EVALUATION AND MODELING OF TRIHALOMETHANES CONCENTRATIONS ON BANI SUEF WATER DISTRIBUTION NETWORK

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ABSTRACT

There is a serious challenge in achieving the balance between destroying pathogenic organisms by chlorination and reduction of trihalomethanes (THMs) under safe limits. This study aimed to develop an empirical mathematical model for the THMs concentrations prediction in water distribution networks (WDN) having multiple water treatment plants (WTPs) by studying the Bani Suef water distribution network (BSWDN), Egypt, as a case study. Various parameters such as; pH, bromide ion, free residual chlorine, temperature and THMs were measured for drinking water samples that were collected from fifteen sampling points according to monthly sampling program was undertaken between February and September 2015. THMs concentrations of all samples were less than 100 µg/L below the WHO guideline values. An empirical mathematical model has been developed based on frequent THMs testing and by statistical analysis using statistical package for social sciences (SPSS) software to validate and improve the developed model to predict THMs at any points on the WDN or at the exit of WTPs on BSWDN according to close agreement with the measured THMs (R^2 = 0.77). Good results have been obtained from a previous mathematical model which was modified and applied to predict THMs only at any points after determining the overall THMs formation yield value for BSWDN (Y = 27.7277 µg/mg) through the field study period.

Keywords: Trihalomethanes, Chlorination, Modeling, Drinking water quality

1 INTRODUCTION

Disinfection is a chemical process which usually involves using disinfectants such as chlorine, chloramines or ozone, which can destroy pathogenic organisms. Disinfection is the most important step in drinking water treatment to supply safe drinking water (WHO 2006). Disinfectant residual maintained in the WDN is practiced mainly for three main objectives; minimize formation of bacteria, provide an additional safeguard against exogenous pathogenic intrusion, and act as an indicator for the integrity of the WDN (Laurent et al. 2005). Chlorine and its compounds are the most commonly used disinfectants for water treatment due to its high oxidizing potential, high half life, and relatively low cost (Gopal et al. 2007). In 1976 it was discovered that disinfection by-products (DBPs) were produced during the disinfection process because of reaction occurs between chlorine and natural organic matters (NOM) found in rivers and canals (Marhaba and Washington 1998). According to Gopal et al. (2007), chlorination DBPs such as trihalomethanes (THMs) and haloacetic acids (HAAs) are well known carcinogenic substances and linked to cancer. In 2006, the United States Environmental Protection Agency (USEPA) provided an explicative article about reducing the THMs and HAAs concentrations in drinking water (USEPA2006). Exposure to THMs concentrations leads to cause not only cancer but also collapse of the functions of the kidney and liver, retarded fetus growth, and birth defects (Shehawy and Awad 2012). Because of these risks WHO requires that THMs concentration at the consumer's tapnot to exceed 100 µg/L. Major components of THMs are;

chloroform ($CHCl_3$), bromodichloromethane ($CHCl_2Br$), chlorodibromomethane ($CHClBr_2$) and bromoform ($CHBr_3$). In general chloroform represents the most expanded of these components (Farren et al. 2003).WDN with surface water sources always contain higher DBPs because of high levels of NOM in these sources than groundwater sources. Water quality through WDN which fed by multiple sources is better than fed by single one (Shehawy and Awad 2012). Since 1976, a lot of researches have been intensive efforts to find various parameters affecting THMs formation within WDN which are as follows: the disinfectant type and dose, pH, water age, water temperature, NOM concentration and total organic carbon (TOC) concentration (Chowdhury et al. 2009; Basiouny et al. 2008). After detailed studies these researches have been reached that if the previous parameters are higher, higher THMs concentrations are expected (Nikolaou and Lekkas 2001; Nikolaou et al. 2004a, b; USEPA 1999 b). These researches have been investigated and developed empirical mathematical models that can estimate THMs in WDN depending on these previous multi parameters (Shehawy and Awad 2012, Ristoiu et al. 2009, Basiouny et al. 2008, Al-Omari et al. 2004 and I. Toroz and V. Uyak 2004).

Two main objectives of this paper are; the first is to apply previous five mathematical models to predict THMs concentrations at BSWDN to reach the best model which give good results according to the measured THMs through the field study period. Another previous mathematical model (sixth model) was applied to estimate THMs at any point on the BSWDN after modifying the calculations of its parameters (due to multiple WTPs) and determining the THMs yield factor Y, micrograms of THMs formed per one mg consumed of chlorine up to the point of THMs measurement (James Philip Cooper, 2009). The second purpose is to develop an empirical mathematical model to predict THMs concentrations at the end of WTPs or at any point of the BSWDN as a function of various parameters such as, free chlorine, TOC, pH and Br-, by statistics analysis using SPSS program.

2 METHODOLOGY

2.1 Study Area and System Description

This research is conducted in BSWDN that feed Bani Suef city and its surrounding villages. Bani Suef is an Egyptian city, approximately 124 km south of Cairo, lies in the west bank of the River Nile located at the northern latitude earth grid 29º 04` and east longitude earth grid 31º 05`, with an altitude varying from 55 m above sea level. The population of Bani Suef City with its surrounding villages is around 578006 capita (banisuef.gov.eg, 2015). BSWDN is fed by six WTPs (surface water sources from River Nile and Ibrahimiya main canal) with total treated water production is about 184,896 m^3/d. There are three elevated tanks (all are not in service) and there are not any booster pumps. Distribution network pipes have lengths about 168 Km with diameters ranged between 125 to 1200 mm of different materials have been shown in the figures 1, 2.General layout of BSWDN is shown in figure 3.

