

Operational Paper

Modelling chlorine residuals at Jabal Amman water supply

Abbas Al-Omari, Manar Fayyad and Aseel Al-Nimer

ABSTRACT

The purpose of the study presented in this paper is to test the ability of WaterCad, which simulates chlorine concentrations throughout water supplies, in predicting chlorine concentrations in the Jabal Amman distribution system and hence provide a tool to water supply operators in Jordan that helps them to better manage chlorine concentrations throughout distribution systems. To achieve this goal a sampling programme that aimed at measuring chlorine concentrations throughout Jabal Amman over time was conducted over a 2-year period. Half of the data collected was used for model calibration and the other half was used for model verification. Results showed good agreement between measured and simulated chlorine concentrations.

An important input for WaterCad is bulk chlorine decay coefficient. So, bulk chlorine decay coefficient for Zai Water Treatment Plant effluent, which supplies water to Jabal Amman, was modelled in terms of initial chlorine concentration, total organic carbon and temperature based on laboratory experiments. The developed mathematical model was used to determine bulk chlorine decay coefficient for the conditions of initial chlorine concentration, total organic carbon and temperature observed at the time of sampling, the determined bulk chlorine decay coefficient was then input into WaterCad.

Key words | chlorine decay coefficient, chlorine modelling, chlorine residuals, distribution system, drinking water quality

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INTRODUCTION

Drinking water quality may be within standards as the water leaves the treatment plant. However, it may deteriorate during distribution because of defective distribution systems, long travel times, or physical, chemical and biological transformations that may take place in the distribution system. One important measure of water quality in distribution systems is chlorine residual. Municipalities are required to maintain minimum chlorine residuals throughout distribution systems for disinfection. However, maintaining this residual is a complicated task because of chlorine decay with time and formation of chlorine by-products, such as trihalomethanes, which are suspected carcinogens.

Owing to the complexity of distribution systems, several computer models that simulate the concentration of

different water quality parameters as a result of transport, mixing and growth or decay in these systems have been developed in the last two decades. These include Al-Omari and Chaudhry (2001), Islam and Chaudhry (1998), Rossman (1993), Cohen and Van der drift (1991), Musa (1991), Males *et al.* (1985), Metzger (1985) and Murphy (1985). These models have been extensively used in the United States, Europe and other parts of the world to model water quality variations as a result of mixing of waters from different sources, to predict chlorine residuals and total trihalomethane concentrations in drinking water supplies and to model the propagation of waterborne substances in distribution networks (Liou and Kroon 1987; Clark *et al.* 1993; Rossman *et al.* 1994; Maslia *et al.* 2000).

However, despite the urgent need to implement a model that helps water authorities in Jordan to predict different water quality parameters such as chlorine residual concentrations as the water travels in the distribution system, no steps have been taken towards achieving this goal yet. The objective of the study presented in this paper is to test the ability of WaterCad in predicting chlorine concentrations throughout Jabal Amman distribution system and hence provide an efficient tool to the operators of water supplies in Jordan that helps them to better manage chlorine residuals in distribution systems.

MATERIALS AND METHODS

Bulk chlorine decay

The accuracy of simulated chlorine concentrations throughout distribution systems depends to a high degree on the accuracy of the input data. An important input for WaterCad is bulk chlorine decay coefficient, which is defined as the rate by which chlorine concentration disappears as water travels in the distribution system as a result of chlorine reaction with chlorine-consuming substances that may exist in the bulk water phase. So, the bulk chlorine decay coefficient for Zai Water Treatment Plant effluent, which supplies Jabal Amman, was first modelled based on laboratory experiments. The first step in modelling bulk chlorine decay coefficient is identifying the predictors, so the effect of initial chlorine concentration, total organic carbon, temperature and pH on bulk chlorine decay coefficient was studied at the lab. Bulk chlorine decay was determined for the following initial chlorine concentrations: 1.0, 1.5, 2.0, 2.5, 3.0 mg l⁻¹. Temperatures considered were 10, 15, 20, 25, 30 and 35°C. pH values of 6.5, 7.0, 7.5, 8 and 8.5, which represent the pH range for drinking water, were considered. TOC varied naturally as a result of the variation in the source water; observed TOC values were 0.96, 1.18, 1.43, 1.46, 1.47, 1.55 and 2.09 mg l⁻¹.

