Effect of Dividing the Water Transmission Pipe Line in Modeling Residual Chlorine, Case Study: Isfahan Water Transmission Line

Yasaman Frozandeh
University of Isfahan
Ali Dehnavi (a.dehnavi@eng.ui.ac.ir)
University of Isfahan https://orcid.org/0000-0001-5036-8805
Ahmad Shanehsazzadeh
University of Isfahan

Research

Keywords: drinking water quality, chlorine residual, coefficients of chlorine decay, decay kinetic models, EPANET-MSX

Posted Date: February 22nd, 2021

DOI: https://doi.org/10.21203/rs.3.rs-214682/v1

Effect of dividing the water transmission pipe line in modeling residual chlorine, case study: Isfahan water transmission line

Yasaman Frozandeh[1], Ali Dehnavi[2,*], Ahmad Shanehsazzadeh[3]

[1]Department of Civil Engineering, University of Isfahan, Iran.

Yac.frz72@gmail.com

[2]Department of Civil Engineering, University of Isfahan, Iran.

a.dehnavi@eng.ui.ac.ir

[3]Department of Civil Engineering, University of Isfahan, Iran

a.shanehsazzadeh@eng.ui.ac.ir

* Correspondence: a.dehnavi@eng.ui.ac.ir

Abstract

In assessing the quality of drinking water in transmission and distribution lines, the study on chlorine reactions is of particular importance. Chlorine decay happens in bulk and wall and it is mainly affected by the water age which depends on the transmission line length. Residual chlorine concentration in Isfahan water transmission line (IWTL) is simulated through three decay models, namely the first order, parallel first order and second order single reactant (SR model) which incorporated in EPANET and EPANET MSX, respectively. The results of the models are compared through two approaches, one is the one-part approach (OPA) whereby chlorine decay simulation is performed taking into account the whole line as one section and the second is multi-part approach (MPA) whereby the line is divided into two sections and decay coefficients of chlorine for each section are separately determined. Results show that in the OPA, the SR model in summer and the parallel model in winter are the best kinetic models. While in the MPA, the results of first order model has the same order of accuracy as the more complex models of parallel and SR models.

In general, the simple first order model in the MPA applied by EPANET2.0 s/w provides acceptable level of accuracy in compare to the complex models applied in

EPANET MSX s/w. The average RMSE volumes are reduced from 0.078 in OPA to 0.029 in MPA in summer and from 0.059 to 0.015 in winter, indicating that the dividing the line in simulation procedure and considering the individual decay coefficient for each part, considerably improves the results, more effectively than the application of advanced decay models.

Keywords: drinking water quality, chlorine residual, coefficients of chlorine decay, decay kinetic models, EPANET-MSX.

1. Introduction

In the design and operation of drinking water distribution systems, the quality of the water is one of the most important concern. Different methods of disinfection is applied to preserve water quality [1–3]. The main reasons to disinfect the drinking water is due to pathogenic microorganisms entering through the drinking water distribution system [4,5]. The residual amount of the disinfectant during storage and distribution of drinking water is the most important factor to select the kind of disinfectant. Chlorine is the most common disinfectant in water supply systems due to its residual preservation, effective performance and economical aspect [4,6]. Chlorine decays along pipes and in storage reservoirs in water content and pipe walls. The reactions of chlorine with organic and inorganic substances in the volume of water is called bulk decay, while the reactions with biofilms and materials on the wall of the pipes and reservoirs is called wall decay [1,2,7]. The bulk decay reactions depend on chemicals and microbiological quality and water age. The water age is the time which takes for a parcel of water to travel from water treatment plant to a node in a the line or in the network [8]. The wall decay reactions are affected by characteristics of the pipes and reservoirs[7,9–11]. These reactions reduce concentration of chlorine. Thus, the risk of microbial contamination increases and more chlorine should be injected to maintain the minimum chlorine content. Increasing chlorine concentration in the water supply accelerates pipe corrosion, changes the water taste and odor and increases disinfection by-products (DBPs) [11,12]. To find optimal conditions for chlorine injection in drinking water distribution systems or transmission lines, the study on the bulk and wall chlorine decay reactions is essential.

The decay of chlorine involves complex reactions that is conventionally simplified to first order kinetic in water quality modeling. To improve this traditional model, different advanced decay kinetic expressions, i.e. n^{th} order, parallel first order, limited first order, single-reactant second order (SR) and two-reactant second order (2R) model are developed [3,13,14]. Eqs. (1) to (7) list the differential expressions of kinetic models (dc_{cl}/dt) proposed for chlorine bulk decay.

$-\boldsymbol{k_b * c_{cl}}$	First Order	(1)
$-\boldsymbol{k_b * \ c_{cl}{}^{n}}$	n^{th} Order	(2)
$-\boldsymbol{k_b}(\boldsymbol{c_{cl}}\ -\ \boldsymbol{c_{cl}}^{*})$	Limited First Order	(3)
$-(\boldsymbol{k_{b1}} \times \boldsymbol{x} * \ \boldsymbol{c_{cl}} + \boldsymbol{k_{b2}} * (\boldsymbol{1} - \boldsymbol{x}) * \boldsymbol{c_{cl}})$	Parallel First Order	(4)
$-\boldsymbol{k} * \ \boldsymbol{c_{cl}} * [\boldsymbol{React}]$	Second Order Single Reactant (SR)	(5)
$-\boldsymbol{k_{bf}} \ * \boldsymbol{c_{cl}} * \ \boldsymbol{c_{sf}} + \ \boldsymbol{k_{bs}} * \ \boldsymbol{c_{cl}} \ * \boldsymbol{c_s})$	Second Order two Reactant (2R)	(6)
$-\boldsymbol{cl_t}\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \boldsymbol{k_i} \ \boldsymbol{x_{i,t}}$	Variable Rate Coefficient (VRC)	(7)

where c_{cl} is the concentrations of chlorine (mg L^{-1}), k_b is bulk decay coefficient ($time^{-1}$), n is order of reaction, $c_{cl}{}^{*}$ is the limited concentration of chlorine (mg L^{-1}), k_{b1} and k_{b2} are bulk decay rate coefficients for fast and slow reactions, respectively ($time^{-1}$), x is a fraction of the initial concentration, [React] is the concentration of the species that react with chlorine, c_f and c_s are the concentrations of fast and slow reducing agents respectively, and k_{bf} and k_{bs} are bulk decay rate coefficients for fast and slow reactions respectively (L mg^{-1} $time^{-1}$). $x_{i,t}$ is the concentration of the i^{th} aqueous species at time t that reacts with chlorine with rate constant k_i [15]. Parallel and second-order 2R models are developed, because some compounds in drinking water e.g. iron are fast reactive, whereas some e.g. manganese are slow reactive [3,10,13]. The required time for fast reactions is about 3 to 4 h [7]. Several studies are performed to investigate on the most suitable bulk decay coefficients [3–5,10,16]. The SR model is simulated by combined concentration of chlorine and other substances in the kinetic equations of decay. Eqs. (8) to (10) formulated by Boccelli et al to simulate SR model [1].

$$aA + bB \rightarrow \rho P \tag{8}$$

$$\frac{dC_A}{dt} = -k_A C_A C_B, \quad \frac{dC_B}{dt} = -k_B C_A C_B \tag{9}$$

$$\frac{k_A}{a} = \frac{k_B}{b} \tag{10}$$

where C_A is the concentration of chlorine, C_B is the concentration of reactive component, k_A is decay rate coefficient for the chlorine, k_B is decay rate coefficient for the reactive component, and a and b are stoichiometry coefficients [1,17].

The first order model is generally applied for the reaction of chlorine wall decay, as Eq. (11):

$$\frac{dC}{dt} = \frac{4k_w k_f}{D(k_w + k_f)} C \tag{11}$$

where k_f is the mass transfer coefficient (length divided by time), k_w is the wall reaction rate coefficient (length divided by time) and D is the pipe's diameter

[5,16,18,19]. The wall decay coefficient depends on characteristics of the distribution pipes such as diameter, age, roughness, pipe material and the volume of biofilm formed on the pipe surfaces [7,9,11].

In order to simulate chlorine decay reactions, the bulk decay coefficient (k_b) and the wall decay coefficient (k_w) need to be specified. The k_b is determined by bottle tests and k_w is determined by calibration of distribution systems or transmission lines through the simulation [2].

EPANET is a series of modeling software package developed by the United States Environmental Protection Agency's (EPA) for the hydraulic and quality simulation of water distribution systems [2,3,5]. The water quality simulation in the EPANET2.0 is limited to only a single chemical species. The Multi-Species extension, EAPANET MSX, which was developed in 2008, provides qualitative simulation with a multi-species approach [14,18–20]. This new extension has brought enhanced capabilities for the simulation of chlorine residuals in water supply systems that allows the modeling of chemical reactions of any level of complexity. In this extension, kinetics of chemical reactions are introduced to the model through a set of Ordinary Differential Equations (ODEs) [21].