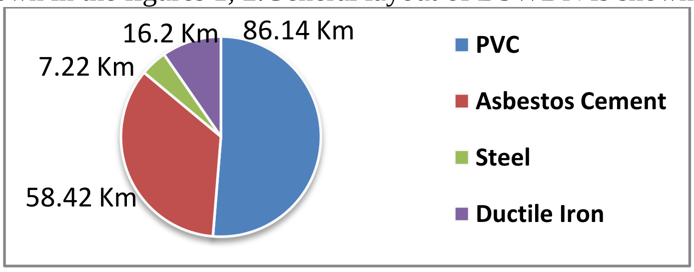


Figure 1. Distribution of pipe materials with lengths (Km) of BSWDN

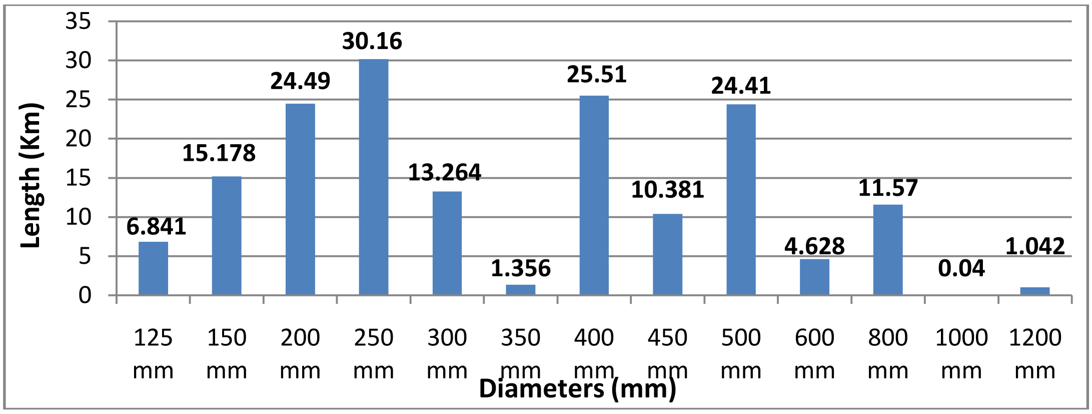
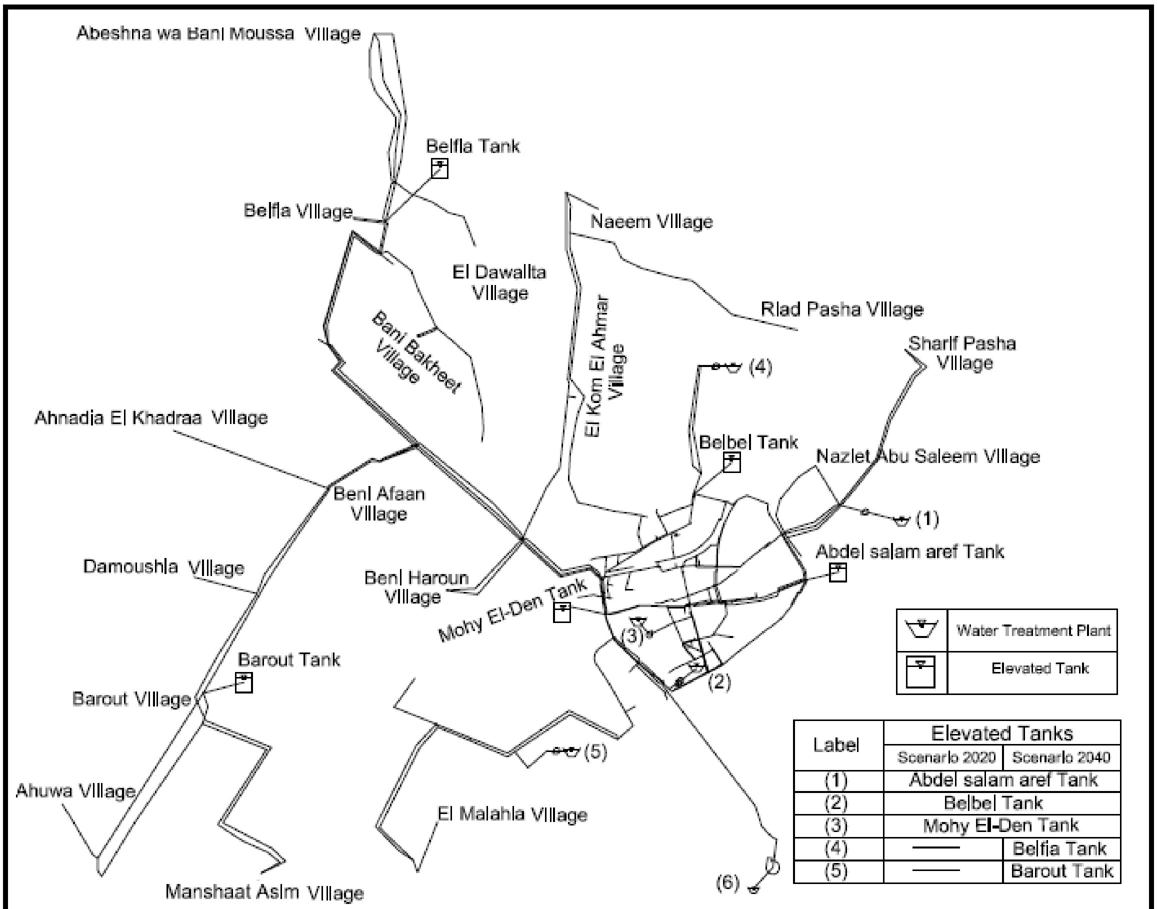


Figure 2. Distribution of pipe diameters (mm) with lengths (Km) of BSWDN



Label	Elevated Tanks	
	Scenario 2020	Scenario 2040
(1)	Abdel salam aref Tank	
(2)	Belbel Tank	
(3)	Mohy El-Den Tank	
(4)	——	Belfia Tank
(5)	——	Barout Tank

Label	Water Treatment Plants	Characteristics						
		Type of treatment	Average yield (L/Sec)		Water source	Main Pumps		
						No.		Head (m)
			2020	2040		2020	2040	
(1)	Abo Sleem	Conventional	500	1500	River Nile	4	6	60
(2)	American	Conventional	600	800	River Nile	4	5	45
(3)	British	Conventional	200		River Nile	3		45
(4)	Halabiya	Direct filtration	160		Ibrahimia Canal	2		45
(5)	New bani suef WTP	Conventional	600		River Nile	4		45
(6)	Riad Pasha	Direct filtration	80		Ibrahimia Canal	2		45

