# Simulation of Chlorine Decay in Water Distribution Networks Using EPANET – Case Study

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#### Abstract

Deterioration of water quality in distribution networks has a great impact on human health and public acceptance of tap water reaching them. Residual chlorine should be maintained through network pipes to prevent contamination and microbial regrowth. This paper investigates the ability of EPANET 2.0, a free software developed by United States Environment Protection Agency (USEPA), to simulate residual chlorine decay through water networks, taking water-age analyses into consideration, and assesses the feasibility of using it as a measuring and controlling tool to estimate and predict chlorine concentration at different water network points. A study was performed on drinking water network of 6<sup>th</sup> of October city, where field measurements were done, while data required as program inputs were taken from the daily records of the 6<sup>th</sup> of October and El-Shaikh Zayed WTPs. The network model was calibrated to minimize error in program results. Errors were evaluated using statistical analyses. The calculated concentrations by the calibrated model were very close to the actual concentrations measured in field at different sampling points for different sampling days. Moreover, EPANET showed that for the water network concerned in this study, chlorine concentrations at network extremities did not recede 0.5 mg/l, the minimum allowable limit established in the Egyptian Code of Practice (ECP), even for those points having water age greater than 24 hours.

Keywords: chlorine decay, water quality, water distribution networks, EPANET, water-age

#### 1. Introduction

In the last few decades, the worldwide awareness about risks arising from degradation of water quality while traveling through transmission and distribution systems increased due to waterborne diseases outbreaks (Cohn *et al* 1999). Chlorine was first applied in Chicago, USA in 1908 (Haas 1999). Chlorination became the most common disinfection method that is usually used to disinfect drinking water, due to its germicidal potency, economy and efficiency. Chlorine disinfectants produce a lasting residual that prevent re-growth of microorganisms that managed escaping from treatment process or entered the distribution system due to external contamination (Gang *et al* 2003).

Decay of chlorine residual, caused by reacting in the bulk of flow and at walls of network elements, may lead to disappearance of disinfectant at network extremities and hence increasing the probability of microbiological contamination of drinking water (Vieira *et al* 2004, Vieira *et al* 2004, and Castro *et al* 2003). However, increasing the chlorine concentration during treatment process can lead to corrosion of water pipes and health hazards caused by increasing concentrations of disinfection by-products (DBPs), especially trihalomethanes (THMs) and haloacetic acids (HAA5), which are claimed to be carcinogenic substances (Gibbs *et al* 2003, Mark *et al* 2008, DBPs (LENNTECH) 2010, and DBPs types (LENNTECH) 2010). Therefore, one of the most important challenges that face water suppliers is to preserve residual chlorine concentration throughout the distribution network within the established maximum and minimum allowable chlorine levels (Gang *et al* 2003).

During the past decades, many studies concerning developing new chlorine decay simulation techniques, modifying existing mathematical models, studying factors affecting chlorine decay, and applying decay models on existing water distribution models were conducted either in the laboratory or in the field. In the first place, chlorine decay was modelled by a first-order kinetic equation (Vieira *et al* 2004), which is included in most of water quality simulation programs. Other models were developed to upgrade the simplicity of the first-order kinetic model, such as a parallel first-order kinetic model, a limited first-order kinetic model, as second-order kinetic model, and an nth order kinetic model (Gang *et al* 2003, and Vieira *et al* 2004). A two-dimensional steady-state transport equation was developed accounting for the bulk decay, including axial convection and radial diffusion, and wall decay (Biswas *et al* 1993). A computer model called DYNAQ was developed based on

the two-dimensional chlorine decay equation to track and evaluate chlorine decay in distribution systems (Vieira *et al* 2004).

Comparing the appropriateness of two different data-driven modeling techniques, linear regression models and multilayer perceptron artificial neural networks (MLPANNs) in predicting residual chlorine concentration it was concluded that among the used statistical measurements, the root mean square error (RMSE), the mean absolute error (MAE), and the maximum absolute error (Max), The RMSE was found to be the best indicator for performance evaluation. The linear regression model has approved high speed of calibration and required small number of parameters for optimization. However, MLPANN model is more suitable as an online tool to aid in the determination of chlorine dosing rates in a water distribution network (Maier *et al* 2000).