Fisher et al. [3] compared three bulk decay models (SR, 2R and VRC model) in the EPANET MSX. According to their results, 2R and VRC models were more accurate [3]. Monteiro et al. [18] evaluated the performance of the 2R model, first and nth order decay kinetics in a transmission line by using EPANET MSX. Their simulation results show that these models described the bulk decay reactions of chlorine consumption with a same accuracy [18]. The chlorine decay was simulated using a second-order model in the EPANET MSX by Ohar et al. [17]. They proposed a new method for designing, installing and disinfection operation in water distribution systems by optimizing the amount of injected chlorine [17]. Tiruneh et al. [5] found that second order kinetics for bulk decay calibration was more accurate than first order model in simulation of the Matsapha town water network. Applying first order model for simulating chlorine wall decay in EPANET s/w, the value of the wall coefficient by trial and error procedure was obtained 0.05 m d^{-1} [5].

Carmen et al. [22] applied EPANET2.0 software to model the residual chlorine in an urban distribution network with a population of 50,000. The bulk decay coefficient was determined 0.85 d^{-1} and the wall reaction coefficients were assigned from 0.013 to 0.057 m d^{-1} [22].

Pedro Castro et al. [23] emphasized on the importance of chlorine wall decay in relation to bulk decay reactions in water distribution network in Luzada, Portugal. The bulk decay coefficient by bottle tests and the wall decay coefficient in the first order reaction were determined as 0.343 d^{-1} and 0.0021 m $second^{-1}$ respectively [23].

Mostafa et al. [4] investigated the effect of water-age as a measuring and controlling tool to estimate chlorine concentration at different water network points. They found that EPANET model is accurate in predicting chlorine concentration at low water age nodes [4].

In this study, the effect of dividing the water transmission pipe line in modeling procedure, on improving residual chlorine prediction is of concern. For this purpose, the chlorine concentration of great Isfahan Water Transmission Line (IWTL) is simulated. The IWTL is the longest and most important water transmission route in the central Iran. First order decay model, parallel first and second order single reactant (SR) models are applied and the results are compared. The EPANET and EPANET MSX s/w are applied for simulation. Bottle tests are carried out to assess chlorine consumption kinetics and estimate bulk decay rate coefficients. The simulations are applied through one-part approach (OPA) and multiple-part approach (MPA). The OPA applies single decay coefficient for whole the line. In the MPA, the transmission line is separated into smaller sections (in this study: two sections) to apply several coefficients

The article is outlined as follow: the case study is introduced in Sec. 2, methodology and experimental work is described in Sec. 3, the results of the Bottle tests for assessing chlorine consumption kinetics are presented in Sec. 3. Simulation procedure in EPANET and EPANET- MSX is described in Sec. 4, followed by the results and discussion in Sec. 5. The conclusion remarks are presented in Sec. 6

2. Case study

Baba-Sheikhali water treatment plant located at the Southwest of Isfahan province, Iran, supplies the drinking water for more than 4 million consumers from Zayandehrod river. Outflow rate of the water treatment plant in summer and winter are about 11.2 and 8.5 m^3 $secund^{-1}$, respectively. The study is performed on the IWTL. The total length of IWTL is 258 km starting from Baba-Sheikhali water treatment plant, ending at Naein city in northeast of Isfahan province (Figure 1). The IWTL with 38 nodes, three pumping stations and two reservoirs is one of the important and strategic water lines in the central Iran. Physical characteristics of some important nodes of the IWTL are tabulated in Table 1.

Table 1: Physical characterizes of important nodes in IWTL

Node number	Node name	Distance from treatment plant site (km)	pipe material between two nodes	pipe age (year)
2	Oshtorjan	17.7	concrete	30
3	Falavarjan	28.7	Prestressed-concrete	30
4	Felman	39.7	Prestressed-concrete, steel	30
5	Hezarjerib (reservoir)	52.7	Prestressed - concrete	22-39 var.
6	Abshar	56.7	Prestressed - concrete	33
7	Gavart (reservoir)	66.7	Prestressed-concrete, steel	14
8	Timyart	101.7	Steel	28
11	Naein (reservoir)	258	GRP-Steel-ductile iron	7-28

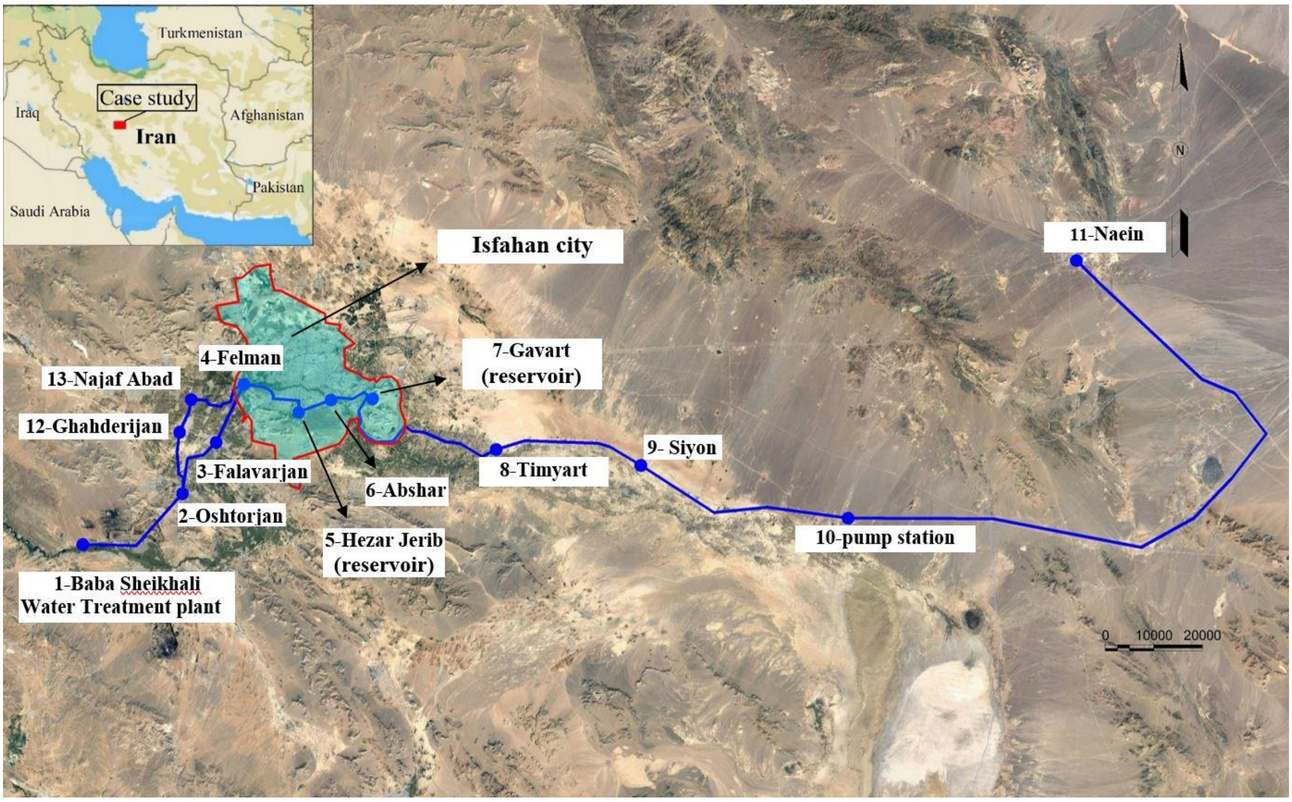


Figure 1: IWTL route

3. Experimental procedure, bulk decay coefficient derivation

Bulk decay coefficient, k_b, is the key parameter in the decay kinetics expressions. Bulk decay coefficients are commonly derived through the bottle tests [9,24]. The results are case specific depending on various parameters [4,10,16]. Jaichan et al. [2] performed thirteen bulk tests at the different water temperatures over a period of 50 h. The Bulk decay coefficient, k_b, ranged from 0.18 to 0.41 d^{-1} [2]. Jico et al. [25] determined the residual chlorine concentration by bottle tests in spring and autumn (water temperature 15 °C), summer (water temperature 25 °C) and winter (temperature 6 °C) as 0.38, 0.4 and 0.3 d^{-1} respectively [25].

In this study, the experimental design consists of collecting a set of samples from the effluent Baba-Sheikhali water treatment plant prior to enter the water transmission line. A Hach pocket colorimeter model 5870012 with Diethyl-P-phenylene Diamine (DPD) as an indicator was applied to measure free residual chlorine concentration of the samples. Tests were performed from the water age 0 to 82 h in summer and 0 to 92 h in winter temperatures. The first sample was measured in place just after it was taken (at t_0) in place. The other bottles were put in incubator and were set at temperatures 6°C and 18°C as an average water temperature in winter and summer, respectively.

Determination of bulk decay coefficients based on water age were derived for OPA and MPA at 6°C and 18°C, where the water age in the OPA is 0-82 h, while in the MPA it is 0-18h in the first part and 18-82h in the second part at T= 18°C.