Figure 3. General layout of BSWDN with six WTPs and three elevated tanks

2.2 Experimental Set-Up

Sampling program started in February and ended in September 2015, was conducted monthly to collect drinking water samples from fifteen points located in BSWDN, six points represented the exit of the WTPs, eight points represented the farthest villages and the last point represented the center of the city. Samples were collected and stored in 40-ml dark brown glasses bottles and closed with Teflon lined screw caps. Each sampling point was represented by 2 samples in 2 bottles with adding sodium thiosulfate ($Na_2S_2O_3$ – 2.5 mg/l) to prevent more formation of THMs by quenching free Cl_2 in the bottle, after that, bottles were saved at 4^0C until making the laboratory analysis using Agilent (7890A) Gas Chromatography (THMs µg/L) and Analytical Technologies-TOC Analyzer (TOC, mg/L). While pH, temperature (C^0), free residual Cl_2 and Br- (mg/L) were measured at the site using HANNA–HI83200 Multi parameter Ion Specific Meter. Modeling of the implemented case of BSWDN was performed using WaterCad, a software developed by Haestad Methods (Bentley WaterCad V8, 2007), by hydraulic solutions ($C_{H.W}$ = 90, 110, 120 and 140 for AC, Steel, DI and UPVC pipes, respectively) to calculate the travel, which used in the previous predictive models to estimate THMs concentrations, (the time water takes from the feeding stations to reach to any point). Figure 4 shows samples location on BSWDN.

Table 1. Samples locations with its codes on BSWDN

Sample Code	Sample Location	Sample Code	Sample Location
ABTw	Abo SleemWTP effluent	MAVd3	Sample (3), Manshaat Asim village
AMTw	American WTP effluent	DVd4	Sample (4), Damoshia village
BRTw	British WTP effluent	AHKHVd5	Sample (5), Ahnasia Elkhadraa village
HATw	Halabiya WTP effluent	DWVd6	Sample (6), Dwalita village
NBSTw	New BaniSuef WTP effluent	NVd7	Sample (7), Naeem village
RPTw	Riad Pasha WTP effluent	BHVd8	Sample (8),Bani Haroun village
ABVd1	Sample (1), Abshna village	BSC	Abd Elslam Aref st., BaniSuef City
AHVd2	Sample (2), Ahwua village		

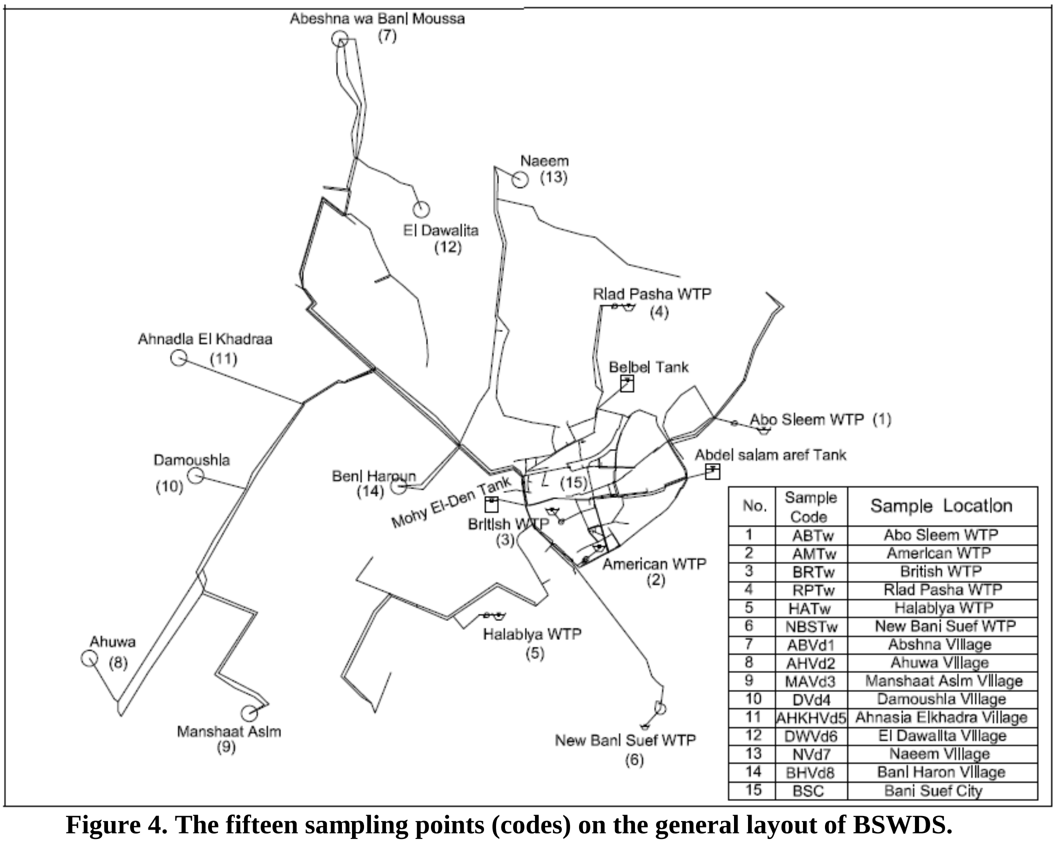


Figure 4. The fifteen sampling points (codes) on the general layout of BSWDS.

3 RESULTS AND DISCUSSIONS

3.1 Analysis of Field Samples

According to sampling program, the following figures 4, 5, 6, 7, 8 and 9 show the concentrations of Cl_2, TOC and Br^- at the exit of the six WTPs and the nine points, respectively, on BSWDN during the field study period.