The performance of single-order decay model and the two-dimensional decay model which is used in EPANET program were investigated and compared in many studies. In London, it was concluded that the EPANET model gives a better fit to the observations than the single decay coefficients when monochloramine decay in a 1.3 km water pipe (Maier *et al* 2000). In Portugal, it was stated that the contribution of wall decay reactions is more significant than bulk decay reactions after comparing EPANET results with real network samples (Castro *et al* 2003). In Japan, EPANET resulted in predicted concentrations were about equal to the observed values (Nagatani *et al* 2008).

EPANET simulating results improved by taking the effect of water prosperities, such as BOD, COD, TOC,  $Fe^{2+}$ , and temperature, into consideration (Castro *et al* 2003). Bulk decay was approved to be affected by many factors, such as DOC, TOC, pH, temperature, flow velocity, and initial chlorine concentration (C<sub>0</sub>), iron (Vieira *et al* 2004, Nagatani *et al* 2008, Kastl *et al* 2003, Al-Jasser, 2007, and Menaia *et al* 2003). Wall decay was approved to be significantly affected by the thickness of the formed biofilm on the inner pipe wall which is, consequently, a function of pipe material, pipe service age, flow velocity, DOC, chlorine dosage, DO, and pH (Castro *et al* 2003, Gibbs *et al* 2003, Al-Jasser *et al* 2007, Meneia *et al* 2003, WHO 1996, Munavalli *et al* 2009, and Mohamed 2004).

This paper studies the potency of using EPANET 2.0 in simulating chlorine decay occurs in water networks, predicting residual chlorine concentration at any point of water network, and accordingly, assesses the feasibility of using it as a measuring and controlling tool to eliminate time delay associated with measuring practices that are currently adopted in WTPs.

Research work is composed of:

- 1) Field measurements,
- 2) Network analysis using EPANET,
- 3) Analysis of field measurements,
- 4) Model Calibration,
- 5) Analysis of the results,
- 6) Chlorine prediction at network extremities.

#### 2. Chlorine Decay Kinetics

The loss of residual chlorine through the water distribution system occurs because of two main reasons (Ozdemir *et al* 2004, Vieira *et al* 2004) first is the external contamination, which happens often during pipelines breaks and maintenance operations, and second is the natural decay, which is divided into the following three mechanisms (Ozdemir *et al* 2002, Castro *et al* 2003, and WHO 1996):

- 1) Bulk reactions with chemical substances present in treated water,
- 2) Wall reactions with the material of the network elements, and
- 3) Natural evaporation in storage tanks.

In the current network model, no elevated tanks exist in the network, so that the third decay mechanism impact was eliminated from the study. Also, the external contamination is ignored due that the current network is fairly recent - about 30 years old - and rarely suffers from pipelines breaks that need excessive maintenance works.

Chlorine decay theory (Ozdemir *et al* 2002, Vieira *et al* 2004, Nagatani *et al* 2008, Al-Jasser 2007, Haestad Methods 2003, and HBRC 2007), which is included in EPANET 2.0 help manuals and used during software quality analysis, account for both bulk and wall reactions as follows:

#### 2.1 Bulk Reactions

Decaying of a substance while moving through a pipe can be generally described as an nth power function of concentration as shown in Eq. (1):

$$r = k_b C^n \tag{1}$$

Where r is the rate of reaction (mass/volume/time),  $k_b$  is the reaction constant (concentration raised to the power of [1-n] divided by time), C is the reactant concentration (mass/volume), and n is the reaction order. Chlorine decay is adequately modelled by a simple first-order reaction (n = 1, kb < 0), according to the program help manuals, and hence the equation becomes:

$$r = k_b C \tag{2}$$

Where r is the rate of reaction (mass/volume/time),  $k_b$  is the reaction constant (1/ time), C is the reactant concentration (mass/volume).

## 2.2 Wall Reactions

The rate of pipe wall reaction is influenced by the mass transfer between the bulk of flow and the wall interface, and the amount of wall area available for reaction. The first factor is represented by a mass transfer coefficient which depends on the molecular diffusivity of the traced substance. Chlorine diffusivity is equal to  $1.44 \times 10^{-5}$  cm<sup>2</sup>/s in water at 25°C. The amount of wall area available for reaction is equal to the surface area per unit volume, which equals 2 divided by the pipe radius.