The result of the measurement of chlorine concentration at 18ºC is shown in Figure 2, where the continuous line is fitted to the whole data in the range 0-82 h. Accordingly, the bulk decay coefficient, k_b is equal to 0.286 d^{-1}. According to the Figure 2, k_b in the first part with water age in range 0-18 h is equal to 0.583 d^{-1} (dotted line) and in the second part where the water age is in range 18-82 h is equal to 0.216 d^{-1} (dashed line).

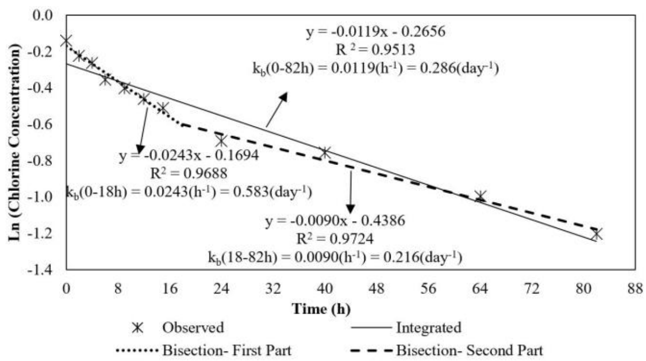


Figure 2: Bulk decay coefficient at 18 ° C with OPA and MPA using the bottle test

The estimation of k_{b1} (the coefficient of fast reaction) and k_{b2} (the coefficient of slow reaction) is necessary to apply the parallel first order model. Therefore, the k_b coefficients for kinetic models at 18° and 6° are calculated as shown in Figure 2. The results are summarized in Table 2.

Table 2: Bulk decay coefficients derived from the bottle test

T (°C)	Approach	Parts	First Order (d^{-1})		Second Order ($L.mg^{-1}.d^{-1}$)		Parallel(d^{-1})			
							Fast		Slow	
			k_b	R^2	k_b	R^2	k_b	R^2	k_b	R^2
18	OPA	All (0-82h)	0.286	0.95	0.590	0.98	0.828	0.98	0.286	0.95
	MPA	First (0-18h)	0.583	0.97	0.821	0.98	0.828	0.98	0.583	0.97
		Second (18-82h)	0.216	0.97	0.557	0.95	-	-	0.216	0.97
6	OPA	All (0-92h)	0.103	0.92	0.144	0.95	0.401	1	0.103	0.92
	MPA	First (0-22h)	0.204	0.95	0.264	0.96	0.401	1	0.204	0.95
		Second (22-92h)	0.062	0.99	0.098	1	-	-	0.062	1

The results of the bottle tests show that k_b in the first and second order reactions is significantly different between the first and second parts of the line Table 2. In addition, they are significantly different from its value for the entire line, which is applied in OPA. Because the chlorination is carried out once in IWTL (in Baba-Sheikhali treatment plant), the concentration of chlorine in the first part is much higher than the concentration in the second part.

The derived coefficients are applied in simulation of bulk decay (Eqs. (1,4,5)). In the parallel model, Eq. (4), k_{b1} is obtained from the first 4 h of reaction and the k_{b2} from the beginning of chlorination up to the end node. In IWTL, in summer at the Falavarjan (node 3 in Figure 1) and in winter at Oshtorjan (node 2 in the Figure 1) water age reaches 3 to 4 h. Thus, these two nodes are respectively considered as the end of fast chlorine reactions in summer and winter.

4. Simulation procedure in EPANET.

IWTL is simulated in EPANET s/w in hydraulic and quality manners. EPANET s/w performs extended period simulation of hydraulic and water quality behaviour. The Hazen-Williams head loss formula is applied in simulation. The water quality model in EPANET s/w applies nth order kinetics to model reactions in the bulk flow and applies zero or first order kinetics to model reactions at the pipe wall [8]. Chlorine residual concentration is then assessed in the line or network by inputting wall and bulk decay coefficients.

4.1. Hydraulic simulation

Applying field pressure data at different nodes, the hydraulic model of the line is calibrated and verified. The comparison between the results of the model and measurements for the selected nodes are summarized in Table 3. The root mean square error (RMSE) of the simulation is 4.09 meters in summer and 4.24 meters in winter. The correlation coefficients (R^2) between the results of the model and measurement are 0.958 and 0.978 for summer and winter, respectively, indicating that the hydraulic simulation is in acceptable level of accuracy.

The schematics of transmission line and the hydraulic simulation results for summer flow condition is shown in Figure 3. The node colors in Figure 3 represent the water age and the numbers adjacent to the lines show the maximum flow rate (L sec^{-1}.). Water age is important in this analysis because when it is increased, the residual concentration of disinfectant decreases and microorganisms' growth increases [2].

Table 3: Results of simulation and measured pressure in some nodes of IWTL in summer

Sampling points	Presure (m)		Error (%)
	measured	predicated	
Felavarjan	34	39.55	16.32
Felman	50	44.99	-10.02
Najafabad	31	36.48	17.67
Abshar	65	65.89	1.36
Timyart	70	67.58	-3.45

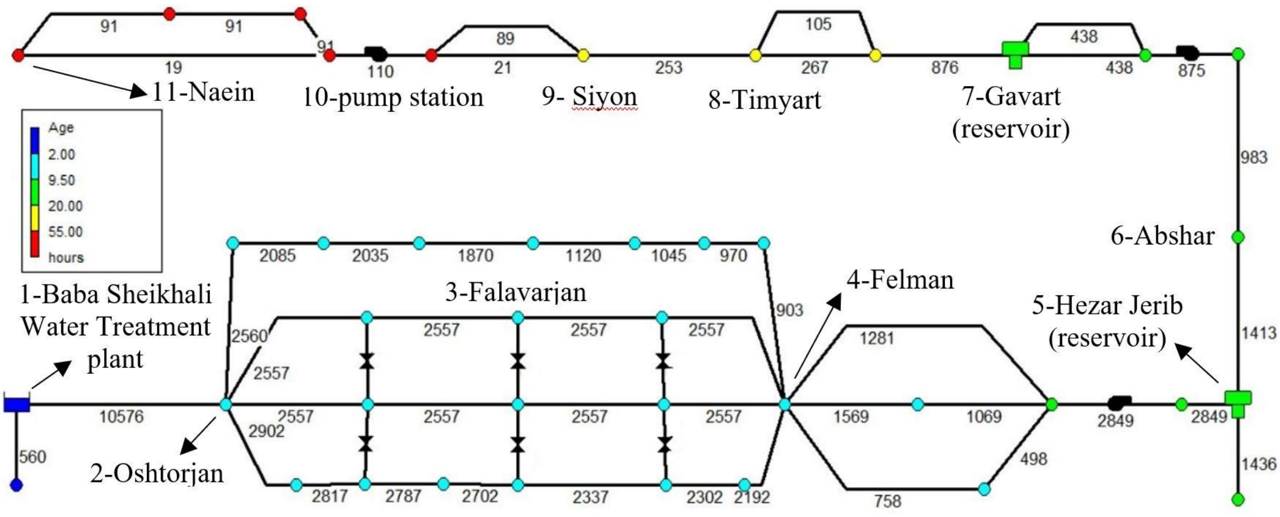


Figure 3: Schematic diagram of IWTL and simulation results in summer

4.2. Residual Chlorine Simulation

Applying the first model in EPANET 2.0 s/w and second order SR model and parallel first order model in EPANET-MSX s/w, the residual chlorine concentration in IWTL is simulated. Since the IWTL is too long, the water residence time in the pipes is lengthy too. This will decline the validity of applying a single decay coefficient for the whole line. Therefore, the IWTL is simulated in two approaches included OPA and MPA. In the OPA, only one bulk decay coefficient and one wall decay coefficient are applied for all pipes in the line. This is a usual method to simulate residual chlorine concentration in transmission lines and water distribution networks [2,4]. In MPA, as a new approach, different bulk and wall decay coefficients are considered. In this study, IWTL line is divided to two parts and therefore, two bulk and wall decay coefficients are considered for simulation.