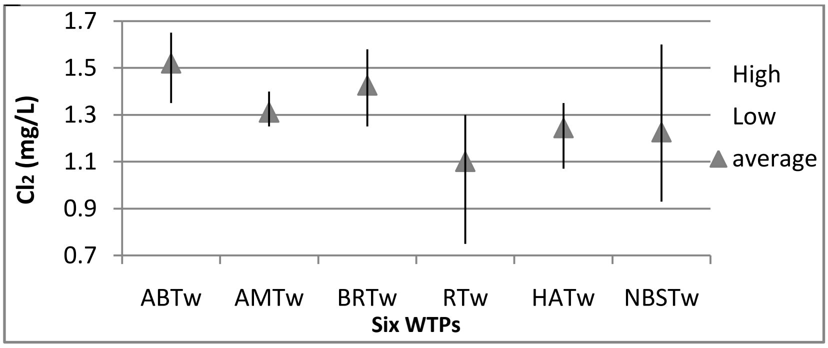


Figure 4. Concentrations of free residual chlorine at the exit of WTPs on BSWDN

The average concentrations of free residual chlorine at the WTPs ranged between 1.1 to 1.52 mg/L

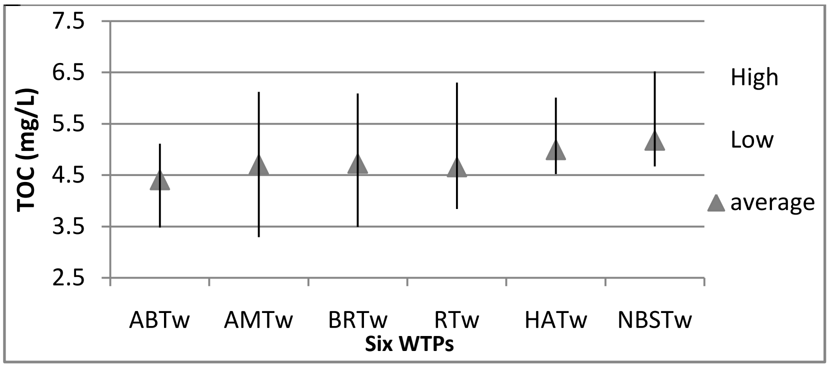


Figure 5. Concentrations of TOC at the exit of WTPs on BSWDN

The average concentrations of TOC at the WTPs ranged between 4.406 to 5.176 mg/L

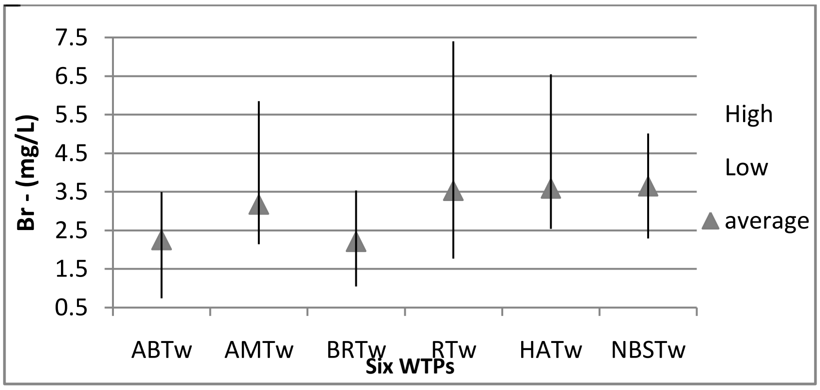


Figure 6. Concentrations of free bromide ion at the exit of WTPs on BSWDN

The average concentrations of Br- at the WTPs ranged between 2.202 to 3.644 mg/L

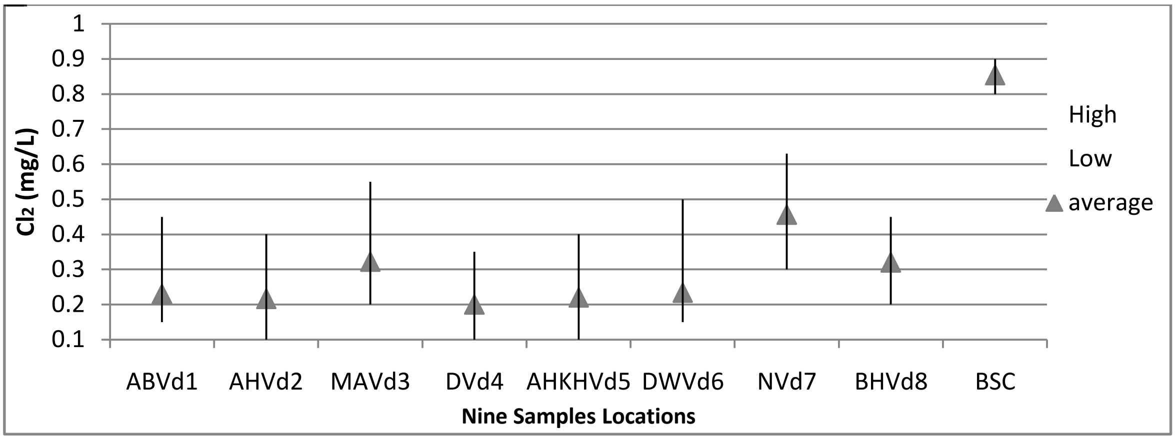


Figure 7. Concentrations of free residual chlorine at the nine points on BSWDN

The average concentrations of free residual chlorine at the nine points ranged between 0.2 to 0.854 mg/L