The rate of reactant reactions that happen in at pipe walls is related to reactant's concentration in the bulk of flow as shown by Eq. (3):

$$R = (A/V) k_w C^n \tag{3}$$

Where R is the rate of reaction (mass/volume/time), (A/V) is the surface area per unit volume within the pipe which equals (4/pipe diameter), C is the chlorine concentration (mass/volume), n is the kinetics order = 0 or 1, and  $k_w$  is the wall reaction rate coefficient (length /time for n=1 and mass/area/time for n=0).

The EPANET is automatically adjusting, to account for mass transfer between the bulk flow and the wall, basing on the molecular diffusivity of reactant under study and the Reynolds number of the flow. In case of zero-order kinetics, which is recommended by the program manuals, the wall reaction rate cannot be greater than the mass transfer rate, resulting in Eq. (4):

$$r = MIN(k_w, k_f C)(2/R)$$
<sup>(4)</sup>

Where r is the rate of reaction (mass/volume/time),  $k_w$  is the wall reaction rate constant (mass/area/time),  $k_f$  is the mass transfer coefficient (length/time), C is the chlorine concentration (mass/volume), and R is the pipe radius (length).

#### 3. Methodology and Experimental Work

#### 3.1 Network Description

The study was performed on the drinking water supply network serving  $6^{th}$  of October City which has an approximate length of 1558.80 km. The treated water is being supplied by two WTPs:  $6^{th}$  of October WTP with a capacity of 86,400 m<sup>3</sup>/day, see Figure 1, and El-Shaikh Zayed WTP with capacity of 450,000 m<sup>3</sup>/day, see Figure 2.

The water distribution network model, which was considered in the current analyses, consists of main and secondary pipelines and feeders, neglecting the network distributaries and laterals. The network model, with a total length of 601,851 m, can be divided into 3 pipe materials as follows:

- 1) Ductile Iron pipes: it is the predominant pipe material, and represents about 573,453 m of the total modeled network length (95.28 %).
- 2) GRP pipes: it represents about 20,525 m of the total modeled network length (3.41 %).
- 3) Pre-stressed pipes: it represents about 7,873 m of the total modeled network length (1.31 %).

Field measurements of residual chlorine were measured instantaneously in field using Photometer 9300 device,

see Figure 3, at 9 selected fixed sampling points, as shown in Figure 4. The measurements were done once a week, on Mondays, between 11:00 am and 1:00 pm from October 2010 to January 2011.



Figure 1. General layout of 6<sup>th</sup> of October WTP and a sketch of the arrangement of its main treated water pipelines







## 3.2 Selection of Sampling Points

Locations of sampling points were selected according to certain factors such as populated zones, sampling point accessibility, existence of additional treatment units and sustainability of sampling points. There were some obstacles in taking water samples from specific areas, such as:

- 1) For the industrial zones, some of the existing factories have an in-door treatment unit which affects the characteristics of the taken water samples; and other factories didn't allow the sampling for security reasons.
- 2) Under-construction zones which are not inhabited yet.

Considering all these factors, the selected fixed points were as follows:

- 1) Dream land compound.
- 2) Classy residential district.
- 3) Second residential district.
- 4) Fourth residential district.
- 5) Sixth residential district.
- 6) Seventh residential district.
- 7) Ninth residential district.



Figure 3. Photometer 9300 device, testing equipment, and reagents



Figure 4. Network model of 6th of October City including locations of sampling points

## 3.3 Determination of Decay Coefficients

• Bulk Decay Coefficient

The bulk flow reactions depend only on chemical composition of distributed water. It is not affected by pipe characteristics or formed biofilm. So a laboratory test was conducted to calculate its value (Ozdemir *et al* 2002, Vieira *et al* 2004, and Haestad Methods 2003).