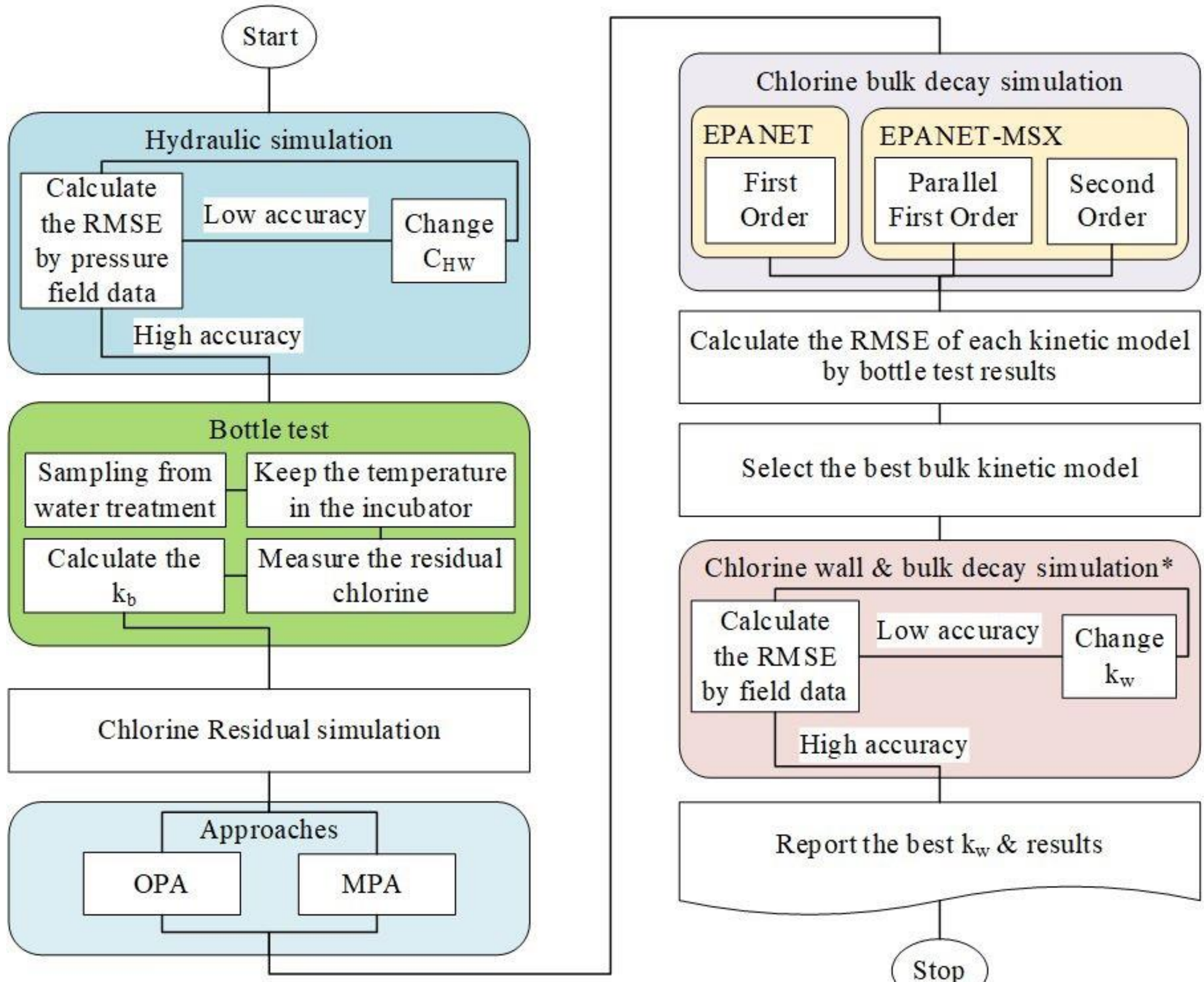
The Gavart reservoir (node 7 in Figure 3) is selected as the separator in MPA for two reasons. First the Gavart reservoir is the last node in the Isfahan city along the IWTL, the second is the number of the available field data to calculate RMSE. Thus, in the MPA, the IWTL from the Baba-Sheikhali treatment plant to Gavart reservoir and from the Gavart reservoir to Naein are considered as the first and second part, respectively. The average water age in the first and second sections is about 18 and 82 h in summer and 22 and 92 h in winter, respectively.

Applying the first order, parallel, and second order SR models, chlorine bulk decay of IWTL is simulated. The first order model Eq. (1) is simulated in EPANET2.0 s/w. The EPANE MSX is applied for simulation of the parallel Eq. (4) and second order SR models Eq. (5).

Wall decay coefficient is estimated by first model kinetic Eq. (11) and the trial and error in the EPANET2.0 s/w to achieve the minimum difference between simulated and measured chlorine concentrations at the study nodes. Field chlorine concentration measured in selected nodes of IWTL by Isfahan Water and Wastewater Organization.

Note that in the OPA, the model is calibrated with a single wall coefficient and in the MPA, two wall coefficients are considered. The best wall coefficient is chosen based on the least RMSE [5,26].

The procedure of hydraulics and chlorine residual concentration for OPA and MPA in EPANET is summarized in Figure 4.



* Depending on the applied kinetics model, wall & bulk decay are simulated in EPANET or EPANE-MSX

Figure 4: Flowchart of Simulation procedure in EPANET

5. Results and discussion

5.1. Evaluating the results of the chlorine bulk decay models

The simulation results of chlorine bulk decay kinetic models for OPA and MPA are compared with the observations in bottle tests in Figure 5 and Figure 6 for summer (T=18 °C) and winter (T= 6 °C) conditions, respectively, where the results of MPA in three simulation models are clearly closer to the observed data in compare to OPA. The RMSE of the results are tabulated in Table 4.

.

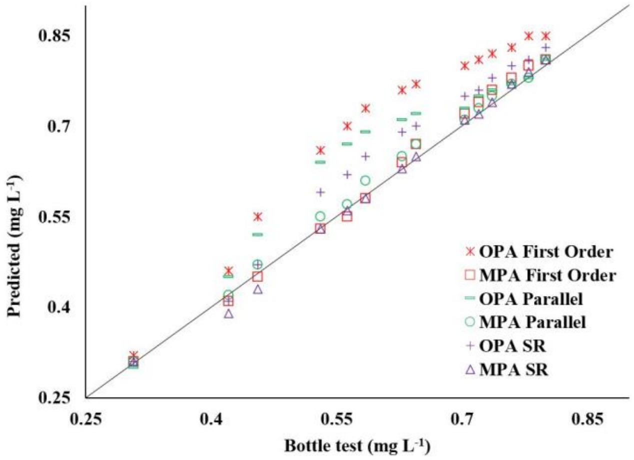


Figure 5: Correlation plot of bottle test and predicted chlorine concentration volumes at T=18°C

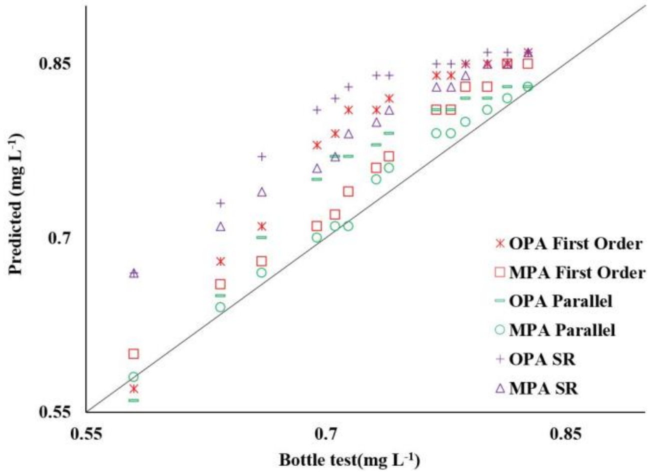


Figure 6: Correlation plot of bottle test and predicted chlorine concentration volumes T= 6 °C

Table 4: RMSE volume between bottle test and predicted chlorine concentrations

Season	Simulated in:		EPANET2.0	EPANET-MSX	
	T (°C)	Approach	First Order	Parallel	SR
summer	18	OPA	0.0954	0.0600	0.0425

		MPA	0.0147	0.0138	0.0116
winter	6	OPA	0.0646	0.0395	0.0900
		MPA	0.0286	0.0114	0.0644

According to Table 4, in the OPA simulation for T=18ºC, the SR and parallel models with respectively RSME of 0.0425 and 0.0600, estimate chlorine consumption more accurate than the first order model with RMSE equal to 0.0954. For T=6ºC in the OPA, the parallel model performs better than SR and first order models.

Applying MPA with different bulk decay coefficients for each part, results in a significant improve in the results, as indicated in Table 4. Therefore, a similar level of accuracy achieved the three simulated kinetic models in MPA and applying first order kinetic model in MPA is more effective than applying more complex kinetic models in OPA. According to Table 4, the SR model in 18ºC and parallel model in 6ºC in both approaches have minimum RMSE and are selected for wall decay coefficient determination.

5.2. Chlorine wall decay simulation

After selecting the best bulk decay models, the wall decay coefficient volume, k_w is estimated for the models. For this purpose, the model is run for a range of k_w to obtain the least RSME. In summer for example, the best wall decay coefficient of 0.04 m d^{-1}

provides the least RMSE of 0.0668 mg L^{-1} for OPA, as shown in Figure 7. In MPA, the wall decay coefficient is obtained for each part separately to reach to the least RMSE. The coefficients are 0.09 and 0.01 m d^{-1} for the first and the second part, respectively.