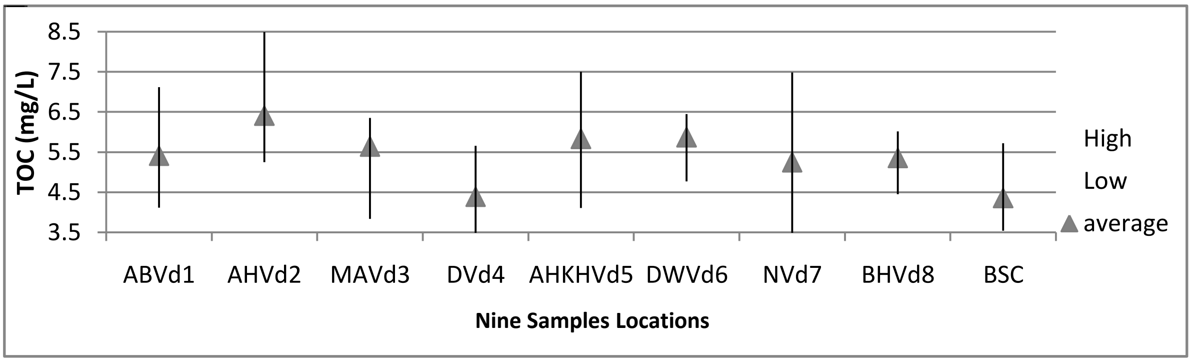


Figure 8. Concentrations of TOC at the nine points on BSWDN

The average concentrations of TOC at the nine points ranged between 4.358 to 6.412 mg/L

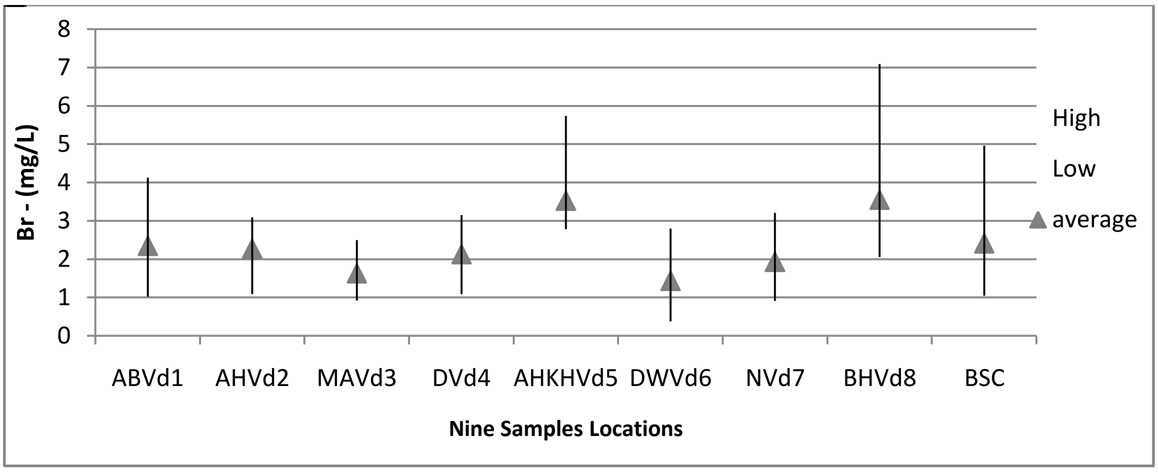


Figure 9. Concentrations of free bromide ion at the nine points on BSWDN

The average concentrations of Br- at the nine points ranged between 1.436 to 3.554 mg/L

THMs concentrations for all samples were under 100 µg/L (allowable limit according to Egyptian limitation). THMs of one sample, at Abeshna Village in 16/4/2015, was 96.65 µg/L (relative high concentrations) because of high TOC concentration and initial THMs from the WTPs. Figures 10, 11 show average THMs concentrations at the six WTPs effluent and the nine points, respectively, during the sampling period.

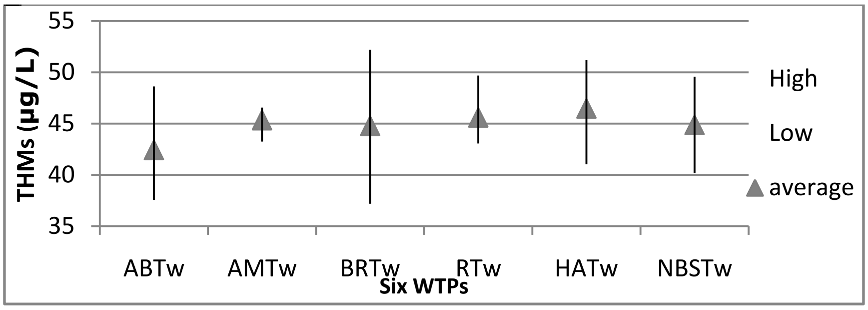


Figure 10. Concentrations of free THMs at the exit of WTPs on BSWDN

The average concentrations of THMs at the WTPs ranged between 42.43 to 46.48 µg/L

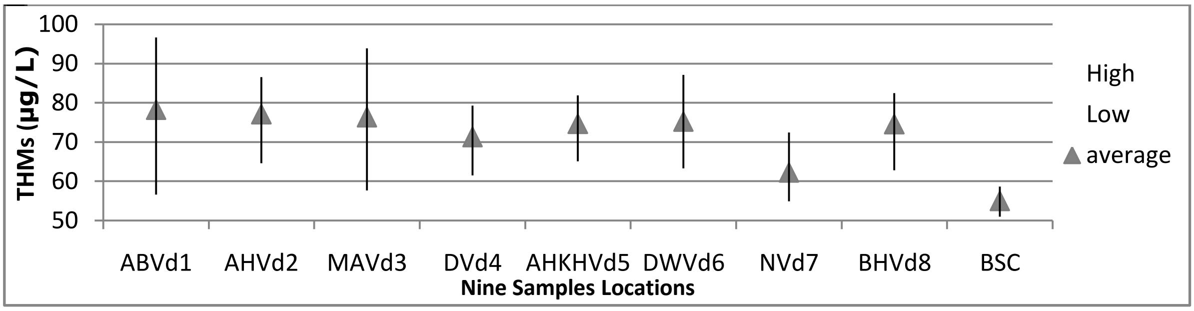


Figure 11. Concentrations of THMsat the nine points on BSWDN

The average concentrations of THMs at the nine points ranged between 55.0 to 78.26 µg/L

Analysis determined that $CHCl_3$ and $CHCl_2Br$ represented about 54.9% to 64.1% and 31.1% to 39.7% of the total THMs concentration, respectively. $CHClBr_2$ represented the reset of THMs. $CHBr_3$with very low concentration. Figures 12, 13 show THMs concentrations with its components at the exit of the six WTPs and at the nine points on BSWDN, respectively, during the sampling period.