Determination of the bulk chlorine decay coefficient is based on first-order reaction kinetics. Bulk chlorine decay is determined by measuring chlorine concentrations over time; a plot of the natural logarithm of chlorine

concentration versus time yields a straight line, the slope of which is the bulk chlorine decay coefficient. There is no standard experimental procedure for the determination of bulk chlorine decay coefficient. So, the procedure outlined by Powell *et al.* (2000) is adopted here.

Chlorine working solutions of 100 mg l⁻¹ chlorine as Cl₂ were freshly prepared by diluting 12–14% sodium hypochlorite solution and were standardized by the iodometric titration method; 100-ml standard solution of free chlorine in the concentration range 0.5–3.0 mg l⁻¹ chlorine as Cl₂ was prepared from about 100 mg l⁻¹ free chlorine solution which was standardized by iodometric titration method. Chlorine concentration was measured by the DPD colorimetric method according to *Standard Methods for the Examination of Water and Wastewater* (1995). pH was adjusted by adding concentrated NaOH or HCl solutions. TOC was determined by UV absorption according to *Standard Methods* (1995).

Sample collection and analysis

In order to compare model simulated chlorine concentrations with actual measurements, a sampling programme of approximately 2 years' duration was conducted. Five to seven samples were collected weekly from different locations at Jabal Amman water supply for the period 17 April 2001 to 4 July 2001 and biweekly for the period 18 July 2001 to 30 January 2002. Another sampling programme started on 27 February 2002 and ended on 23 October 2002; for every sampling event eight samples were collected from two locations at the network over time. Samples were analysed for total chlorine at the site, and for total organic carbon (TOC) at the lab. Temperature and pH of the samples were measured at the site. Chlorine concentration at the reservoir that supplies Jabal Amman was measured for every sampling event. Sample locations were selected on the following bases: distribution of samples over as much of the entire network as possible, availability of a tap that draws water from the network directly (not from roof storage) and easy access.

Total chlorine concentration was determined by titration at the site. TOC was determined by ultraviolet (UV) light absorption according to *Standard Methods*

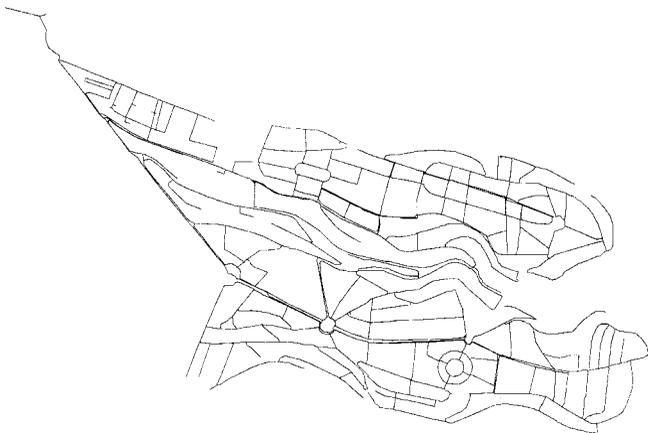


Figure 1 | Jabal Amman network.

(1995). UV absorption was measured at a wavelength of 254 nm.

Running WaterCad

The model used for the purpose of this study is WaterCad, which is a software developed by Haestad Methods (2000) that simulates flow and constituent concentration in water distribution systems. Input data to the model include: (1) pipe characteristics (length, diameter, roughness and chlorine decay coefficient, bulk and wall); (2) node characteristics (elevation and demand); (3) reservoir elevation; and (4) characteristics of any other devices such as pumps, tanks and valves.

A WaterCad file for Jabal Amman was obtained from Lema, which is the company responsible for the operation and maintenance of the Amman water supply system. This network is shown in Figure 1. The original network consists of 4,468 pipes and 5,799 nodes. To make the network manageable, the network was first skeletonized by removing pipes smaller than 100 mm. Skeletonization resulted in reducing the network to about 1,000 pipes and 911 nodes. Nodal elevations were obtained from a digital map. Nodal demands were calculated based on the population density for Jabal Amman, the area around each demand node and per capita use. Bulk chlorine decay coefficient was calculated by Equation (5). Overall chlorine decay