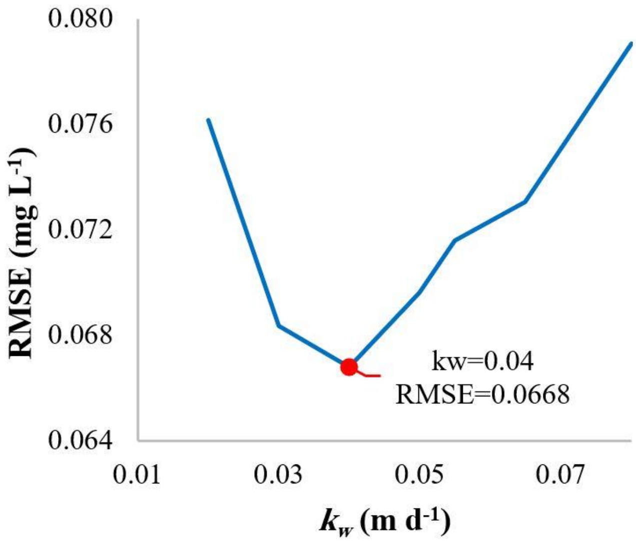


Figure 7: RMSE of simulation in wall first order model in the OPA in summer, T=18 °C

The volumes of k_w in the applied models is tabulated in Table 5. Comparison of simulated chlorine concentration volumes in the OPA and MPA simulation with the field measurements are shown in Figure 8 where volumes in the MPA are closer to the measured volumes than the OPA. For the best bulk kinetic models (SR in summer and parallel in winter), the results clearly indicate the superiority of the MPA compared to conventional approach of OPA.

According to Table 5, the RMSE volumes in the SR and parallel are reduced from 0.0668 to 0.0294 in the summer and from 0.0543 to 0.015 in the winter in the OPA and MPA respectively.

Therefore, determining different bulk and wall decay coefficients for the IWTL due to the long route (258 km), wide range water velocity and different pipe characteristics, significantly improve the accuracy of the simulation results.

In order to compare the simulation results of the best kinetics and the simple first order model in the MPA, the simulation with the first order model is also performed. Comparison between the simulation results of the simple first order model and the advance kinetic models in the MPA, does not significantly improve the results, compare RMSE of 0.0294 and 0.0290 in summer and 0.015 and 0.016 in winter for the first order model and the others, respectively.

Table 5: Wall decay coefficients by simulation

<table>
<tr><th rowspan="2">T (°C)</th><th rowspan="2">Approach</th><th rowspan="2">Parts</th><th colspan="4">Best bulk kinetic model (SR or Parallel)</th><th colspan="3">First Order Model</th></tr>
<tr><th colspan="2">k_b</th><th>k_w</th><th>RMSE</th><th>k_b</th><th>k_w</th><th>RMSE</th></tr>
<tr><td rowspan="3">18</td><td>OPA</td><td>All(0-82h)</td><td colspan="2">0.590</td><td>0.04</td><td>0.0668</td><td>0.286</td><td>0.08</td><td>0.090</td></tr>
<tr><td rowspan="2">MPA</td><td>First(0-18h)</td><td colspan="2">0.821</td><td>0.09</td><td rowspan="2">0.0294</td><td>0.583</td><td>0.15</td><td rowspan="2">0.029</td></tr>
<tr><td>Second(18-82h)</td><td colspan="2">0.557</td><td>0.01</td><td>0.216</td><td>0.005</td></tr>
<tr><td>6</td><td>OPA</td><td>All(0-92h)</td><td>0.401</td><td>0.103</td><td>0.08</td><td>0.0543</td><td>0.103</td><td>0.08</td><td>0.064</td></tr>
</table>

	MPA	First(0-22h)	0.401	0.204	0.1	0.015	0.204	0.13	0.016
		Second(22-92)	-	0.062	0.05		0.062	0.04	

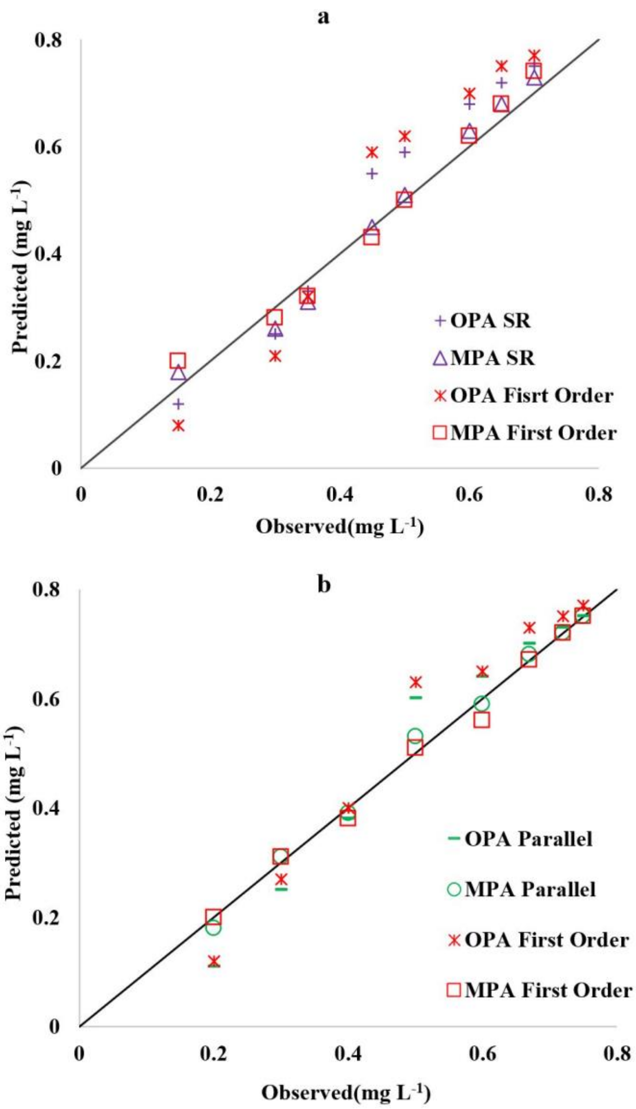


Figure 8: Comparison between observed and predicted chlorine concentration (mg L^{-1}) in a) T=18°C and b) T=6°C

6. Conclusions

Residual chlorine simulation is conducted in Isfahan Water Transmission Line (IWTL). The total length of IWTL is 258 km and maximum flow rate is more than 11

$m^3\ s^{-1}$. Hydraulic simulation of IWTL is performed through EPANET2.0 s/w and the results are verified against pressure data collected at a number of nodes along the line. Bulk decay coefficient is determined by bottle test in 6 and 18°C corresponding to winter and summer water temperature, respectively. Residual chlorine concentration is simulated via two approaches: one-part approach (OPA) and multi-part approach (MPA) and the results are compared. Number of decay kinetic models are applied in the simulation, including first order model (in EPANET2.0) and Parallel and SR models (in EPANET MSX). The optimum wall decay coefficient is determined through the calibration of the models with the measured chlorine concentration at the selected nodes on the line. In the OPA, the parallel kinetic model in winter (RMSE=0.0543) and the SR model in summer (RMSE=0.0668) are the best kinetic models with the least RMSE compared to the field data. In the OPA, the bulk decay coefficients of 0.401 and 0.103 d^{-1} and wall decay coefficient of 0.08 $m\ d^{-1}$ are derived, for the whole line in winter and they are 0.590 $L\ mg^{-1}\ d^{-1}$ and 0.04 $m\ d^{-1}$ in summer respectively.

In the MPA, no significant advantages found between the kinetic models. In the former approach, RMSE of the first order and the best kinetics models are 0.0290 and 0.0294 in summer, and 0.016 and 0.015 in winter. Applying different coefficients for each part (MPA) is more effective than applying most sophisticated kinetics models.

In the MPA, the bulk decay coefficient for the first and second parts is 0.204 and 0.062 d^{-1} and the wall decay coefficient is 0.13 and 0.04 m d^{-1} in winter and 0.583, 0.216, 0.15, 0.005 respectively in summer.

Average RMSEs are changed from 0.078 to 0.029 in summer and 0.059 to 0.015 in winter between OPA and MPA respectively, indicating a considerable improvement in the accuracy of the simulation. In the simulation of the water transmission lines with the common OPA, advanced models behave more accurately than the first order model, while different kinetic models do not differ much in the MPA. It means that applying the simple and conventional first order model incorporated in EPANET2.0, results in an acceptable level of accuracy, provided that the appropriate decay coefficient is applied for each parts of the line. Further research determines the optimum number of divisions and the location of separation points on the line.

<u>Declarations</u>

Availability of data and materials

Not applicable.

Competing interests

Not applicable.

Funding

Not applicable

Authors' contributions

Not applicable.

Acknowledgements

Appreciations are extended to Mr. Akbary (deputy) and Ms Jahanfard (Engineer) at Isfahan Water and Wastewater Organization (IWWO) for providing the data, according to the joint plan No. 3554 between IWWO and the University of Isfahan.

References

1. Boccelli DL, Tryby ME, Uber JG, Summers RS. A reactive species model for chlorine decay and THM formation under rechlorination conditions. Water Res. 2003;37:2654–66.

2. Ahn J, Lee S, Choi K, Koo J. Application of EPANET for the determination of chlorine dose and prediction of THMs in a water distribution system. Sustain Environ Res. 2012;22:31–8.

3. Fisher I, Kastl G, Sathasivan A. Evaluation of suitable chlorine bulk-decay

models for water distribution systems. Water Res. 2011;45:4896–908.

4. Mostafa NG, Matta ME, Halim HA, L.Monteiro. Simulation of Chlorine Decay in Water Distribution Networks Using EPANET – Case Study. Civ Environ Res. 2013;3:100–16.