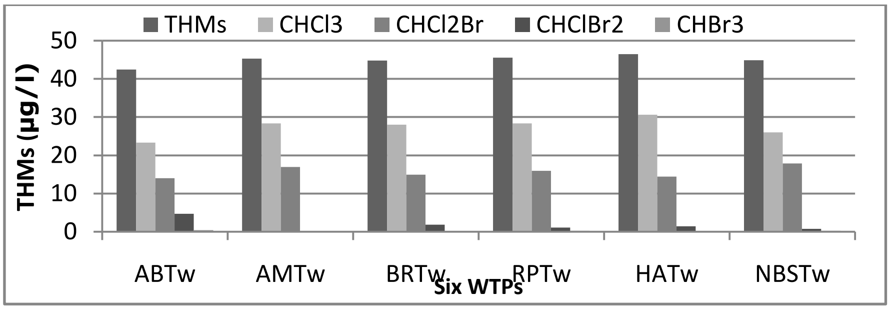


Figure 12. Averaged measured THMs with its components (µg/L)at the six WTPs

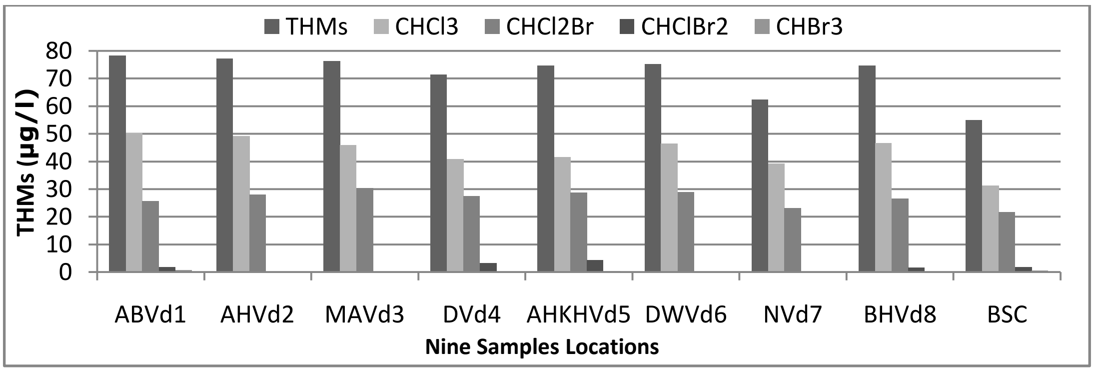


Figure 13. Averaged measured THMswith its components (µg/L) at the nine points

3.2 Prediction of THMs

3.2.1 Previous Empirical Mathematical models for THMs prediction

In this study, five previous empirical mathematical models have been applied to predict THMs concentration at BSWDN as shown in next table (2).

Table 2. Predicted THMs from empirical models and goodness of fit statistics

No.	Empirical Models	n	k	R^2	R^2_{adj}
1	$THMs = (0.0143)(Temp)^{0.128}(t)^{0.36}(pH)^{2.729}(TOC)^{0.203}$ (Basiouny et al. 2008)	4	45	**- 12.16**	**- 11.266**
2	$THMs = (0.00441)(Temp)^{3.172}(Cl2)^{0.538}(pH)^{0.722}(t)^{0.309}$ (Ristoiu et al. 2009)	4	45	**- 230369.6**	**- 76789.23**
3	$THMs = (4.527)(t)^{0.127}(Cl2)^{0.595}(TOC)^{0.596}(Br)^{0.103}(pH)^{0.66}$ at temperature = 20 ^{0}C, $C_T = C_{20}\, e^{t(kT - k20)}$ C_T THMs concentrations at temperature(T^0C) C_{20} THMs concentrations at temperature (20^0C) K_T THMs growth rate at temperature (T^0C) K_{20} THMs growth rate at temperature ($20\ ^0$C) t Contact time(minutes) **Temp (^{0}C)** / **Kt (mint $^{-1}$)**: 15 / 0.0020; 20 / 0.0024; 25 / 0.0029; 30 / 0.0037 (Al-Omari et al. 2004)	5	45	**- 515.87**	**- 468.88**
4	$\log(THMs) = 1.078 + 0.398\log(TOC) + 0.158\ \log(Temp) + 0.702\ \log(CL)$ **CL;** is the sum of pre and post chlorine dose at WTPs. (I. Toroz and V. Uyak 2004)	3	45	**- 41.84**	**- 39.89**
5	$THMs = -11.19\,(Cl2) - 0.14(TOC) + 7.3135\,(pH) + 4.99(Br) - 0.959$ (Shehawy and Awad 2012)	4	45	**- 1.19**	**- 1.0386**

Contact or travel time (t) was estimated by the model of the implemented case of BSWDN using WaterCAD program.

So, it`s clearly shown that all of these models can`t be used at BSWDN. Figure 14 shows the difference between the measured and predicted THMs from each one.

