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MODELING OF TRIHALOMETHANES IN BENHA WATER SUPPLY NETWORK

نمذجة مركبات التراي هالوميثان في شبكة مياه الشرب بمدينة بنها

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الملخص العربي

في هذا البحث تم ايجاد وتقييم تركيز مركبات التراي هالوميثان (Trihalomethane) الموجودة في شبكة مياه الشرب بمدينة بنها. ولقد تم عمل ذلك معمليا بقياس تركيز مركبات التراي هالوميثان شهريا في ستة أماكن مختلفة وموزعة في شبكة مياه الشرب لمدينة بنها. ولقد تم تقييم تلك النتائج بعمل نموذج رياضي يمكن به تقدير تركيز مركبات التراي هالوميثان التي توجد في شبكة مياه الشرب لمدينة بنها باستخدام القياسات الميدانية لجرعة الكلور المبدئي والكربون العضوي الكلي وأيون البروم وزمن المكث ودرجة الحرارة والعد الكلي للطحالب والرقم الهيدروجيني خلال فترة الدراسة في الشبكة. ولقد تم تقييم النموذج الرياضي بمقارنة نتائجه بالنتائج التي تم قياسها معمليا في الشبكة خلال فترة الدراسة. ولقد تم ايضا استخدام برنامج EPANET للحصول على زمن انتقال مياه الشرب من محطة التنقية حتى الأماكن التي تم عندها قياس تركيز مركبات التراي هالوميثان. ولقد تم استخدام ذلك الزمن في النموذج الرياضي. و أظهرت النتائج تشابه النتائج المقاسة معمليا مع النتائج المستنتجة باستخدام النموذج الرياضي حيث كان الاختلاف بينهما يتراوح ما بين 4,5% إلى 9,9%. لذلك يمكن استخدام ذلك النموذج الرياضي للتنبؤ بخواص المياه في شبكات توزيع مياه الشرب وتحديد تركيز مركبات التراي هالوميثان فيها.

ABSTRACT

The presence of total trihalomethane (THMs) in Benha Water Supply Network (BWSN) was determined and evaluated in this research. Six sampling points located at different distances from the main water reservoirs, were selected in BWSN in order to follow the evolution of THMs. The gained information from the monthly sampling and laboratory analysis program was used to formulate relationship of total trihalomethanes (THMs) concentration in terms of initial chlorine dose, total organic carbon, bromide ion concentration, contact time, temperature, algae, and pH. To define the accuracy level of the developed model, the predicted THMs concentrations from the developed model were compared to actual THMs concentrations measured during the monitoring period. The developed mathematical model and software (EPANET), which was used to determine water age, were used to predict THMs concentrations throughout BWSN. The results showed close agreement between the measured and calculated THMs concentration. Hence the difference in the average calculated values and measured values during the study period ranged from (4.6% to 9.9 %). The model can provide reasonable results for most of the functioned variables and can be used to have a rapid assessment of the trihalomethanes formation.

Keywords

Trihalomethanes Modeling, Chlorine modeling, Drinking water quality, Distribution systems.

INTRODUCTION

Disinfection by-products (DBPs) are formed when chlorine is added to water that contains naturally-occurring aquatic organic matter. The DBPs created by this reaction include two important groups: haloacetic acids (HAAs) and trihalomethanes (THMs). Both are of significant concern because they include known or suspected human carcinogens. As trihalomethanes are related to the well being of the community, there has been intensive efforts in the last three or four decades to study their formation in drinking water, and simulate their propagation systems.

A very powerful technique that is starting to be used by utilities for assesment the levels of THMs is mathematical modeling of DBP formation. Power function models have been widely applied to complex and poorly understood chemical systems such as the reactions between chlorine and disinfection byproduct precursors. An example is the general multiparameter model that includes terms for quantity of organic matter (TOC), reactivity of organic matter (UVabs), time, chlorine dose, pH, bromide and temperature (Amy et al., 1987 and Clark et al. 2001).