5. Tiruneh AT, Debessai TY, Bwembya GC, Nkambule SJ, Zwane L. Variable Chlorine Decay Rate Modeling of the Matsapha Town Water Network Using EPANET Program. Water Resour Prot. 2019;11:37–52.

6. Goyala R V., Patelb HM. Optimal location and scheduling of booster chlorination stations for drinking water distribution system. Appl Water Eng Res. 2017;5:51–60.

7. Al-Jasser AO. Pipe Service Age Effect on Chlorine Decay in Drinking-Water Transmission and Distribution Systems. Water Res. 2007;41:387–96.

8. Rossman L. EPANET 2 user's manual. Envionmental Prot Agency. 2000;1–200.

9. Abokifa AA, Yang YJ, Lo CS, Biswas P. Water quality modeling in the dead end sections of drinking water distribution networks. Water Res. 2016;89:107–17.

10. Vieira P, Coelho ST, Loureiro D. Accounting for the influence of initial chlorine concentration, TOC, iron and temperature when modelling chlorine decay in water supply. Water Supply Res Technol - AQUA. 2004;53:453–67.

11. Hallam NB, West JR, Forster CF, Simms J. The potential for biofilm growth in water distribution systems. Water Res. 2001;35:4063–71.

12. Li C, Yu JZ, Zhang TQ, Mao XW, Hu YJ. Multiobjective optimization of water quality and rechlorination cost in water distribution systems. Urban Water J. 2015;12:646–52.

13. Haas CN, Karra SB. Kinetics of wastewater chlorine demand exertion. J Water Pollut Control Fed. 1984;56:170–3.

14. Fisher I, Kastl G, Sathasivan A. A comprehensive bulk chlorine decay model for simulating residuals in water distribution systems. Urban Water J. 2016;14:361–8.

15. Fisher I, Kastl G, Sathasivan A, Jegatheesan V. A variable rate coefficient chlorine decay model. Environ Sci Technol. 2009;43:408–14.

16. Boulos PF, Vasconcelos JJ, Rossman LA, Clark RM, Grayman WM. Kinetics of chlorine decay. Am Water Work Assoc. 1997;89:54–65.

17. Ohar Z, Ostfeld A. Optimal design and operation of booster chlorination stations layout in water distribution systems. Water Res. 2014;58:209–20.

18. Monteiro L, Figueiredo D, Dias S, Freitas R, Covas D, Menaia J, et al. Modeling of chlorine decay in drinking water supply systems using EPANET MSX. Procedia Eng.

2014;70:1192–200.

19. Seyoum AG, Tanyimboh TT, Siew C. Assessment of water quality modelling capabilities of EPANET multiple species and pressure-dependent extension models. Water Sci Technol Water Supply. 2013;13:1161–6.

20. Fisher I, Kastl G, Sathasivan A, Jegatheesan V. Suitability of chlorine bulk decay models for planning and management of water distribution systems. Crit Rev Environ Sci Technol. 2011;41:1843–82.

21. Shang F, Uber JG, Rossman LA, K. EPANET Multi-Species Extension User's Manual. 2008;115.

22. Georgescu AM, Georgescu SC. Chlorine concentration decay in the water distribution system of a town with 50000 inhabitants. UPB Sci Bull Ser D Mech Eng. 2012;74:103–14.

23. Castro P, Neves M. Chlorine decay in water distribution systems case study–Lousada network. Electron J Environ Agric Food Chem. 2003;2:261–6.

24. Powell JC, Hallam NB, West JR, Forster CF, Simms J. Factors which control bulk chlorine decay rates. Water Res. 2000;34:117–26.

25. Ahn JC, Kim YW, Lee KS, Koo JY. Residual chlorine management in water

distribution systems using network modelling techniques: Case study in Seoul City. Water Sci Technol Water Supply. 2004;4:421–9.

26. Forouzandeh Y, Dehnavi A, Shanehsazzade A. Application of Multiple-part Method length of line to Improve the Simulation of Chlorine Decay in Big Isfahan Water Conveyance Line. Water and Wastewater. 2020;31:1–11.

Figures

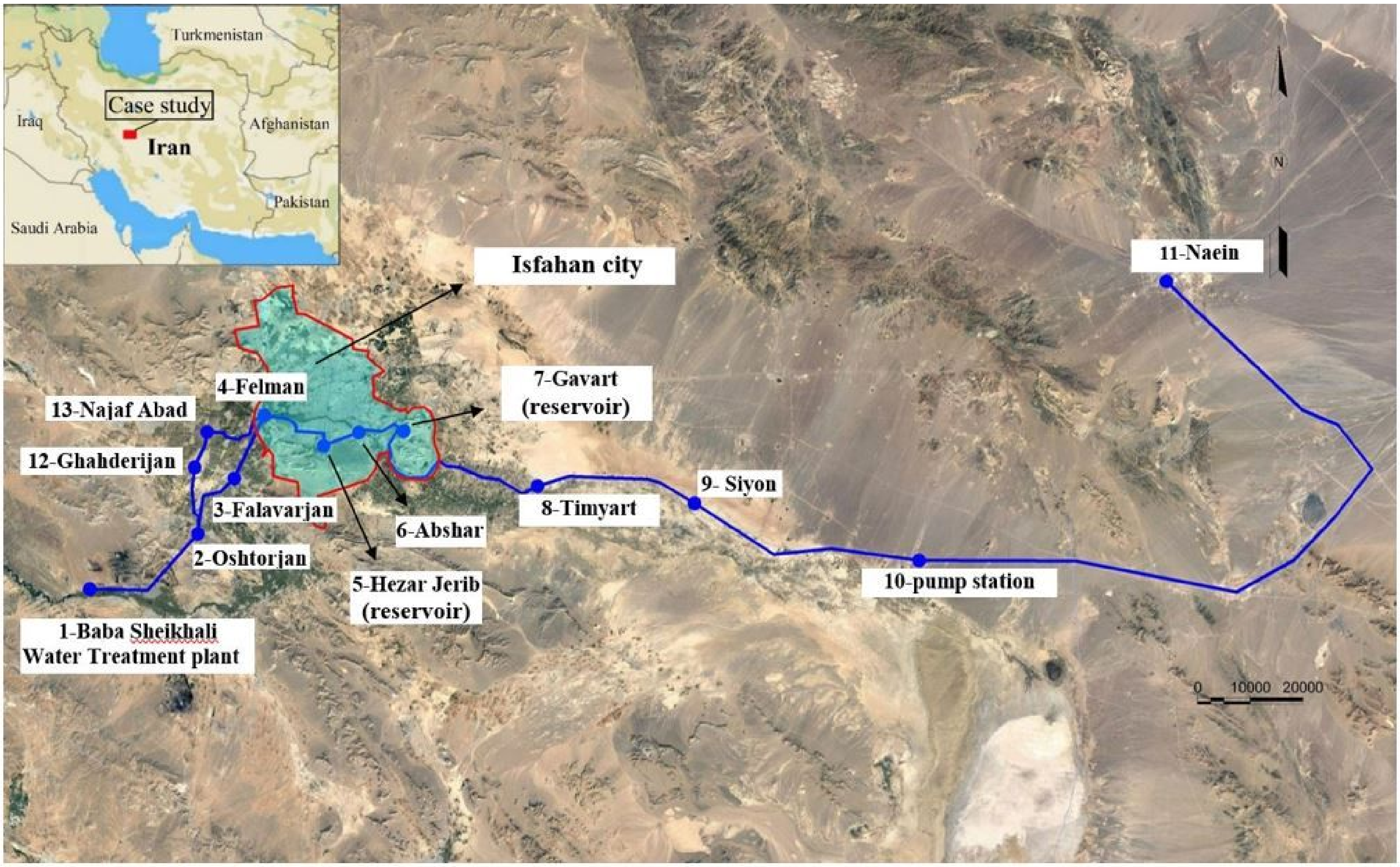


Figure 1

IWTL route Note: The designations employed and the presentation of the material on this map do not imply the expression of any opinion whatsoever on the part of Research Square concerning the legal status of any country, territory, city or area or of its authorities, or concerning the delimitation of its frontiers or boundaries. This map has been provided by the authors.

