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Detection of Pipes Decreasing Residual Chlorine Via Wall Reaction Coefficient in Water Distribution Networks

Su Dağıtım Şebekelerinde Bakiye Kloru Azaltan Boruların Cidar Reaksiyon Katsayısına Bağlı Olarak Tespit Edilmesi

Miraç Eryiğit

Bolu Abant Izzet Baysal University, Faculty of Engineering, Department of Environmental Engineering, Bolu, Türkiye

Abstract

This paper intended to build an optimization model utilizing the modified clonal selection algorithm (one of the famous heuristic optimization techniques) to detect pipes which reduces a residual chlorine in the water distribution networks (WDNs). MATLAB programming language was used to code the model linked with EPANET. The model performance was evaluated in a two-loop hypothetical WDN under steady-state flow conditions. In nodes of this hypothetical WDN, free chlorine concentrations were assumed to be measured since an objective function depends on model calibration. Pipes decreasing residual chlorine concentrations were determined by running the model which minimizes a total of concentration differences between estimated and measured free chlorine in each node. In order to find these pipes, pipe wall reaction rate coefficients were utilized. The model was run 10 times to obtain average reaction rate coefficient of each pipe in the WDN. After 10 runs, mean estimated and actual/real reaction rate coefficient values were almost equal (R2=0.99). The optimization model appeared to be viable for detecting pipes causing a residual chlorine loss in the WDN.

Keywords: Artificial immune systems, model calibration, pipe wall reaction coefficient, residual chlorine, water distribution network.

Öz

Bu çalışmada, su dağıtım şebekelerindeki bakiye kloru azaltan boruların tespit edilmesi için modifiye klonal seçim algoritması (çok bilinen sezgisel optimizasyon tekniklerinden biri) kullanan bir optimizasyon modeli inşa edilmesi amaçlanmıştır. Model, EPANET ile bağlantılı olarak MATLAB yazılım dilinde kodlanmıştır. Modelin performansı, kararlı/sabit akım koşulları altında iki gözlü farazi bir su dağıtım şebekesinde değerlendirilmiştir. Amaç fonksiyonu, model kalibrasyonuna dayalı olduğu için şebekenin düğüm noktalarında serbest klor konsantrasyonlarının ölçüldüğü kabul edilmiştir. Bakiye klor konsantrasyonlarını azaltan borular, her bir düğüm noktasındaki ölçülen ve tahmin edilen serbest klor konsantrasyonları arasındaki farkların toplamının minimize edilmesine bağlı olarak model tarafından belirlenmiştir. Boruların belirlenmesi için boru cidarı reaksiyon hız katsayılarından yararlanılmıştır. Model 10 kez çalıştırılarak su dağıtım şebekesindeki her bir borunun ortalama reaksiyon hız katsayıları elde edilmiştir. Model 10 kez çalıştırıldıktan sonra, ortalama tahmin ve gerçek reaksiyon hız katsayı değerlerinin hemen hemen aynı olduğu sonucuna varılmıştır (R2=0.99). Su dağıtım şebekesindeki bakiye klor kaybına neden olan boruların tespit edilmesi için optimizasyon modelinin uygulanabilir olduğu görülmüştür.

Anahtar Kelimeler: Yapay bağışıklık sistemleri, model kalibrasyonu, boru cidar reaksiyon katsayısı, bakiye klor, su dağıtım şebekesi.

1. Introduction

The chlorine used to disinfect drinking and domestic water is a vital and critical chemical in terms of the public health. Water should be supplied and distributed as disinfected from water tanks/reservoirs to settlements/residences/cities by water distribution networks (WDN). But the chlorination should be appropriately applied to avoid toxic effects of the chlorine. The total residual chlorine consists of free chlorine (hypochlorite ion/OCl- and hypochlorous acid/HOCl) (more oxidizing/more powerful disinfectant) and chloramines (more stable and long-lived/durable) remained after a certain residence time of water, and it should be