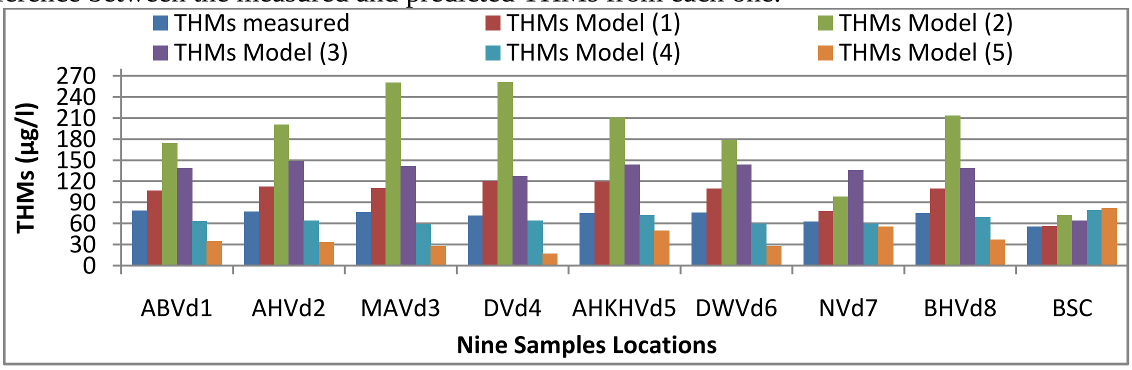


Figure 14. Averaged measured andpredicted THMs by the five empirical models

3.2.2 Development of the Previous Empirical Mathematical Model for Predicting THMs (James Philip Cooper, 2009)

A previous empirical mathematical model has been already developed and applied in two cities Norwalk and Barberton, Canada (James Philip Cooper, 2009) for predicting THMs at any point on the WDN in terms of initial THMs ($THMs_0$) leaving the feeding source and the amount of the consumed chlorine at the same point after determining the overall THMs formation yield (**Y**) in μg/mg by the measurements of sampling period of this study.

$$(THMs)_{at\ any\ point} = (THMs_0)_{av} + \mathbf{Y} \times (Cl_2\ consumed)$$

$$\text{and, } (Cl_2)_{consumed\ at\ any\ point} = initial\ (Cl_2)_{av} - free\ residual\ (Cl_2)_{measured\ at\ this\ pint}$$

Predicting THMs at any time on BSWDN by applying this model can be performed in two main steps;

1-Calculating $THMs_0$ and Cl_2as average concentration from the six WTPs as follow;

$$\frac{(THM1 * Q1) + (THM2 * Q2) + (THM3 * Q3) + (THM4 * Q4) + (THM5 * Q5) + (THM6 * Q6)}{(Q1 + Q2 + Q3 + Q4 + Q5 + Q6)}$$

$$\frac{(C1 * Q1) + (C2 * Q2) + (C3 * Q3) + (C4 * Q4) + (C5 * Q5) + (C6 * Q6)}{(Q1 + Q2 + Q3 + Q4 + Q5 + Q6)}$$

Where; THM1 and C1 are the concentration of the $THMs_0$ and the initial Cl_2 in the exit flow (Q1) from ABTw. Similarly (THM2 and C2)in Q2, (THM3 and C3)in Q3, (THM4 and C4) in Q4, (THM5 and C5)in Q5 and (THM6 and C6)in Q6forAMTw, BRTw, HATw, RPTw and NBSTw, respectively.

2-Calculating the overall THMs formation yield (**Y** factor) during the sampling period (table 5 illustrates the results of $THMs_0$ and Cl_2 to calculate **Y**, from 27 measurements represented the first three months of measurements).

Table 5. Determining the overall THMs formation yield (Y factor)

Date	THMs av (μg/l)	Cl_2av (mg/l)	Y (μg/mg)
15 / 2 / 2015	45.413	1.275	32.13
16 / 4 / 2015	47.82	1.50	25.64
9 / 5 / 2015	43.64	1.281	25.41
Average **Y**	(32.13+25.6431+25.41) / 3 = **27.7277 μg / mg**		

By determining the average concentrations of $THMs_0$ and Cl_2 at 8/6/2015 and 16/9/2015 were (41.61,1.268) and (44.352, 1.344), respectively.

Table 7. Predicting THMs concentrations for last months of measurements

Samples code	8 / 6 / 2015		16 / 9 / 2015	
	$THMs_{measured}$	$THMs_{estimated}$	$THMs_{measured}$	$THMs_{estimated}$
ABVd1	65.93	77.459	56.67	64.291
AHVd2	76.45	78.845	64.62	65.678
MAVd3	63.80	73.022	57.70	61.518
DVd4	79.25	76.073	66.55	67.064
AHKHVd5	75.22	77.459	65.14	65.678
DWd6	71.46	75.518	63.33	62.905
NVd7	72.41	67.754	59.96	61.518
BHVd8	65.51	73.30	62.85	64.291
BSC	54.31	58.05	58.66	51.814