Elshorbagy (2000) modeled the formation of different THMs under reprehensive extreme conditions of chlorine concentration, temperature and bromide ion concentration. Clark (1998) developed a mathematical model that predicts the concentration of THMs as function of pH, temperature, initial chlorine concentration, and total organic carbon (TOC). Montogomery Watson (1993) modeled the formation of different THMs in terms of TOC, pH, temperature,

chlorine concentration, bromide ion concentration and contact time.

There is no available information concerning the trihalomethane concentration levels in the Benha Water Supply Network (BWSN). One aspect of this research is to investigate the development of mathematical models for predicting the formation of THMs in BWSN. The modeling consists of establishing empirical or mechanistic relationships between THMs levels in treated water, and the parameters of water quality and its operational control that can be linked to their formation. This paper presents a study on the influence of several parameters on the formation and evolution of THMs in BWDS, and to develop a mathematical model based on easily routinely and daily measured water parameters that could use to expresses THMs concentration. In this paper, the developed mathematical models with software (EPANET) are used to predict THMs concentrations at different locations of BWSN and then compare predicted concentrations to actual measurements.

MATERIALS AND METHODS

Benha Water Supply Network

The water supply network of Benha city, is consisted of 18.52 Km of different types and diameters pipelines, which constructed in the range of 1938-1998. Water is pumped from the clear water reservoir into the service area by the pump station contains three centerifugal pumps with a total capacity of 800 Lit/Sec. The main pipes of BWSN were

replaced by new pipes of ductile iron for pipes diameters 300 mm and 400 mm and precast concrete for pipes from 500 mm to 800 mm at 1997, as shown in Figure 1. Benha city has a population of 175,343 capita in 2004 and expected to increase to 347,000 capita in target year 2024. The Benha water network was designed to cover the city water demand until the target year 2024, with average water consumption fluctuate in the range of 185-195 Lit/capita/day and fire demand of 50 Lit/sec. The main sources of treated water for Benha city is New Benha Water Treatment Plant (NWTP) which produces 800 Lit/sec. For the hydraulic simulation of main pipes of BWSN, the pipes lengths were scaled from map of Benha city and actual pipes diameters were used. Based on the age and type of pipes the Hazen-Williams roughness coefficient for each pipes was assigned, the average water use rate through the service area of main pipes were assumed according to the type, density, and number of building units surrounding each junction node in the distribution network.

Sampling Locations and Periods

The locations of sampling points in this study are chosen at eleven points, five points in the water treatment plant, from sample No. 1 to sample No. 5 at clear water reservoir in NWTP. The other six sampling points is in water supply networks, as illustrated in Figure 1 at six locations. The first point at Al Amn (sample No. 6), the second point at Benha rail way station (sample No. 7), the third point at El Ramad Hospital (sample No. 8), the fourth point at El Vielal (sample No. 9), the fifth point at old Benha water treatment plant (sample No. 10), the six point at Benha Higher Institute of Technology (sample No. 11). Samples locations were selected on these bases: distribute sapling locations as much as possible over the entire network, availability of a tap that draws water from the network

directly, and easy access. The sampling period was chosen to cover the seasonal variations during a year to meet the effects of the changes of operations and weather conditions. Analyses and measurement of the measured parameters were made for 11 sampling dates every month from April 2004 to August 2005.

Computer Programs

Two software computer programs were employed for the hydraulic analysis of Benha water supply network and statistical treatment of data and predicting mathematical modeling.

Epanet Software Package

Epanet computer program was developed by the USEPA (Environmental Protection Agency). The program performs extended period simulation of hydraulic and water quality behavior within pressurized pipe networks. Epanet tracks the flow of water in each pipe, the pressure at each node, the height of water in each tank, and the concentration of a chemical species throughout the network during a simulation period comprised of multiple time steps. In addition to chemical species, water age and source tracing can also be simulated. Extended-period hydraulic simulation method was used to compute flows, pressures, and velocities for all pipes in the network. Using Epanet alternative hydraulic parameter values and a trial-and-error approach for model calibration, and also to predict water age and chlorine residual at each water sample in water supply network. These assumptions resulted in the demand patterns shown in Figure 3.