To estimate the first-order decay coefficient for bulk decay ( $k_b$ ), a water sample was taken from the distribution network. The water sample was then divided into 13 separated sub-samples each of 10 ml and put in a closed non-reacting glass bottles. After that, the 13 sub-samples were subjected to residual chlorine test successively using Photometer 9300. The first sub-sample was tested just after it was taken (at  $t_0$ ) followed by the other 12 sub-samples with a time gap of one hour between each ( $t_1, t_2, t_3 \dots t_{12}$ ), see Figure 5 (a).

This procedure was applied on 8 random water samples taken from the different sampling points during the sampling period. The measured chlorine concentrations were plotted versus time as indicated in Figure 5 (b). Then the bulk decay coefficient was taken equal to  $-0.033 \text{ h}^{-1}$  which has the highest regression coefficient (R<sup>2</sup> = 0.974) and corresponds to  $-0.792 \text{ day}^{-1}$ . The negative sign refers to reduction of chlorine residuals with time.





Figure 5. Determination of bulk decay coefficient in laboratory: (a) testing procedure, (b) first-order adjustment of the testing results for a certain sample

#### • Wall Decay Coefficient

Measuring wall decay coefficient in laboratories is difficult as it depends on water temperature and actual pipe wall conditions, such as: material, diameter, age, roughness, inner coating material, and biofilm formation. To overcome this difficulty, the wall coefficient was assumed to be the same for all network pipes, as the modeled network consists mainly from ductile iron pipelines, except for few GRP or pre-stressed pipes. Also, all network pipes were buried late 1970s, except for few pipelines which connect the existing network with El-Shaikh Zayed W.T.P. which were buried in late 1990s. An initial value of kw was assumed to be equal to - 4.0 mg/m<sup>2</sup>.day (Nagatani *et al* 2008), then it was corrected by trial and error to fit with the observed concentrations measured at different sampling points (as discussed later in model calibration).

#### 3.4 Hydraulic Modelling

The hydraulic model of the distribution network of  $6^{th}$  of October City (pipes, junctions, reserviors, and pumps) was taken form a consultant engineering office which was responsible for making a hydraulic modeling of the existing network and then improve and upgrade the network to overcome the current problems and to fit with the future needs of the city.

The water network was modeled for the maximum daily consumption data as the critical design case based on Egyptian Code for design and implementation of pipeline networks for drinking water and sanitation (HBRC 2007), see Figure 6, which differs from consumption data for the field-experimental working days.

In order to overcome this difference, data of flow rates exiting the water treatment plants serving 6th of October City over the 12 field-experimental weeks were collected and then data of both pumps and demands at network junctions were adjusted to fit with daily consumptions of 6<sup>th</sup> of October city assuming a daily consumption pattern based on Egyptian Code (HBRC 2007).



Figure 6. Water consumption pattern during the maximum daily demand

#### 4. Results and Discussions

#### 4.1 Analysis of Field Measurements

For each sampling point, variations in chlorine concentrations measured in field were analyzed. To evaluate these variations values of both standard deviation and coefficient of variation were calculated for each sampling point through the experimental period as illustrated in Table 1.

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Sampling Point	1	2	3	4	5	6	7	8	9
σ (mg/l)	0.25	0.26	0.19	0.17	0.14	0.22	0.22	0.16	0.23
C.V.	0.19	0.20	0.15	0.13	0.17	0.19	0.18	0.17	0.21

Table 1. Standard deviation and coefficient of variation values for different sampling points

The maximum value of standard deviation is 0.26 mg/l with a corresponding C.V. of 0.2 and occurs at sampling point (2). The standard deviation analysis indicates that the data points tend to be very close to the mean (due that the standard deviation is closer to zero than to unity) and hence it is concluded that chlorine concentrations measured in field are centralized for all sampling points and accordingly for the entire network.

## 4.2 Model Calibration

Model calibration was done to adjust the network model with field measurements in order to obtain reasonable results that simulates actual system behavior. In this study, model calibration was done to obtain the most suitable value of daily wall decay coefficient which contributes in chlorine decay throughtout the distribution network. The starting value was assumed to be equal to  $-4.0 \text{ mg/m}^2$ .day, as mentioned earlier.