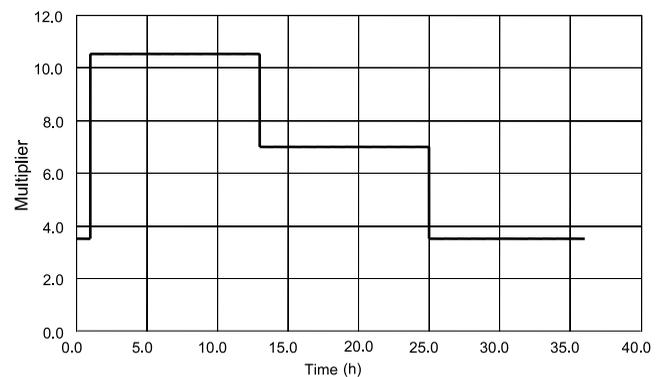


Figure 2 | Demand pattern for nodes close to the reservoir.

coefficient was calculated by WaterCad, by the following equation (Haestad Methods 2000):

$$k = k_b + \frac{k_w + k_f}{R_{Hi}(k_w + k_f)} \quad (1)$$

where k is overall chlorine decay coefficient, time^{-1} ; k_b is bulk chlorine decay coefficient, time^{-1} ; k_w is wall reaction rate constant, $\text{L} \cdot \text{time}^{-1}$; k_f is mass transfer coefficient between bulk flow and pipe wall, $\text{L} \cdot \text{time}^{-1}$; and R_{Hi} is hydraulic radius of pipe i , length. k_w and k_f are calculated by WaterCad. Readers interested in the details of the calculation should refer to Haestad Methods (2000).

Owing to water scarcity in Jordan, water is pumped to consumers for about 36 h a week. Consumers store water in roof storage tanks for use over the week until the next pumping period. It is important to note that samples were collected from the network during this pumping period. The model was also run for the same period when there is flow in the network.

Demand variation over time was estimated based on the assumption that nodes close to the reservoir receive half of their water need during the first 12 h, one-third of their need during the next 12 h and one-sixth of their need during the last 12 h. For nodes in the downstream half of the network, it is assumed that these nodes receive one-sixth of their need during the first 12 h, one-third of their need during the second 12 h and one-half of their need during the last 12 h. These assumptions resulted in the demand patterns shown in Figures 2 and 3. As will be

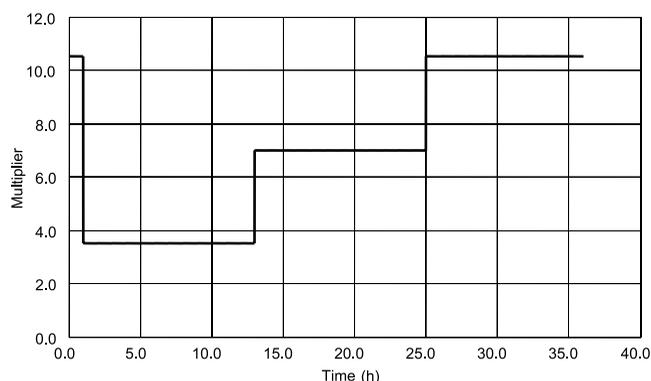


Figure 3 | Demand pattern for nodes far from the reservoir.

seen later, these assumptions resulted in a reasonable agreement between measured and model simulated concentrations.

Model calibration

Before computer models can give reliable results they should first be carefully calibrated. Several researchers have given different definitions of calibration (Eggener and Polkowski 1975; Walski 1983). However, the common thing in all definitions is that calibration means adjustment of model parameters such as Hazen-Williams coefficient of the pipes and/or nodal demands so that the difference between measured and calculated values is minimized for a wide range of boundary and operating conditions. In this study pipe wall decay coefficient and nodal demands were adjusted by trial and error so that the difference between measured and simulated chlorine concentration is minimized. Half of the data (chlorine concentrations) collected in this study was used for model calibration and the other half was used for model verification.

RESULTS AND DISCUSSION

Bulk chlorine decay coefficient

Effect of initial chlorine concentration

Chlorine was added to Zai effluent samples to achieve five different initial concentrations: 1.00, 1.50, 2.00, 2.50 and

Table 1 | Bulk chlorine decay coefficient for different initial chlorine concentrations

Initial chlorine concentration, mg l^{-1}	Bulk decay coefficient, h^{-1}
0.88	0.0554
1.31	0.0394
1.75	0.0306
2.25	0.0258
2.80	0.0225

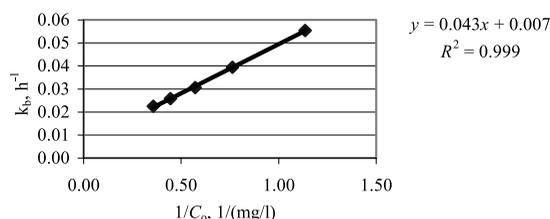


Figure 4 | Relationship between reciprocal of initial chlorine concentration and bulk decay coefficient.