Statistical Analyses

The Statistical Package for the Social Sciences (SPSS) software package used for conducting statistical analyses, manipulating

data, and generating tables and graphs that summarize data. SPSS contains several tools for manipulating data, including functions for recoding data and computing new variables as well as merging and aggregating datasets (STSC 1989).

Water Quality Analytical Method

Sampling Collection and Handling, Equipments, and Measured Parameters

(Chlorine Residual, TOC, Bromide Ion, THMs, pH, Algal Count, conductivity, Temperature, Turbidity and Total Solids) are presented in details in the Master of Science Thesis of Mohamed Rabee Ghazy (2005). The physicochemical characterization and other DBPs of both the raw and treated water were performed in accord to the Standard Method for the Examination of Water and Wastewater, APHA, AWWA (1998).

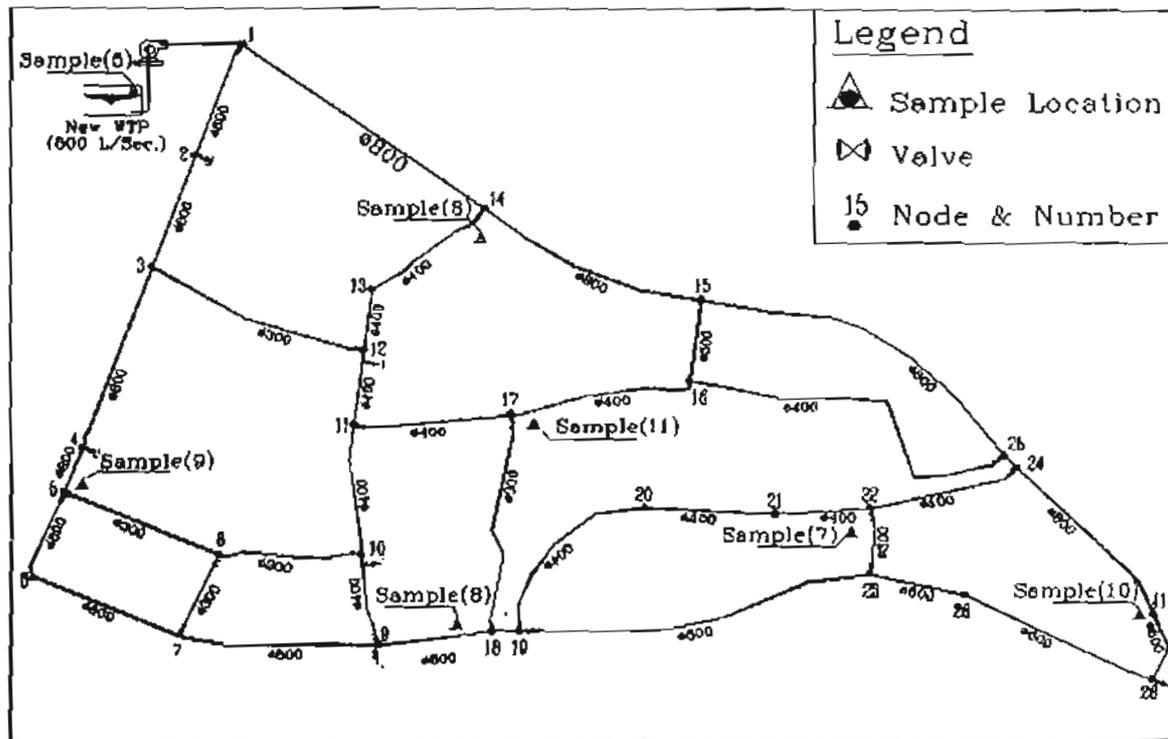


Figure (1) Sample Locations at Benha Water Supply Network

Study Approach

The study presented in this paper consists of four parts; the first part is a laboratory study that aims at studying the formation of THMs at the laboratory scale for different combinations of initial residual chlorine concentration, total organic carbon, bromide ion concentration, contact time, temperature, algae count, and pH. The second part is the

development of mathematical model of which utilizes the laboratory results obtained in the first part to express THMs concentration in terms of initial residual chlorine concentration, total organic carbon, bromide ion concentration, contact time, temperature, algae count, and pH. The third part is a sampling program that aims at measuring THMs concentration throughout Benha water supply network over time. The

fourth part uses the developed mathematical model along with Epanet to predict THMs concentrations throughout Benha water supply network, after that predicted THMs concentrations are compared to actual concentrations obtained by the sampling program.