*Corresponding author: miraceryigit@hotmail.com

Miraç Eryiğit orcid.org/0000-0002-7035-7078

provided as desired concentrations (e.g., 0.3-0.5 mg/l free chlorine) in the nodes of the WDNs (see Askenaizer 2003, Oğur et al. 2004 for the chemical reactions). The guidelines of World Health Organization (WHO) on water quality suggests limit concentrations of residual chlorine (as free chlorine) in the drinking water to the range 0.2–5 mg/l (WHO 2022). As well as free chlorine decay due to reactions with natural organic matters in the bulk flow over time, the metal pipes of the WDNs are corroded over time and cause to reduce the concentration of the residual chlorine since free chlorine oxidizes iron (Fe) released from pipe wall corrosion or pipe wall reactions/decay with biofilm (Rossman 2000, Han et al. 2017, Fisher et al. 2017a, Xu et al. 2018). Therefore, both health risk occurs and costs increase due to extreme chlorine consumption.

In the literature, there are many studies regarding residual chlorine modelling in the WDNs (Onyutha and Kwio-Tamale 2022, Elsherif et al. 2023, Hossain et al. 2022, Ardila et al. 2023). Rossman et al. (1994) improved a mass-transfer-based model which considers first-order reactions of chlorine to occur both in the bulk flow and at the pipe wall for predicting chlorine decay in the WDNs. Islam et al. (1997) proposed a new computer model using an inverse method to model chlorine concentration in the pipe networks. Rodriguez and Sérodes (1998) applied two empirical models to simulate and predict residual chlorine concentrations in the urban water systems. Li et al. (2003) built a model of residual chlorine decay in the WDN considering a chlorine consumption in reactions with chemicals in a bulk water, in corrosion process, bio-films occuring on a pipe wall, and the chlorine mass transport from a bulk water to a pipe wall. Gibbs et al. (2006) used different data-driven techniques (artificial neural networks and linear regression model) to predict concentrations of chlorine in the Hope Valley WDN (South Australia). Helbling and VanBriesen (2009) performed modeling residual chlorine related to a microbial contamination in the WDNs. Monteiro et al. (2014) carried out a chlorine decay modelling in drinking water supply systems by using EPANET MSX. Kim et al. (2014) investigated the relationship between a temporal variation in a chlorine concentration and hydraulic conditions for a pilot scale WDN (Similarly, Kim et al., 2015). Blokker et al. (2014) predicted residual chlorine concentrations in WDN under the effect of stochastic water demands. Chelsea (2016) modelled residual chlorine and trihalomethanes using EPANET for the City of Akron's WDN (Ohio, US). Fisher et al. (2017b) implemented a bulk chlorine decay model (the augmented two-reactant (2RA) model) for simulating residuals in the WDNs. Monteiro et al. (2020) modelled pipe wall decay of chlorine residuals in a full-scale water supply system using the traditional first-order and EXPBIO models. García-Ávila et al. (2021) proposed a model of residual chlorine decay to forecast chlorine concentration levels in a real WDN during the COVID-19 pandemic. Fisher et al. (2021) modelled residual chlorine and trihalomethane profiles in the WDNs after pre-chlorination of the water treatment plant. Absalan et al. (2022) performed predictions of chlorine and trihalomethanes in the WDN in southern Quebec (Canada). Abhijith and Ostfeld (2022) developed a novel computer-based tool (EPANET-C) to simulate variations in residual chlorine concentrations in the WDNs. Wu and Dorea (2022) applied basic chlorine decay kinetic models in the literature for humanitarian emergency water supply. Yimer et al. (2022) conducted modelling of residual chlorine in the Arada sub-city supply system (Addis Ababa water supply distribution systems, Ethiopia) by using Water CAD. Onyutha (2022) predicted residual chlorine concentrations in drinking water using machine and deep learning techniques. Wang (2022) optimized the chlorine injection mass to maintain chlorine in the WDN by using a fuzzy chance-constrained optimization model. Huang and Wang (2023) developed a double-sided fuzziness chance-constrained programming model to cut down costs of the disinfectant booster under uncertainty. Kyritsakas et al. (2023) designed a data-driven model that uses different machine learning algorithms for the prediction of chlorine losses in water distribution trunk mains. Wang et al. (2023) proposed an improved VRC-3R- residual chlorine decay model in the UV/Cl2 process in the WDN. Wongpeerak et al. (2023) applied a novel method based on a simple theoretical analysis (theoretical disinfectant mass loss models) to simulate residual chlorine concentrations in the real WDNs in Thailand. Enriquez et al. (2023) estimated chlorine and trihalomethanes concentrations in the trunk network of Bogota's WDN (Colombia) by using evolutionary polynomial regression models and artificial neural networks. Belcaid et al. (2023) presented a new methodology for chlorine decay modeling in the WDN of Mohammedia City (Morocco). Helm et al. (2024) implemented machine learning models by developing a gradient-boosting method to forecast a free chlorine residual in a drinking water treatment plant (Georgia, U.S.). Li et al. (2024) improved a novel gated graph neural network model/approach for a chlorine prediction in nodes of a real WDN (Yantian WDN, China).