For each sampling day, chlorine concentrations at each sampling point were calculated at different  $k_w$  values (-1, -4, -7, and -10). After that the error between field measurements and the EPANET estimated concentration was calculated (two values were considered *Error* and *Error*<sup>2</sup>). Finally, an average of the two  $k_w$  values result in zero *Error* and *Error*<sup>2</sup> was calculated for each sampling day and considered as the optimum  $k_w$  value to run EPANET analysis for that certain day.

## 4.3 Comparison of EPANET Results and Field Measurements

Free chlorine concentrations at each sampling point from both EPANET results and field measurements were drawn versus time (sampling days) on the same sheets. Also, absolute errors resulted from the calibrated EPANET model at each sampling point were calculated to obtain the error range resulted from EPANET for each sampling point. Moreover, statistical calculations were done on the absolute values of resulted errors to calculate the maximum absolute error (Max), the minimum absolute error (Min), the mean absolute error (MAE), the root mean square error (RMSE), and the standard deviation ( $\sigma$ ), see Figure 7.

Errors between the calculated chlorine concentrations obtained from the calibrated model and field measurements may be occurred due to some of analysis approximations, such as:

- 1) Variations in daily water demand pattern while a constant pattern was adopted when using EPANET.
- 2) Difference in measurement devices and accuracy between water treatment plants' devices and the study's device.
- 3) Adopting stepwise presentation for 2-hrs-gaped chlorine records taken from water treatment plants.
- 4) Constant values of k<sub>b</sub> and k<sub>w</sub> were adopted in EPANET neglecting temperature effect on kb (due that the study was performed during winter) and pipe material effect on k<sub>w</sub> (due that 95% of the network is ductile iron).





Figure 7. Field measurements and EPANET results of free chlorine concentration at sampling point no. (3): (a) comparing measured and calculated values and resulted errors, (b) statistical analyses of the resulted errors

MAE

RMSE

Max

## 4.4 Error Analysis Based on Point Location and Water-age

0.0

Mm

Chlorine decay, without neglecting other affecting factors, is a time-based phenomenon which depends mainly on how much time is available for bulk reactions to take place and how long the drinking water is in contact with the pipe wall to allow wall reactions to take place. As the flow velocities in network pipes changes every hour according to the hourly consumption pattern and , also, changed daily according to the daily flow rates supplied in the water network, the time spent by water since it exits the WTP until it reaches the sampling point is the governing factor in comparison.

For a given sampling day, water-age was evaluated for each sampling point using EPANET at the moment of time when chlorine concentration was measured in field. Flow conditions and water consumption rates needed for the analysis were discussed previously in section 3.5. After getting water-age of each point the average of the 12 points' was calculated and named "Average Water-Age", see Table 2.

Sampling Point No.	Water-Age from EPANET (hrs)
1	5.00
2	2.00
3	2.00
4	3.00
5	4.00
6	3.00
7	4.00
8	5.00
9	3.00
Average water-age	3.40

Table 2.	Average	dailv	water-age	for sa	mpling	dav	(1)
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This step was repeated for the 12 sampling days, and then the sampling points' locations were classified as shown in Table 3. For each sampling day, points that have water-age that is always above the "Average" for the whole 12 sampling days were named "*Near*". Points that have water-age that is always below the "Average" for the whole 12 sampling days were named "*Far*". And finally, points that have water-age that is hesitating around the "Average" during the whole 12 sampling days were named "*Intermediate*".

Table 3.	Classification	of sampling	points based	on water-age	analysis.
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Point classification	Near	Intermediate	Far
Sampling Point No.	2, 3, 4, 6, and 9	1 and 7	5 and 8

Figure 8 shows the statistical results for different sampling points where sampling points on horizontal axis were arranged according to their location classification. It was noticed that for near points the resulted errors were generally smaller than those at far points.

#### 4.5 Chlorine Prediction

Since selection of sampling points' locations was affected by some constrains, evaluation of the effectiveness of the current chlorination system applied in the existing water treatment plants serving  $6^{th}$  of October Water Network was pursued by predicting chlorine concentration at different network nodes at different locations inside and outside the study area using the calibrated model. Both locations, inside and outside, are very important due that both not only water quality, but also, consumer location in the water distribution network can influence the perception of water consumer greatly (Turgeon *et al* 2004).