Modeling Trihalomethanes Formation

The data obtained from the monthly water parameters measurement of NBWTP, BWSN, and bench scale study water parameters measurements was used to create a mathematical model to predict the concentration of trihalomethane in water treatment plant and water supply network. A multiple stepwise regression method was applied for the development of the empirical power mathematical function models. A Power function equation is a transformed equation derived from multiple linear regression, the only difference is the input and output parameters are transformed to logarithm values. The standard regression enters all input variables into the regression equation in one single step, while stepwise regression adds or deletes from the model at each step of the regression until the best regression model is obtained. Commercial software SPSS package, which performs multiple regression analysis, was used to model THMs concentration in terms of initial residual chlorine concentration, total organic carbon, bromide ion concentration, contact time, temperature, algae count, and pH. SPSS utilizes the least square method which minimize the square difference between modeled and experimental THMs concentration to obtain the best fit.

RESULTS

The results of THMs content of water samples and their species at the selected locations from Benha water supply network are obtained. The available results showed a wide variations in the concentration levels of THMs throughout the period of investigation, especially for samples location 7, 10, and 11, which illustrated deferent trend for the other samples. The mean concentration levels and ranges of THMs are presented in Table (1). The general trend of THMs species distribution followed the order $CHCl_3 > CHCl_2Br > CHClBr_2$. The concentration of Chloroform ($CHCl_3$) was the principal constituent of THMs and presented 58.0 % - 64.0 % of THMs as shown in Figure 2. The results of THMs concentration in the treated water in the network did not exceeded the 100 $\mu\text{g/L}$ level recommended by the Egyptian Standards for drinking water.

Hydraulic Simulation of Benha Water Supply Network

The Epanet program was used to perform extended period simulation of hydraulic and water quality behavior of BWSN. The data input to Epanet program includes pipe characteristics such as length, diameter and friction coefficient, nodal elevations, nodal demands, water consumption pattern which assumed as shown in Figure (3), and characteristics of any other devices such as pumps, elevated tank, and valves, as illustrated in Figure (1). The results of hydraulic analysis at sampling time (11.0 hr a.m) are given in Table (2). The main object of hydraulic results which is used to predictive the mathematical models is time age at each sample locations.

Table (1) Mean Concentration Levels of THMs at Benha Water Supply Network

Sampling locations	n	CHCL ₃ (µg/L)			THMs(µg/l.)		
		Range	Mean	S.D.	Range	Mean	S.D.
Location (5)	9	28.4 - 47.92	38.74	7.56	53.2 - 70.45	63.57	6.39
Location (6)	9	32.07 - 48.90	39.06	6.05	52.99 - 73.00	64.93	6.86
Location (7)	9	16.85 - 41.42	34.80	7.14	27.17 - 68.04	57.94	11.98
Location (8)	7	33.87 - 52.25	45.69	6.24	66.18 - 81.50	74.71	5.85
Location (9)	8	33.26 - 56.92	48.3	8.57	65.0 - 87.43	78.02	7.84
Location (10)	6	7.45 - 19.58	15.6	4.32	7.45 - 33.19	25.73	9.33
Location (11)	7	24.84 - 50.19	39.35	10.72	37.77 - 81.09	62.77	14.74