These studies generally focused on modelling of residual chlorine concentrations (not detecting pipes which decrease the concentrations). By considering this gap in this broad literature, this study aimed to develop a heuristic optimization model based on model calibration to detect pipes which reduce residual chlorine concentrations (as free chlorine) in nodes of the WDNs (considering pipe wall reaction coefficients).

2. Material and Methods

2.1. Algorithm

The heuristic optimization model was coded by linking with EPANET software in MATLAB programming language. EPANET, a commonly known WDN simulation software, was chosen for the hydraulic calculations since it is simple and efficient (also, it can be linked with MATLAB). It was developed as a tool for understanding the movement and fate of drinking water constituents within WDNs and can be used for many different applications in distribution systems analysis (Rossman 2000). As for MATLAB, it is a programming and numeric computing platform used by engineers and scientists to analyze data, develop/improve algorithms, and build models.

The model uses the modified clonal selection algorithm (modified Clonalg) (one of the artificial immune systems) developed by Eryiğit (2015) as a heuristic optimization method. (See Figure 1). This algorithm mimics the clonal selection theory of the natural immune system. In Figure 1, Ab is the antibody population randomly created, f is the antibody's antigenic affinity (representing an objective function), C is the cloned antibody population, C* is the mutated antibody population. The algorithm process can be briefly defined as follows (Eryiğit 2015, Eryiğit and Sulaiman 2022):

1) An antibody set/population (Ab) is randomly generated.
2) An objective function (f) is computed to be minimized or maximized (optimization) for each individual in Ab.
3) All individuals are cloned/copied.
4) All antibody clones (C) are exposed to the maturation (mutation) process which is inversely proportional to their antigenic affinities. Besides, new antibody genes are generated for the clones in this step.
5) An objective function (f) is recalculated for each matured clone in C*.
6) The matured/mutated clones owning the highest affinity (best individuals) are chosen to replace the antibodies which own the lowest affinity in Ab.

This loop goes on until the iteration reaches a maximum number (or a certain error/difference between worst and best individuals in Ab). Hence, the optimum result can be obtained.