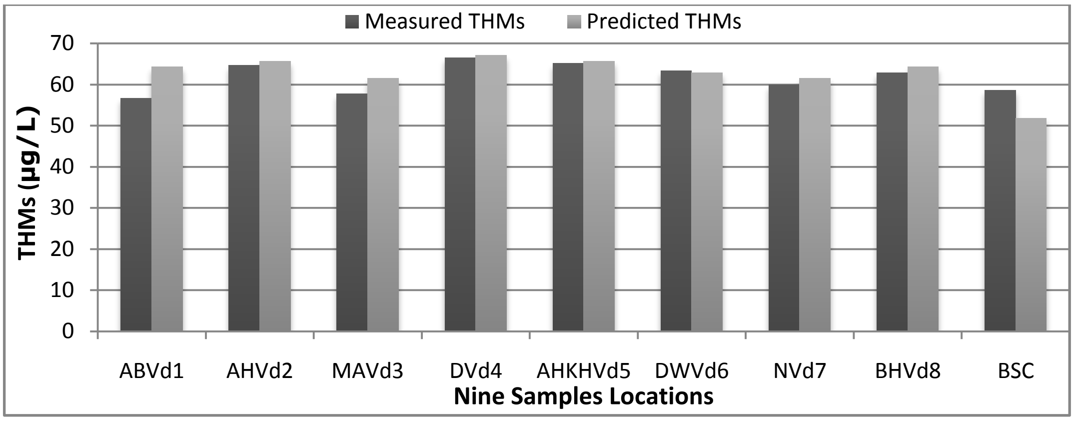


Figure 17Averaged measured andpredicted THMs by the model (6) at 8 / 6 / 2015

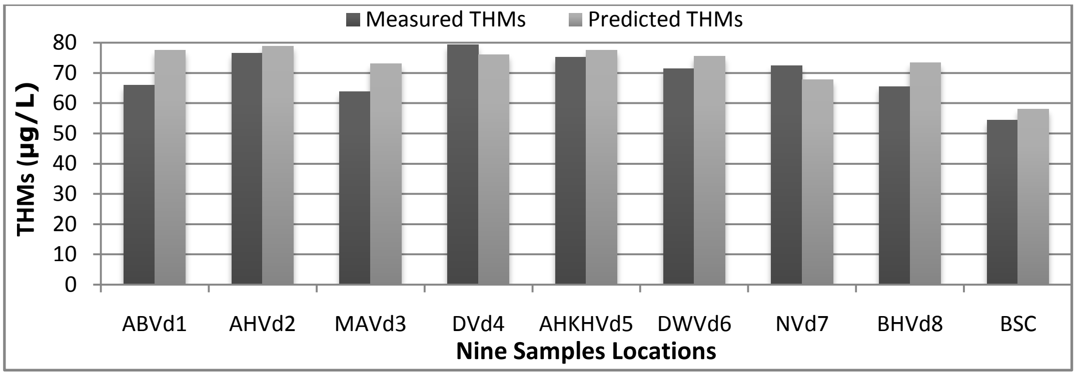


Figure 18. Averaged measured andpredicted THMs by the model (6) at 16 / 9 / 2015

3.2.3 Prediction of THMs Concentration by New Developed Empirical Mathematical Model

Statistical Package for Social Sciences (SPSS) software was used to create a multiple linear regression model for THMs formation. New empirical model has been developed to predict THMs (µg/L) as function of parameters such as; free residual Cl_2, TOC, Br- (mg/l) and pH, during the sampling period, as follow;

$$THMs = \mathbf{a1}*(Cl_2) + \mathbf{a2}*(TOC) + \mathbf{a3}*(Br) + \mathbf{a4}*(pH) + \mathbf{a5}$$

Where; **a1= - 25.824004, a2 = 1.817187, a3 = - 0.066221, a4 = - 0.402593 and a5 = 73.57234.**

Figures 15, 16 show the measured and predicted THMs from this new model at the six WTPs and the nine points on BSWDN, respectively. The statistics parameters are determined; **n=75**, **k=4**, $\mathbf{R^2=0.774}$ and $\mathbf{R^2_{adj}=0.761}$, respectively.

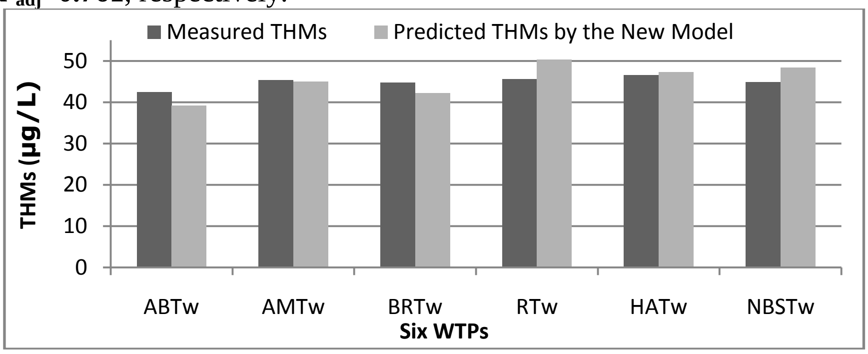


Figure 15. Averaged measured andpredicted THMs by new Developed model

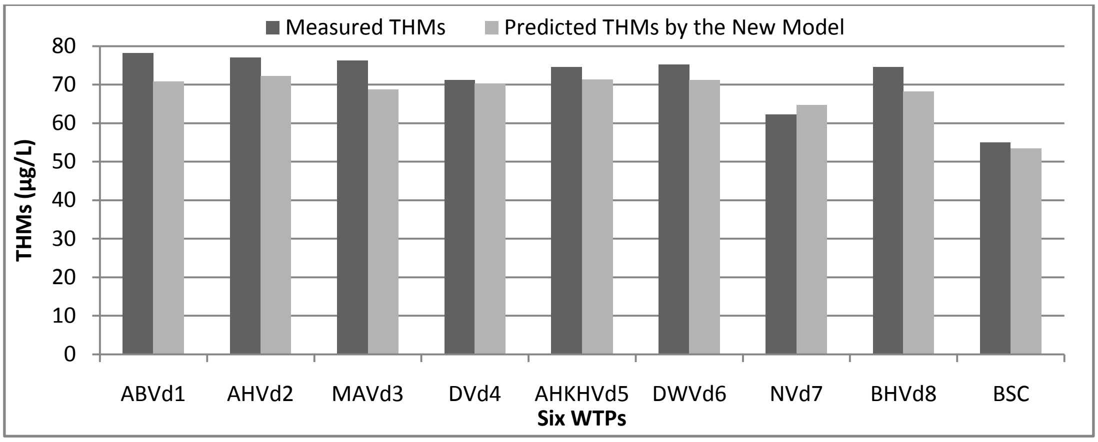


Figure 16. Averaged measured andpredicted THMs by the new Developed model

4 CONCLUSION

THMs concentrations of all samples were less than 100 µg/L (the allowable limit according to the Ministry of Health No.458 of 2007). Chloroform ($CHCl_3$) and bromodichloromethane ($CHCL_2Br$) represented about 59.9 % and 35.4 %, respectively, which are the major fraction of THMs in BSWDN. Five of six previous empirical mathematical models couldn`t give acceptable results for THMs prediction at BSWDN because the water quality, operational conditions and models parameters at WDN of these models are not similar to BSWDN, while the results of the predicted THMs concentration at any point on BSWDN obtained from the sixth model, that was modified and applied after calculating the overall THMs formations yield for BSWDN during the sampling program period (Y=27.72 µg/mg), were close agreement with the measured THMs concentrations. A new empirical mathematical model was developed by multiple regression models using SPSS program to estimate THMs at the ends of WTPs or at any point on BSWDN with R^2 = 0.77 as follow:

$$THMs = \mathbf{25.824}*(Cl_2) + \mathbf{1.817}*(TOC) + \mathbf{-0.066}*(Br) + \mathbf{-0.403}*(pH) + \mathbf{73.572}$$

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