S.D = Standard Deviation, n = number of samples

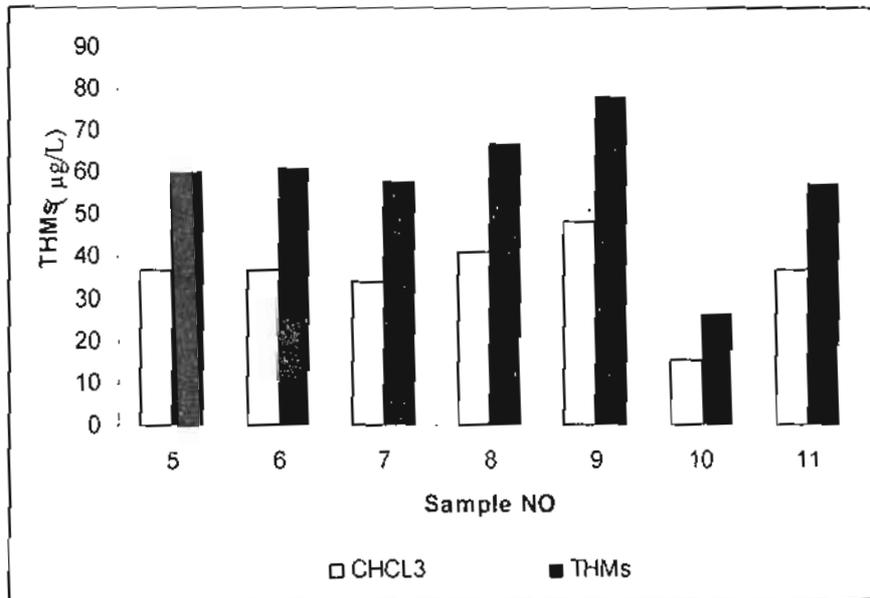


Figure (2) Mean of concentration Levels of THMs and CHCL₃ at Benha Water Supply Network

Table (2) Time Age of network sampling points at sampling time (11 Hrs am)

Sample Stations	Node	Time Age (Hrs)	Total Time (Hrs)
Clear water reservoir in NWTP - (sample 5)	0.0	0.0	7.4
Al Amn - (sample 6)	14	0.29	7.69
Benha rail way station - (sample 7)	22	1.58	8.98
El Ramad Hospital - (sample 8)	9	1.16	8.56
El Vielal - (sample 9)	4	0.4	7.80
Benha Higher Institute of Technology - (sample 11)	17	1.85	9.25

Total Time = Time Age from WTP to sample point + time period of treatment processes in WTP (about 7.40 Hrs)

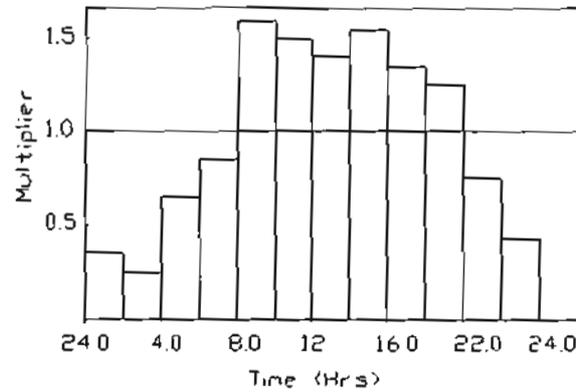


Figure (3) Demand Pattern for Benha Water Supply Network

Mathematical Modeling of THMs at Benha Water Supply Network

The data collected from the monthly water parameters measurement of the concentration levels and distribution of THMs species at BWSN, for water samples were analysed from December 2004 to August, 2005. These data was used to create a mathematical model to predict the

concentration of THMs and its species at any site of the distribution system. A global simple statistical regression analysis was used to develop a mathematical model that expresses THMs concentration, total organic carbon, bromide ion concentration, contact time, temperature, chlorine residual, algae, and pH. The following data were obtained:

N	R	R ²	Adjusted R ²	Std. Error of the Estimate
27	0.943	0.889	0.848	0.034

The correlation matrix of the tested variables parameters is presented in Table (3), which showing a high significant positive linear correlation (Sig=0.001) of Temperature, Time (Sig=0.0008), pH (Sig=0.00), and

Algae (Sig=0.00). The results showing also, a not significant negative linear correlation (Sig=0.315) of Bromide ion and significant negative linear correlation for free chlorine Cl₂ (Sig=0.0054).