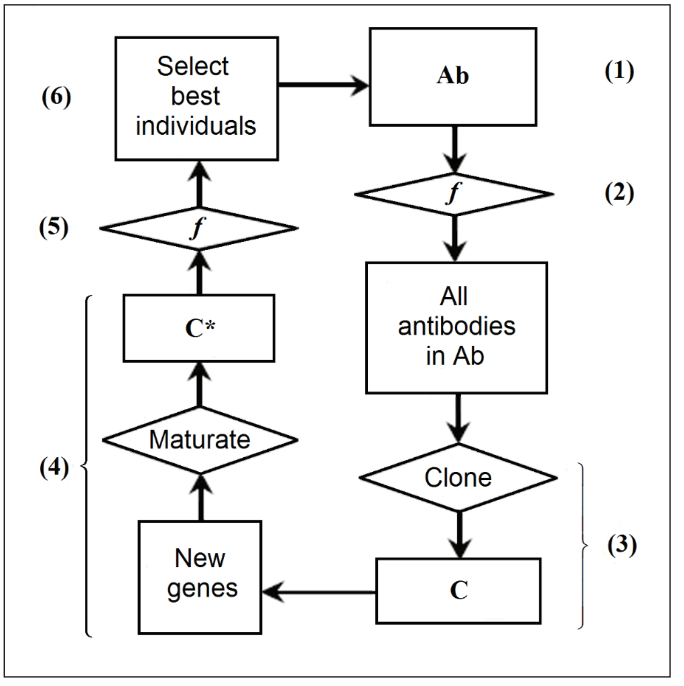

Figure 1. The flow diagram of the modified Clonalg (Eryiğit 2015).

In the modified Clonalg (step 4), new genes are produced for each antibody clone by taking in consideration a certain probability which is referred to "probability rate" (PR) depending on an optimization problem. The antibody clone number can be computed as below (De Castro and Von Zuben 2002):

$$N_c = \sum_{i=1}^{N_{Ab}} round(\beta \cdot N_{Ab}) \qquad i = 1, \cdots N_{Ab} \tag{1}$$

where N_c is the total clone number, β is the coefficient of multiplying, and "round" is a rounding operator for the integer.

A mutation rate can be obtained as the following (De Castro and Von Zuben 2002):

$$\alpha_i = \exp(-\rho \cdot f_i) \tag{2}$$

where α_i is the mutation rate, ρ is the coefficient of decay, and f_i is a value of the antigenic affinity (value of the objective function) normalized between 0 and 1.

Population Ab is defined as shown below:

$$\begin{bmatrix} Ab_1 & = x_{11}\cdots & & \cdots x_{1nd} \\ \vdots & \vdots & x_{1j} & \vdots \\ Ab_i & = x_{i1} & & x_{ind} \\ \vdots & \vdots & \ddots & \vdots \\ Ab_{N_{Ab}} & = x_{N_{Ab}1}\cdots & x_{N_{Ab}nd} & \cdots x_{N_{Ab}nd} \end{bmatrix} \rightarrow \begin{bmatrix} f_1 \\ \vdots \\ f_i \\ \vdots \\ f_{N_{Ab}} \end{bmatrix} \quad (3)$$

$i = 1, \cdots N_{Ab} \quad j = 1, \cdots nd$

where N_{Ab} is the total antibody number (population Ab), x_{ij} is the gene of Ab_i (decision variable of f_i), nd is the gene number of Ab_i. In this study, x_{ij} corresponds to the wall reaction rate coefficient (K_w) of each pipe in the WDN. f was minimized depending on pipe wall reaction coefficients (genes) produced and mutated/matured through the algorithm processes. The objective function (f) is based on model calibration in the study:

$$minimize \sum_{i=1}^{NRC} 10^3 \left| RC_{ipred} - RC_{iobs} \right| \quad (4)$$

where RC_{ipred} is the i-th predicted residual chlorine, RC_{iobs} is the i-th observed residual chlorine, NRC is the number of observed residual chlorine values in nodes of the WDN.

2.2. Implementation

The optimization model was applied to a two-loop hypothetical WDN consisting of 6 nodes (junctions), 8 pipes and one reservoir under steady-state gravity flow conditions in EPANET (See Figure 2). The data of the WDN was given in Table 1. This scenario includes some assumptions as follows:

1) Free chlorine concentrations are assumed to be measured in the WDN nodes in each hour for 24 hours.
2) Bulk reaction coefficient (K_b) in the WDN is assumed as -0.01/day (most of the chlorine decay in the network is occurring in the reservoir and residual chlorine concentration is 1 mg/l).
3) Pipe corrosion and biofilm are dominant in the system because of pipe age and material.
4) All pipe wall reaction coefficients in the WDN are unknown.

