mm in order to be able to mount fire hydrants on them. In this case, the water velocity on certain sections (especially when consumption is zero) is low and the decrease in chlorine concentration becomes more pronounced. If we take into account any possible network extensions, at the present moment, in the network extreme points, the ensured chlorine concentration should have a value of 0.2 mg/L, in order to have continuity in the future pipes that are to be connected.

Finally, it is recommended to increase the chlorine concentration at injection point or to modify the sections geometrical characteristics, in order to improve the water quality for the entire system. It is to be specified that the study was carried out for a future water supply system, so the model calibration could not be carried out and the obtained results are to be considered as only preliminary results.

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