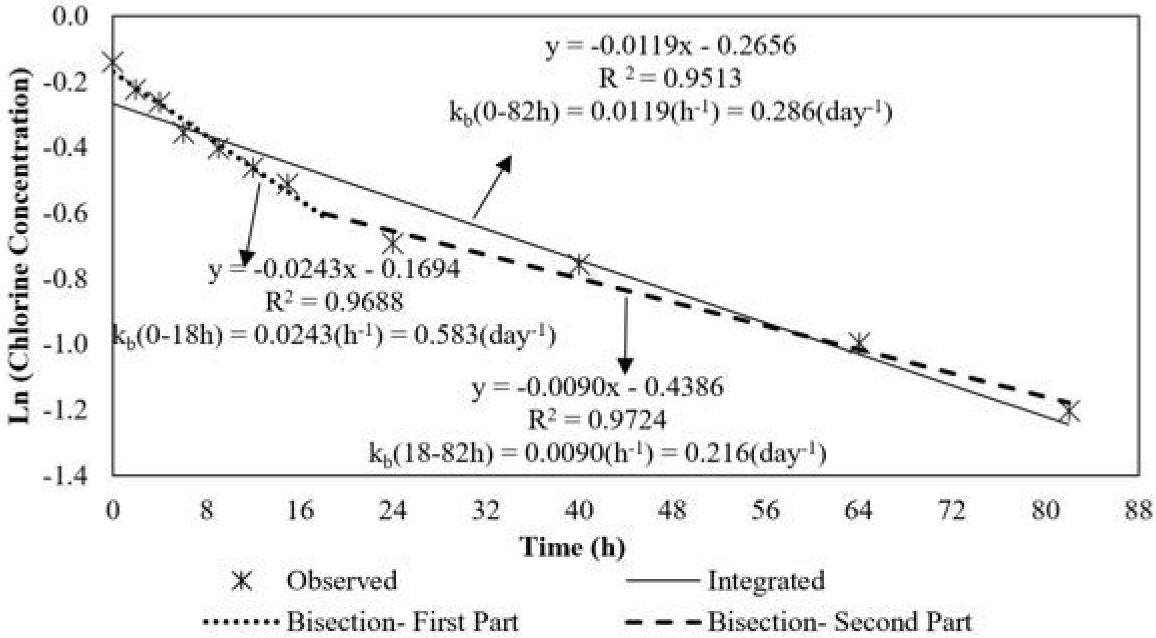


Figure 2

Bulk decay coefficient at 18 ° C with OPA and MPA using the bottle test

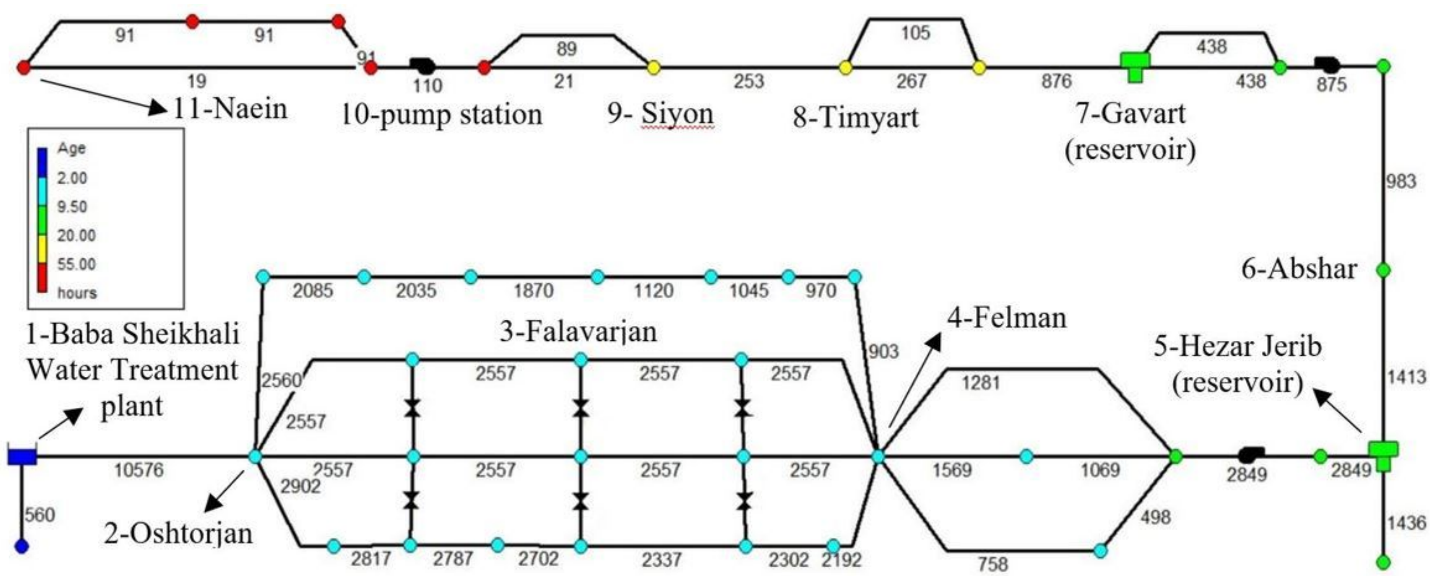
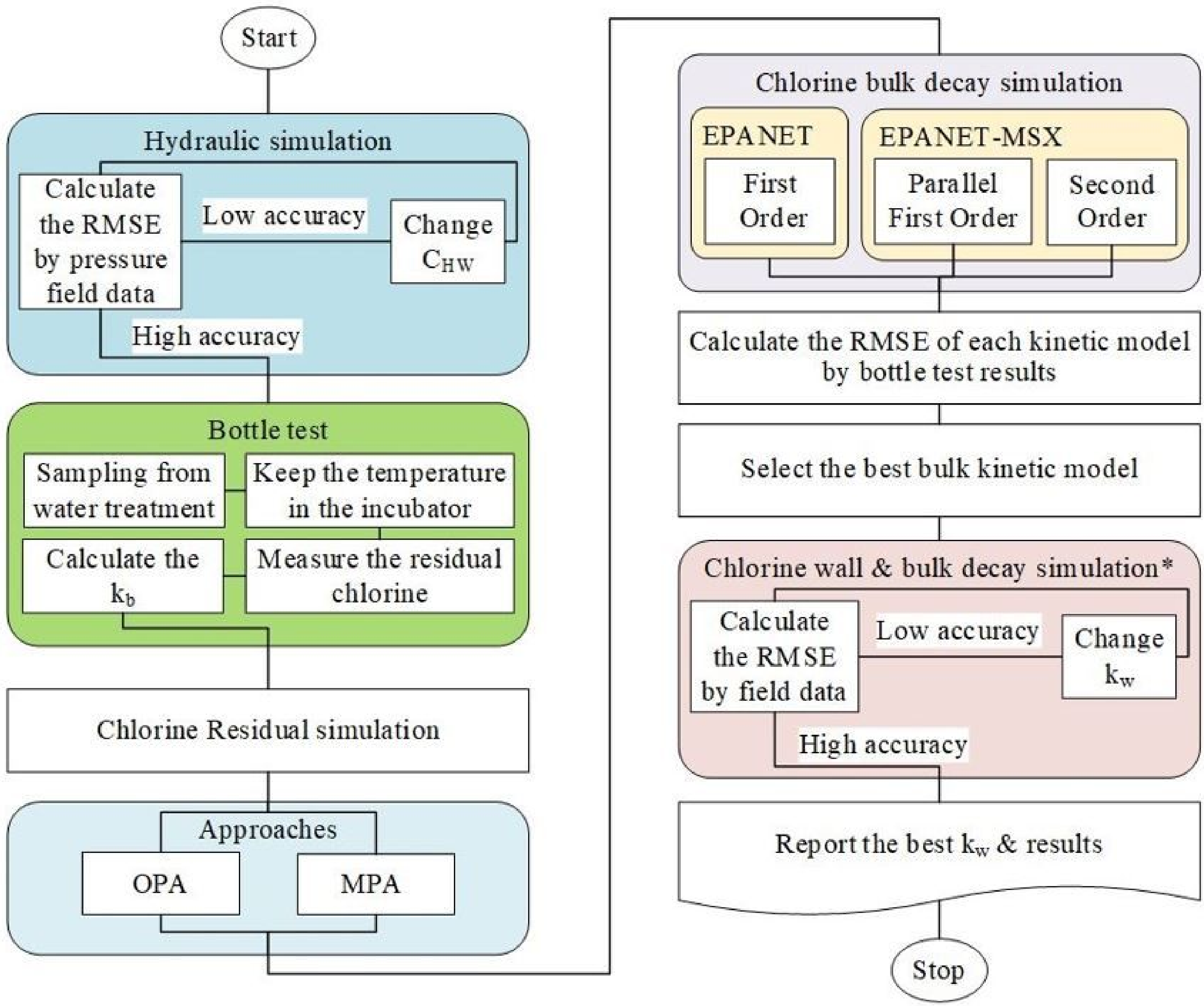


Figure 3

Schematic diagram of IWTL and simulation results in summer



* Depending on the applied kinetics model, wall & bulk decay are simulated in EPANET or EPANE-MSX