The residual chlorine concentrations (as free chlorine) measured in the nodes after 24 hours and pipe wall reaction coefficients (K_w) are shown in Figure 2. First-order (n=1) reactions/decay kinetics ($R = K_b \cdot C^n$ and $R = (A/V) \cdot K_w \cdot C^n$ for bulk and wall reactions (R), respectively. A/V: The surface area per unit volume within a pipe, C: The reactant concentration) were used for the chlorine, and lower and upper limits for pipe wall reaction coefficient were assigned as -1.5 and 0 m/day, respectively (Rossman 2000, Rossman et al. 2020). The optimization model reaches a global minimum (f) by assigning coefficient values in this range [-1.5, 0] to the pipes of the WDN during the iteration.

The analyses were carried out by using a computer with Intel Core I5-8300H CPU 2.3 GHz, and the model was run 10 times with maximum iteration number (I_{max}) of 1000 for examining a model stability. In this study, N_{Ab}, β, ρ, and PR were assigned as 30, 1, 0.5, and 0.2, respectively.

3. Results and Discussion

There are 8 pipes in the WDN. Their wall reaction coefficients are assumed to be unknown. As it is seen in Figure 2, Pipe 1, 3, 5 and 8 (red lines with -1.5 m/day) cause a higher loss of residual chlorine concentration while

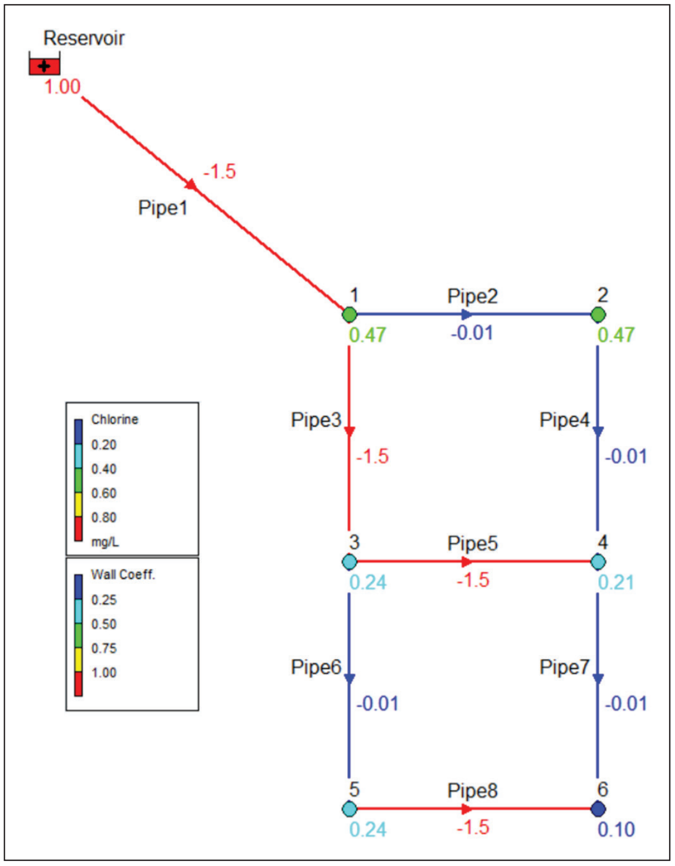

Figure 2. Layout and operational data of the two-loop hypothetical WDN.

Table 1. The main characteristics of the two-loop hypothetical WDN.

Node	Elevation (m)	Base Demand (l/s)	Pipe	Length (m)	Diameter (mm)	C_p
Reservoir	150	-	1	5000	450	130
1	80	20	2	3000	250	140
2	70	20	3	3000	300	130
3	70	20	4	3000	150	140
4	60	20	5	3000	200	130
5	60	20	6	3000	250	140
6	60	20	7	3000	150	140
			8	3000	150	130

Table 2. Results of predicted wall reaction coefficient for each pipe in the WDN after 10 runs.