Table (3) The correlation matrix of simple regression analysis

		THMs	Temp.	CL ₂	Time	pH	TOC	Algae	Br
Pearson Correlation	THMs	1.00	0.56	-0.48	0.58	0.88	0.02	0.59	-0.10
	Temp.	0.56	1.00	-0.06	-0.03	0.56	-0.38	0.26	0.12
	CL ₂	-0.48	-0.06	1.00	-0.77	-0.37	0.04	-0.43	-0.21
	Time	0.58	-0.03	-0.77	1.00	0.45	0.04	0.56	0.02
	pH	0.88	0.56	-0.37	0.45	1.00	-0.20	0.54	-0.18
	TOC	0.02	-0.38	0.04	0.04	-0.20	1.00	0.15	-0.47
	Algae	0.59	0.26	-0.43	0.56	0.54	0.15	1.00	-0.18
	Br	-0.10	0.12	-0.21	0.02	-0.18	-0.47	-0.18	1.00
	Sig. (1-tailed)	THMs	.	0.0011	0.0054	0.0008	0.0000	0.4671	0.0006

The predictive mathematical model for the simple statistical regression analysis can be expressed as follows:

$$THMs = (0.010) (Temp)^{0.119} (Time)^{0.337} (pH)^{3.0} (TOC)^{0.258} (CL_2)^{1.067 \times 10^{-4}} (Algae)^{-1.86 \times 10^{-2}} (Br)^{9.534 \times 10^{-4}} \dots (1)$$

Where: THMs (µg/L) and Time (min), CL₂ Residual (mg/L), Br (mg/L), Temperature (C⁰), Algae (count), and TOC (mg/L).

The previous mathematical model can be simplified by using stepwise multiple regression analysis which only uses the most significant variables. The results illustrated

that, the most significant parameters are Time, Temperature, pH, and TOC. The following data were obtained:

Model	R	R ²	Adjusted R ²	Std. Error of the Estimate
1	.919	.844	.824	3.690E-02
2	.939	.882	.860	3.289E-02

Model-1 Predictors: (Constant), pH, Time, Temp.

Model-2 Predictors: (Constant), pH, Time, Temp., TOC

The mathematical equation for this correlation can be expressed as follows (R=0.939):

$$THMs = (0.0143) (pH)^{2.729} (Time)^{0.36} (Temp)^{0.128} (TOC)^{0.203} \dots (2)$$

Where: THMs (µg/L) and Time (min), CL₂ Residual (mg/L), Temperature (C⁰), and TOC (mg/L).

Hence it is difficult to measured TOC variable by operators of Benha water works so, this model can be modified as follow with (R =0.919):

$$THMs = (0.02) (pH)^{2.729} (Time)^{0.368} (Temp)^{9.499 \times 10^{-2}} \dots (3)$$

Where: THMs (µg/L) and Time (min), Temperature (C⁰).

The calculated THMs concentrations versus observed once are presented in Figure (4), for simple regression analysis mode.

DISCUSSION

The Mathematical Models of Benha Water Supply Network

The available results of the concentration levels and distribution of THMs species at

BWSN which used to test the effect of TOC, bromide ion concentration (Br), contact time, temperature, chlorine residual, algae, and pH on THMs formation. The results showing that, THMs concentration had significant correlations with the previous parameters. They had strongly significant positive correlations with time (r = 0.58, Sig = 0.0008 < 0.05), pH (r = 0.88, Sig = 0.000 < 0.05), Algae (r = 0.59, Sig = 0.0006 < 0.05), and Temperature (r = 0.56, Sig = 0.0011 < 0.05). However, they had no

significant positive correlations with TOC ($r = 0.02$, $Sig = 0.467 > 0.05$). On the other hand, they had strongly significant negative correlations with residual chlorine ($r = -0.48$, $Sig = 0.005 < 0.05$) and not significant negative correlations with Bromide ion concentration ($r = -0.10$, $Sig = 0.315 > 0.05$). These results are in agreement with the

several previous studies (Abdel-Shafy M., Grünwald A. 2000, Windsor Sung et al. 2000 and others). A global simple regression analysis was used all the measured parameters to test a predictive of THMs concentrations with the following mathematical expression:

$$THMs = (a) (pH)^b (TOC)^c (Algae)^d (Time)^e (Temp)^f (CL2)^g (Br)^h \dots\dots(4)$$