Figure 4

Flowchart of Simulation procedure in EPANET

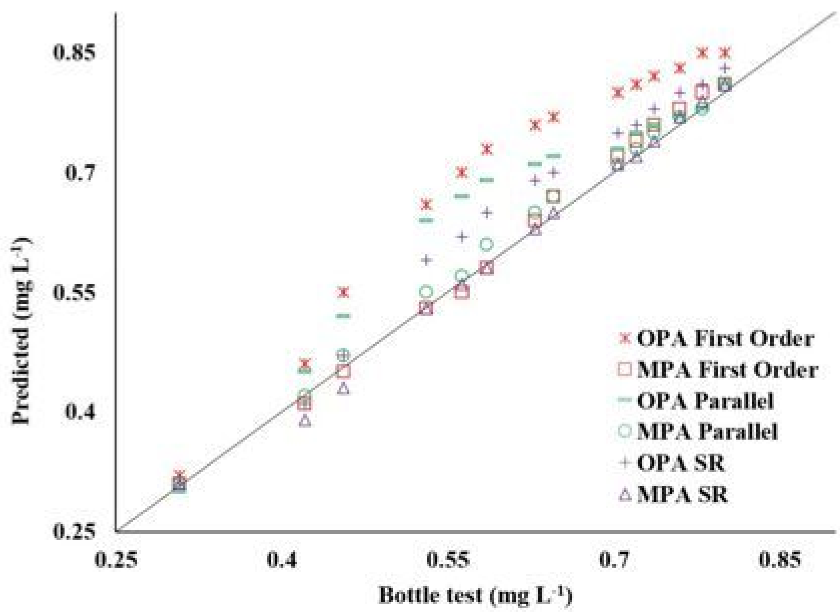


Figure 5

Correlation plot of bottle test and predicted chlorine concentration volumes at T=18°C

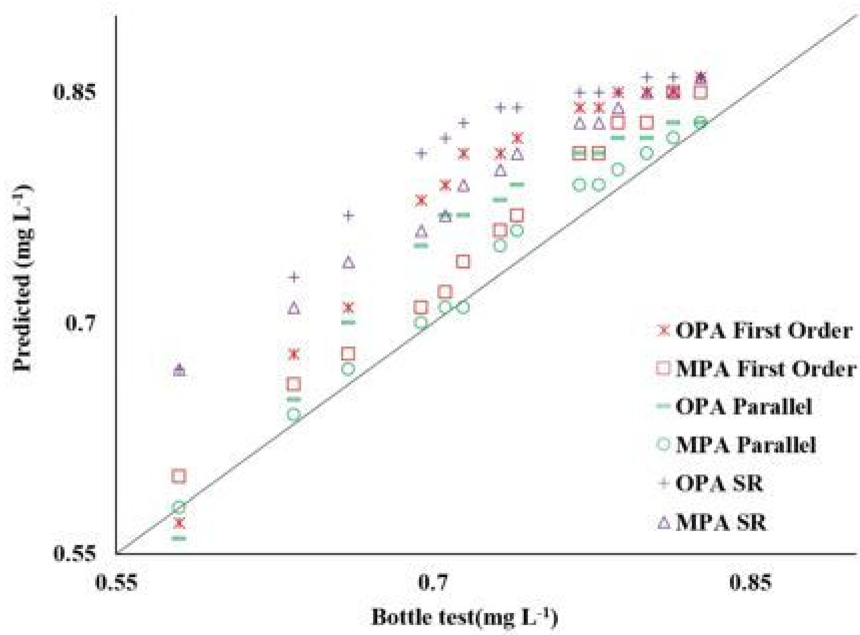


Figure 6

Correlation plot of bottle test and predicted chlorine concentration volumes T= 6 °C

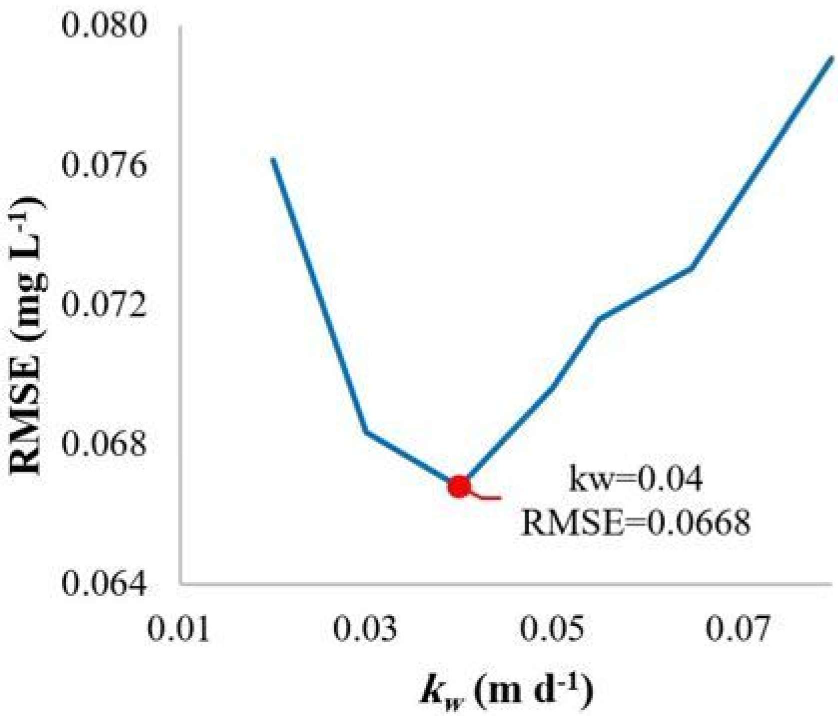


Figure 7

RMSE of simulation in wall first order model in the OPA in summer, T=18 °C

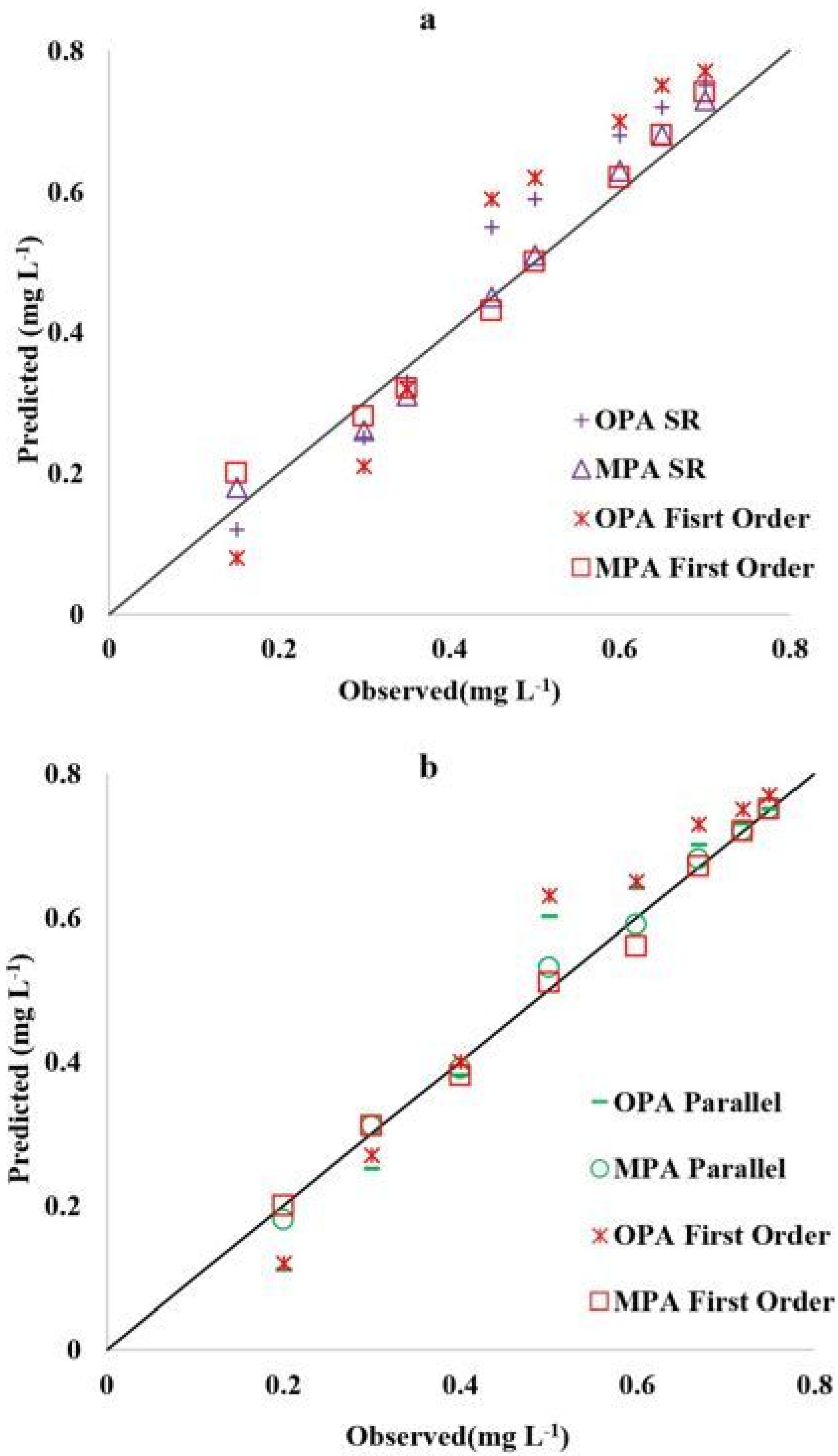


Figure 8

Comparison between observed and predicted chlorine concentration (mg L-1) in a) T=18°C and b) T=6°C