3.00 mg l^{-1} . Samples were incubated in a water bath at 20°C , pH of the samples was kept at 7.5 and TOC of the samples was 1.46 mg l^{-1} . Chlorine decay coefficient was determined for each initial chlorine concentration by plotting the natural logarithm of the concentration versus time. Chlorine decay coefficients for the five initial concentrations are given in Table 1.

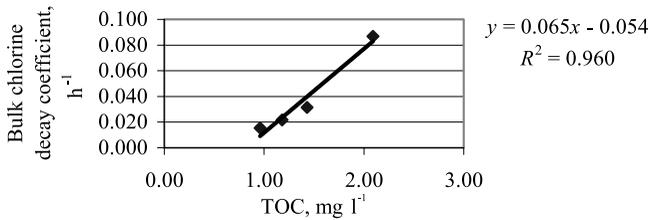
Figure 4 shows the relationship between bulk chlorine decay coefficient and the reciprocal of initial chlorine concentration. The coefficient of determination was found to be 0.999, which shows very strong correlation between $1/C_0$ and the bulk chlorine decay coefficient. This finding agrees with those of Powell *et al.* (1999) and Hau *et al.* (1999).

Effect of total organic carbon content

TOC varied naturally as a result of the natural variation in the source water. Four TOC values were observed: 0.96, 1.18, 1.43 and 2.09 mg l^{-1} . Initial chlorine concentration was adjusted to 2.0 mg l^{-1} for all the samples. Samples

Table 2 | Bulk chlorine decay coefficient for different TOC values

TOC, mg l ⁻¹	Bulk decay coefficient, h ⁻¹
0.96	0.0154
1.18	0.0218
1.43	0.0314
2.09	0.0868

**Figure 5** | Linear relationship between TOC and bulk chlorine decay coefficient.

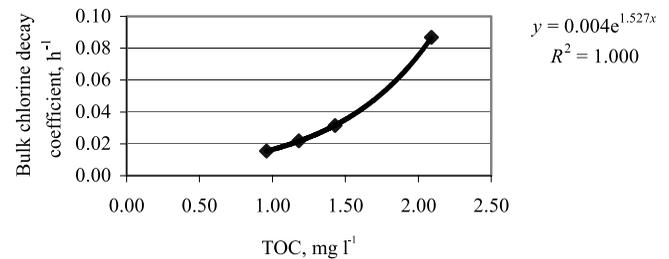
were incubated in a water bath at 20°C, and pH was kept at 7.5.

Chlorine decay coefficients for the four TOC values were determined by plotting the natural logarithm of chlorine concentration versus time. Chlorine decay coefficients are summarized in Table 2.

Two mathematical models were tried to best describe the relationship between TOC and bulk chlorine decay coefficient, a straight line of the general form $y = ax + b$ and a logarithmic model of the form $y = Ae^{-ax}$. The best fits for the two models are shown in Figures 5 and 6, respectively.

Although the logarithmic model has a higher coefficient of determination than the straight line model, the straight line model has a coefficient of determination of 0.96, which is also high. However, the problem with the straight line model is that it does not pass through the origin; in other words, at a TOC value of zero, the model predicts k_b of 0.054 h⁻¹ which is high and may not be attributed to experimental error.

To overcome this, Powell *et al.* (1999) proposed the following model to describe the relationship between k_b and TOC:

**Figure 6** | Logarithmic relationship between TOC and bulk chlorine decay coefficient.

$$k_b = e(\text{TOC} - f) \quad (2)$$

The logarithmic model shown in Figure 6 predicts a k_b value of 0.0036 h⁻¹ at a TOC value of zero, which is small and may be attributed to experimental error, in addition to the fact that the logarithmic model has a higher coefficient of determination. The logarithmic model is adopted in this study.

Effect of temperature

The chlorine decay coefficient was determined for the following temperatures: 10, 15, 20, 25, 30 and 35°C. All samples were chlorinated to 2.00 mg l⁻¹, TOC was 1.55 mg l⁻¹ and pH was kept at 7.5. Chlorine decay coefficients for these temperatures obtained by plotting chlorine concentrations versus time are given in Table 3.