The constants parameters (a, b, c, d, e, f, g, and h) which have been obtained from the statistical analysis of the available data as following:

$a = 0.0101$, $b = 3.0$, $c = 0.258$, $d = -1.86 \times 10^{-2}$, $e = 0.337$, $f = 0.119$, $g = 1.067 \times 10^{-5}$, and $h = 9.534 \times 10^{-3}$.

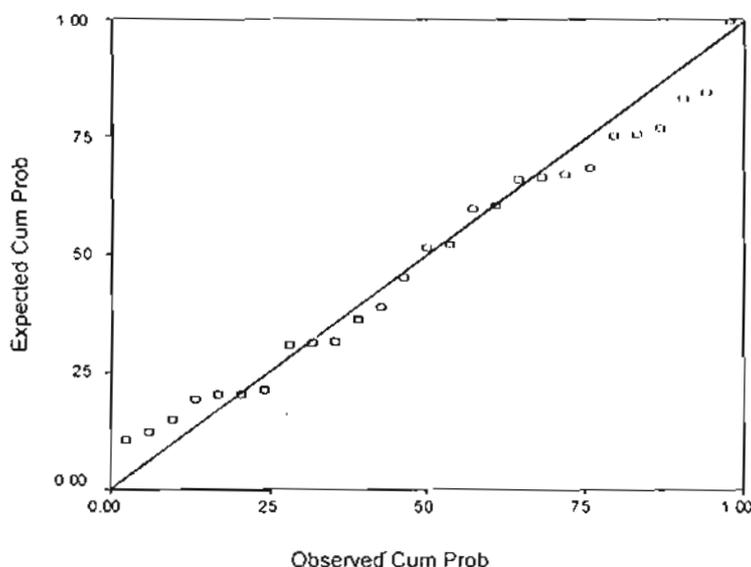


Figure (4) Comparison of observed and predictive THMs concentration by equation (3)

The correlation of applying this mathematical equation with these constants was high correlation ($R = 0.943$) and strongly significant ($Sig = 0.001 < 0.05$). The previous mathematical model can be simplified by using stepwise multiple

regression analysis which only uses the most significant variables. the results illustrated that, the most significant parameters are time, pH, TOC and temperature only and can be expressed as follows:

$$THMs = (a) (pH)^b (TOC)^c (Time)^d (Temp)^e \dots\dots(5)$$

The constants parameters (a, b, c, d, and e) which have been obtained from the

statistical analysis of the available data as following:

$$a = 0.0143, b = 2.729, c = 0.203, d = 0.36, e = 0.128$$

The correlation of applying the this mathematical equation with these constants was high correlation (R=0.939) and similar to which findings by several investigator (Rodriguez et al. 2000, Abbas Al-Omari et al. 2004).

Since the measurement of TOC is not simple and need to qualified persons and equipments so the previous model can be simplified as follows:

$$THMs = (a) (pH)^b (Time)^c (Temp)^d \dots\dots(6)$$

Where the constants parameters:

$$a = 0.02, b = 2.729, c = 0.368, \text{ and } d = 9.499 \times 10^{-2}$$

The correlation of applying this mathematical equation was also high correlation (R=0.919) and without significant difference from the original model in equation 5. So the operators can use these models to predict the THMs concentration during any point of BWSN.

predictive calculated values of the bench experimental model (Basiouny, et al. 2007) and field study model are presented in Table (4) and illustrated in Figure (5). The results illustrated that, there are very close agreement between the observed THMs concentration and predictive calculated values from filed study model. Hence the difference in the average calculated values and observed values during the study period ranged from (4.6% to 9.9 %). Whereas the results have shown poor agreement between the observed and predictive calculated values from bench scale model. Hence the difference ranged from (15.75 % to 30 %).