Run No	f	Pipe 1 (m/day)	Pipe 2 (m/day)	Pipe 3 (m/day)	Pipe 4 (m/day)	Pipe 5 (m/day)	Pipe 6 (m/day)	Pipe 7 (m/day)	Pipe 8 (m/day)	Run Time (min)
1	0.34	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.02	-1.5	38.3
2	0.21	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.02	-1.5	38.7
3	0.30	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.02	-1.5	39.0
4	0.27	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.01	-1.5	38.8
5	0.27	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.01	-1.5	38.4
6	0.80	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.13	-1.01	38.4
7	0.15	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.01	-1.5	38.5
8	0.37	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.01	-1.5	38.5
9	0.24	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.01	-1.5	38.4
10	0.31	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.01	-1.5	38.3
Mean	0.32	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.02	-1.45	38.5
Std	0.180	0	0.0004	0	0.001	0	0.0004	0.037	0.154	0.23
Min	0.15	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.13	-1.5	38.3
Max	0.80	-1.5	-0.01	-1.5	-0.01	-1.5	-0.01	-0.01	-1.01	39.0

Pipe 2, 4, 6 and 7 (blue lines with -0.01 m/day) cause a lower loss in the WDN. After the model was run 10 times, results obtained in each run were given in Table 2. Also, the comparison of mean predicted coefficients and actual pipe wall coefficients was shown in Table 3 and Figure 3. As it is seen in Table 2, the model was able to determine accurately wall reaction coefficients of all pipes in all runs except run 6 (ratio of 9/10 runs). This demonstrates that the optimization model is stable. Mean predicted and actual values are almost equal each other (R^2=0.99) (See Table 3 and Figure 3). Consequently, the pipes reducing residual chlorine concentrations in the WDN were successfully detected by the model (Pipe corrosion and biofilm are assumed to be dominant in the network). By detecting these pipes, it can be said that we also specify the old/worn

Table 3. A comparison of mean predicted and actual pipe wall reaction coefficients.

Pipe	*Mean Predicted Coefficient (m/day)	Actual Coefficient (m/day)
1	-1.5	-1.5
2	-0.01	-0.01
3	-1.5	-1.5
4	-0.01	-0.01
5	-1.5	-1.5
6	-0.01	-0.01
7	-0.02	-0.01
8	-1.45	-1.5

*Average of 10 runs

out pipes (especially corroded metal pipes) which may cause pressure losses in the WDN because a higher Darcy-Weisbach roughness coefficient or a lower Hazen-Williams C-factor results in a greater frictional head loss in a flow along the pipe (Rossman 2000). The pipe wall reaction coefficient (K_w) can be assigned as the function of the roughness coefficient for each pipe in EPANET. For this, site-specific field measurements should be performed. In this study, Hazen-Williams C-factors (C_p) for the frictional head loss were selected independently from the pipe wall reaction coefficients (K_w) because the hypothetical WDN was applied.

On the other hand, the optimization model can detect the pipes which decrease residual chlorine with mean run time of 38.5 minutes. Run time depends on iteration number (or error/difference between minimum and maximum affinity values of antibodies in the population) and population number as well as the algorithm structure. Better results (ratio of 10/10 runs) might be obtained by increasing population and iteration numbers (or assigning lower error value). But, this makes the run time longer. So, N_{Ab} of 30 and I_{max} of 1000 were enough to obtain acceptable/satisfying results during the analyses.