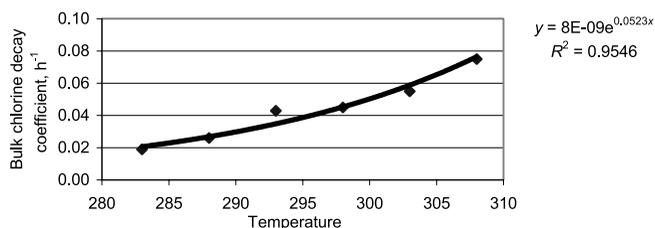
The best model that describes the dependency of bulk chlorine decay coefficient on temperature is found to be exponential, which is shown in Figure 7. This finding is in agreement with that reported in the literature. The constant 0.0523 corresponds to E/RT in the well-known Arrhenius equation multiplied by $1/T$. This model predicts a 1.7-fold increase in k_b as temperature increases from 10 to 20°C.

Effect of pH

Chlorine decay coefficients were determined for five pH values: 6.5, 7.0, 7.5, 8.0 and 8.5, which represent pH values for drinking water. All samples were chlorinated to 2.00 mg l⁻¹, water bath temperature was kept constant at

Table 3 | Bulk chlorine decay coefficient for different temperatures

Temperature, °C	Bulk decay constant, h ⁻¹
10	0.0192
15	0.0257
20	0.0426
25	0.0451
30	0.0546
35	0.0752

**Figure 7** | Relationship between bulk chlorine decay coefficient and temperature.**Table 4** | Bulk chlorine decay coefficient for different pH values

pH	Bulk decay coefficient, h ⁻¹
6.5	0.0339
7.0	0.0336
7.5	0.0342
8.0	0.0345
8.5	0.0339

20°C, TOC of the samples was 1.47 mg l⁻¹. Chlorine decay coefficient was determined for every pH by plotting the natural logarithm of chlorine concentration versus time. The k_b values determined are given in Table 4. Table 4 shows that differences in k_b values for the different pH values considered in this study occur at the fourth digit. These differences may be neglected for two reasons: first,

these differences are within the experimental error; second, k_b value up to three digits is accurate enough for all practical purposes. So, for the range of variables considered in this study, pH effect on k_b was found to be insignificant, which is in agreement with the findings of Powell *et al.* (1999) who considered a pH range of 6.8 to 9.1.

Mathematical modelling of bulk chlorine decay coefficient

A mathematical model that describes the behaviour of bulk chlorine decay coefficient was developed using Minitab software, which performs multiple regression analysis. The model considers initial chlorine concentration, TOC and temperature as predictors. A plot of the best fit for observed and model calculated chlorine decay coefficients was made. The slope of the straight line indicates the degree of agreement between observed and calculated k_b values, the closer the slope to one the higher the agreement between observed and calculated values. The model assumes the following relationship between bulk chlorine decay coefficient and the predictors:

$$k_b = AC_0^a \cdot Be^b \cdot \text{TOC} \cdot Ce^{c/T} \quad (3)$$

where A, B, C, b, and c are constants. The above equation can be rewritten as:

$$k_b = DC_0^a \cdot e^{b \cdot \text{TOC}} \cdot e^{c/T} \quad (4)$$

where D is constant. Multiple regression analysis was performed to determine the constants in Equation (4): $D = 41,233 \text{ (mg l}^{-1}\text{)}^{-1} \text{ h}^{-1}$, $a = -0.76$, $b = 1.388 \text{ (mg l}^{-1}\text{)}^{-1}$, and $c = 4590.5 \text{ K}$. Substituting these values into Equation (4) yields the following equation:

$$k_b = 41233 C_0^{-0.76} e^{1.388 \text{ TOC}} e^{-4590.5/T} \quad (5)$$

Figure 8 shows the best fit between observed and calculated k_b values. The coefficient of determination of the best fit between observed and model calculated k_b values is 0.99 and the slope of the straight line is 0.98, which

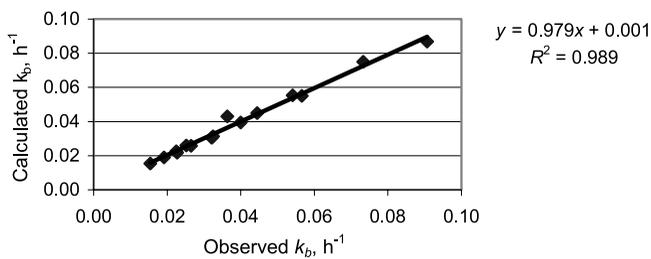


Figure 8 | Calculated versus observed k_b values.