Figure 8. Statistical analyses of the resulted errors at different sampling points according to sampling point classification

For network nodes outside the study area, the selection stressed on those nodes located at network extremities. This selection was adopted to help in identifying the required improvements needed for the existing network, especially as hydraulic studies are being performed to increase the amount of supplied treated water by constructing a new water treatment plant including upgrading the existing network to accommodate the increasing flow rates.

The selected prediction nodes were divided into two groups as shown in Figure 9:

- <u>Group (1)</u>: nodes locate outside the study area, from node (A) to (D).
- <u>Group (2):</u> nodes locate inside the study area, node (E) and (F).

The chlorine concentrations at the selected prediction nodes, from A to F, were predicted using the calibrated model for 4 randomly-selected days; day (3), (7), (10), and (12); throughout the 24-hours working hours. The average daily chlorine concentration and the average daily water-age for each point of sampling and prediction points were calculated to study the effect of water-age on the predicted chlorine concentrations. The predicted average daily chlorine concentrations were then compared with results at three different sampling points (points (1), (3), and (5)). For each day of the 4 randomly-selected sampling days, the average daily chlorine concentration and the average obtained from EPANET were drawn as shown in Figure 10.





Figure 9. Location of both prediction and sampling points on network model







(b) Day (12) - Avg. Daily Chlorine Concentration 2.0 1.5 1.0 mg/l 0.5 0.0 3 F 1 E 5 A в С D Points

Points





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The vertical axes represent either the average daily chlorine concentration in (mg/l) or the average daily waterage in (hrs), while the horizontal axis represents both sampling and prediction points arranged in ascending order according to the average daily water-age of each point.

The following notes were concluded:

- 1) The average daily chlorine concentration, at both of the selected prediction-points and the sampling points, decreases as the average water-age increases.
- 2) For prediction points located at network extremities (i.e. A, B, C, and D) and according to EPANET results, predicted chlorine concentrations did not recede the minimum allowable chlorine limit established by the Egyptian Code (HBRC 2005), even when water-age exceeds 24 hours.
- 3) Within the study area, the average daily water-age did not exceeded 10 hours and the average daily chlorine concentrations were higher than the minimum allowable chlorine limit.
- 4) The average water-age in day (3) was a little bit smaller than that of days (7), (10), and (12) as the total flow rate was higher.

#### 5. Conclusions

Based on the study results it can be concluded that:

- 1) Good water quality, with respect to chlorine concentration, is achieved within the study area.
- 2) Error resulted from the calibrated EPANET model was centralized during the study.
- 3) Errors between model results and field measurements could be due to:
  - i. Variations in daily water demand pattern while a constant pattern was adopted when using EPANET.
  - ii. Difference in measurement devices and accuracy between water treatment plants' devices and the study's device.
  - iii. Adopting stepwise presentation for 2-hrs-gaped chlorine records taken from water treatment plants.
  - iv. Constant values of  $k_b$  and  $k_w$  were adopted in EPANET neglecting temperature effect on kb (due that the study was performed during winter) and pipe material effect on  $k_w$  (due that 95% of the network is ductile iron).
- 4) The statistical measurements of Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) were found to be better indicators than Min, Max, and  $\sigma$  when evaluating the resulted error from the calibrated EPANET model.
- 5) At network nodes having low water-age, EPANET model showed good accuracy in simulating chlorine decay and predicting chlorine concentration.
- 6) In 6<sup>th</sup> of October distribution network, chlorine concentration at network nodes that have an average daily water-age greater than 24 hours did not recede the minimum allowable limit established by the Egyptian Code of Practice (HBRC 2005).
- 7) In case of expanding the populated zones beyond the current area in 6<sup>th</sup> of October distribution network, it is recommended to check whether chlorine concentrations at extremity points will or will not recede the minimum allowable chlorine concentration.
- 8) When modifying the existing 6<sup>th</sup> of October distribution network to account for increasing in future water demands, it is recommended to avoid increasing water-ages at network extremities in order not do decrease the available chlorine concentration. This could be achieved by choosing an appropriate location for the new WTP and improving water circulation.

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