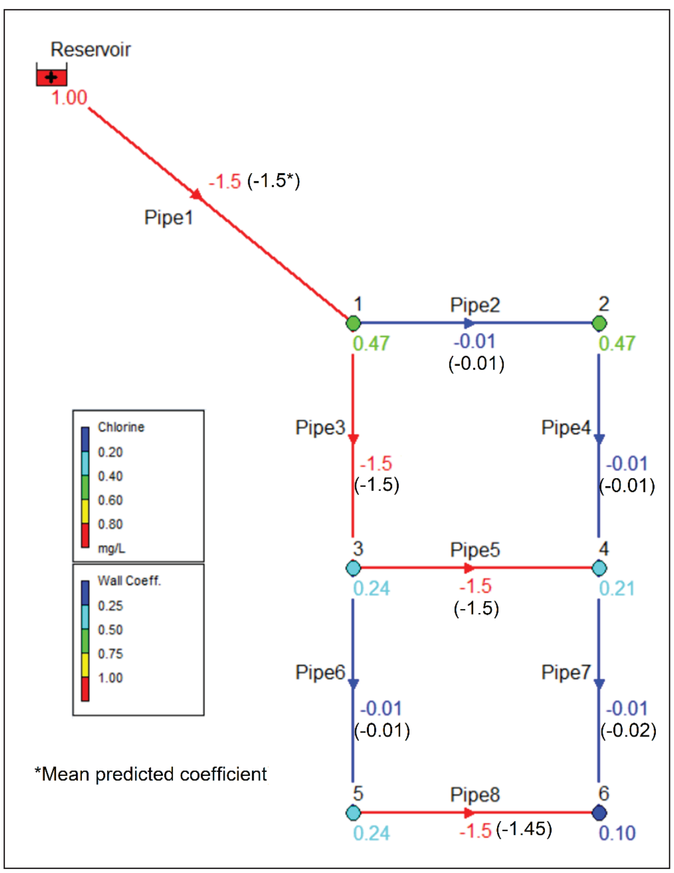

Figure 3. Mean predicted and actual pipe wall reaction coefficients (m/day).

The optimization model obtained good results under steady-state flow conditions. Of course, flows are not steady/constant in real WDNs. However, dynamic flow conditions could be neglectable for this study because the bulk flow reaction was assumed to be too low (-0.01/day) in the WDN (most of the chlorine decay is occurring in the reservoir) according to the scenario.

In the related literature, mostly residual chlorine concentrations have been modeled in the WDNs. The present study differs from the others because pipes reducing the chlorine concentrations were detected instead of modelling the concentrations in the WDNs. Thus, it can be said the paper is the first optimization study based on K_w in terms of the detection of the pipes decreasing the residual concentrations. While reviewing the literature, it is seen that average K_w value of -0.066 m/day was (coincides with the range [-1.5, 0]) experimentally determined by García-Ávila et al. (2021). But experimental methods could be expensive and time-consuming. Zaghini et. al. (2024) assumed an overall rate coefficient K (1/time) combining K_b and K_w due to the difficulties of the accurate estimation of individual K_b and K_w decay contributions. They obtained K values between -0.4 and -1.1 (1/day) for the multiple-source WDNs. But K_w values were uncertain since they were included in the overall rate coefficients. Therefore, the pipes reducing the chlorine concentrations were unknown.

4. Conclusion and Suggestions

The worn-out pipes in the water supply have a risk to the public health due to corrosion and biofilm (pathogens etc.) and increase the costs of the chlorination. These pipes should be detected and renewed as quickly as possible. For this problem, the optimization model could be utilized. In this study, wall reaction coefficients (K_w) of the pipes in the WDN were determined by utilizing the model calibration. Thus, the pipes reducing residual chlorine concentrations were able to be detected by the optimization model considering their reaction coefficients (since pipe corrosion and biofilm are dominant in the present WDN). This also indicates that these pipes are old (especially corroded pipes) and decrease pressure heads desired in the nodes of the WDN. Consequently, the model is useful to detect pipes which decrease both residual chlorine concentrations and pressures by measuring only free chlorine in the nodes of the

WDN in case of domination/dominance of corrosion and biofilm. K_w coefficients could be assigned as the function of the roughness coefficient/C-factors (C_p) for each pipe of the real WDN to show relationship between the pipes causing the frictional head losses and chlorine losses in the future studies.

The optimization model was run under steady-state flow conditions. Therefore, it might need to be tested under non-steady state flow conditions in real WDNs in the future studies. However, this study is a pioneer in terms of detection of pipes resulting in chlorine losses in the WDN and inspires the researchers about this subject.

Author contribution: The entire study was performed by the author.

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