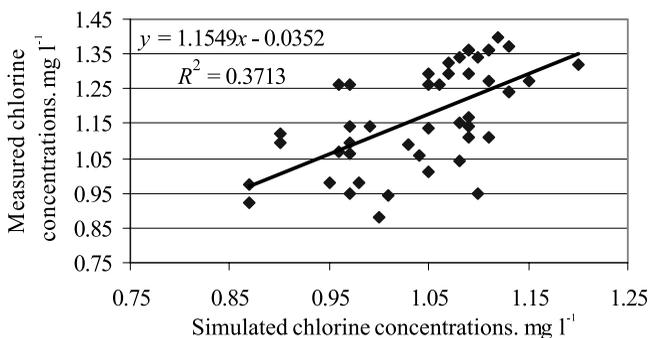


Figure 9 | Simulated versus measured chlorine concentrations for Jabal Amman network before calibration.

means high agreement between observed and calculated k_b values.

Chlorine concentrations at Jabal Amman network

WaterCad was run to determine chlorine concentrations throughout the Jabal Amman network. As mentioned above, half of the chlorine concentrations collected during sampling was used for model calibration, the other half was used for model verification. Figure 9 shows a comparison between measured and simulated chlorine concentrations for the second set of data before calibration, and Figure 10 shows simulated versus measured chlorine concentrations for the second set of data after calibration. The slope of the straight line, which shows the agreement between simulated and measured chlorine concentrations, is 1.15 for Figure 9 and 0.89 for Figure 10, which means that model calibration improved the agreement between simulated and measured chlorine concentrations. The

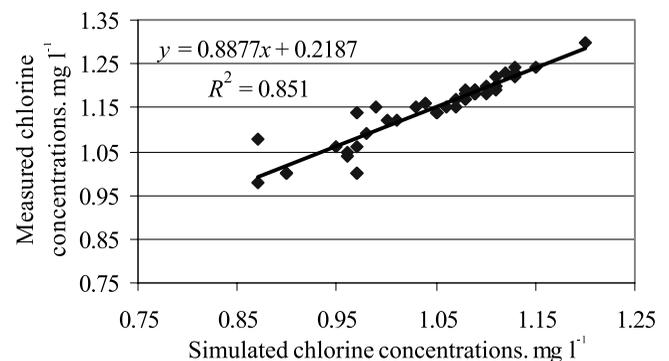


Figure 10 | Simulated versus measured chlorine concentrations for Jabal Amman network after calibration.

coefficient of determination (R^2) improved from 0.37 to 0.85 as a result of model calibration.

CONCLUSIONS

Chlorine concentrations throughout Jabal Amman water supply were simulated by WaterCad and compared with actual measurements. In order to run WaterCad, the bulk chlorine decay coefficient for Zai Water Treatment Plant effluent, which supplies the Jabal Amman network, was modelled in terms of initial chlorine concentration, total organic carbon and temperature. Laboratory experiments showed that initial chlorine concentration, total organic carbon and temperature are the important predictors in modelling bulk chlorine decay coefficient. pH was eliminated as a predictor as it was found to be insignificant for the range used in this study.

In order to test the ability of the model to predict chlorine concentrations throughout the Jabal Amman network, a sampling programme was conducted over a period of approximately 2 years. Water samples were taken at different locations and times from the Jabal Amman water supply and tested for chlorine residuals among other parameters. Results showed good agreement between simulated and measured chlorine concentrations for the Jabal Amman water supply, which means that WaterCad can be

used as a reliable tool for predicting chlorine concentrations throughout networks. The results also showed that model calibration improved agreement between measured and simulated chlorine concentrations significantly.

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SYMBOLS AND ABBREVIATIONS

A, B, C	constants
a	constant (mass/volume) $^{-1}$ time $^{-1}$
b	constant, °C
C _o	initial chlorine concentration, mass/volume
E	activation energy, J mol $^{-1}$
k	overall chlorine decay coefficient, time $^{-1}$
k _b	bulk chlorine decay coefficient, time $^{-1}$
k _f	mass transfer coefficient between bulk flow and pipe wall, L · time $^{-1}$
k _w	wall reaction rate constant, L · time $^{-1}$
R	universal gas constant, J k · mol $^{-1}$
R ²	coefficient of determination
R _H	hydraulic radius, L
T	temperature, °C
TOC	total organic carbon, mass/volume

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