Applicability of Predictive Mathematical Models for Water Supply Network

The results of the average concentration of THMs levels at BWSN in sampling Stations 5, 6, 8, and 9 according to the observed values during the period of study and the

Table (4) Comparison of THMs average concentration according to observed values and Predictive calculated models values for water supply network.

Item		Sample Station			
		Sample(5)	Sample(6)	Sample(8)	Sample(9)
Models	Field Study Model Values	66.70	68.87	70.90	70.29
	Bench Exp. Model Values	88.20	93.28	92.60	92.61
	Observed Values	63.60	64.94	67.00	78.02
Difference	Field Study Model	4.6 %	5.7%	5.5%	9.9 %
	Bench Exp. Model	27.9 %	30 %	27.76 %	15.75 %

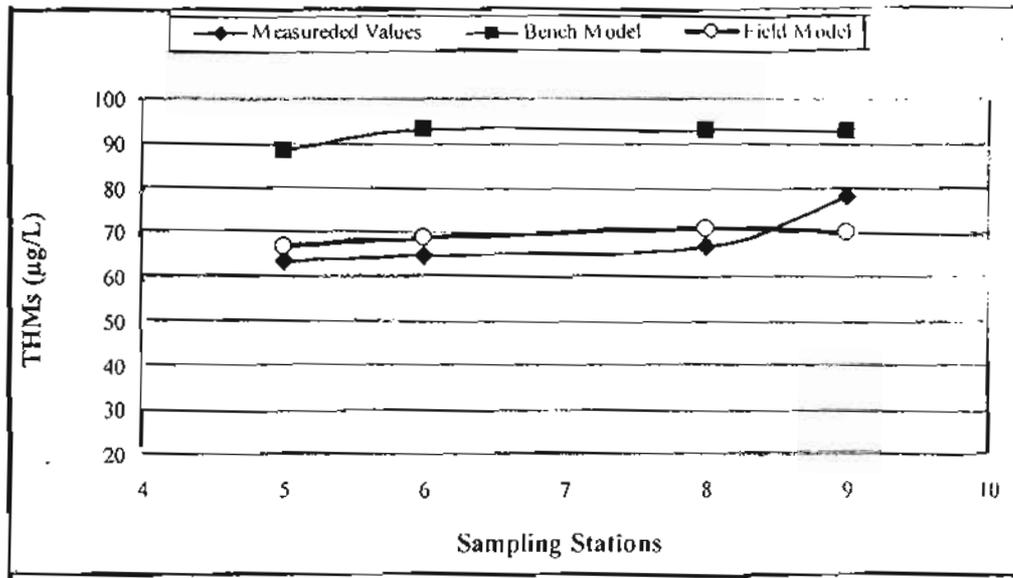


Figure (5) Comparison between predictive THMs concentrations from bench. field study models, and observed values for water supply network

CONCLUSIONS

- The concentration levels of THMs in Benha water supply networks were generally within the permissible concentration recommended by the WHO and Egyptian Standards.
- Chloroform (CHCl_3) and dichlorobromomethane (CHCl_2Br) were the major fraction of THMs in Benha water works.
- THMs formation for Benha water supply network was modeled in terms of initial residual chlorine concentration, total organic carbon, bromide ion concentration, contact time, temperature, algae count, and pH by performing regression analysis on experimental data.
- The developed mathematical model along with Epanet was used to calculate THMs concentrations throughout Benha water supply network.
- THMs concentrations calculated by the use of the model developed in this

study and Epanet were compared to measured concentrations obtained during a sampling program for Benha water supply network.

- The results showed close agreement between the measured and calculated THMs concentration. Hence the difference in the average calculated values and measured values during the study period ranged from (4.6% to 9.9 %).
- The model can provide reasonable results for most of the functioned variables and can be used to have a rapid assessment of the trihalomethanes formation.

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