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Developing a Multiple Regression Model for Predicting Trihalomethane Concentrations in Drinking Water Supply: A Case Study

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Abstract:

This study was carried out to monitor the concentrations of trihalomethanes (THMs) in both raw and treated water, and to develop a model for predicting THM concentration in drinking water systems within the largest drinking water treatment plant in Bangladesh. A mathematical model was developed using the multiple linear regression (MLR) approach. THM concentration was designated as the dependent variable, while various water quality parameters—namely pH, temperature, COD, TOC, DOC, UV254, SUVA, ammonia nitrogen, bromide, chlorine contact time, chlorine dose, and residual chlorine—were defined as independent variables. Multiple linear regression analysis of the data indicated that COD, ultraviolet light absorbance at 254 nm (UV254), initial chlorine dose, and ammonia concentration were the most significant variables. COD was found to be the most influential parameter responsible for THM formation, followed by UV254, chlorine dose, and ammonia-N. The residual free-chlorine concentration, pH, reaction time, bromide ion, DOC or TOC or SUVA had little or no significance. Analysis of combinations of the TOC, DOC, SUVA, COD and the ultraviolet absorbance indicated that use of COD along with the ultraviolet absorbance alone provided the best prediction of the experimental data. The relationships between the variables were initially examined using simple correlation analysis. Multiple regression analysis was then applied to evaluate the statistically significant variables in the system. The significance level for including a variable in the model was set at 0.05. The developed model provided satisfactory estimations of THM concentrations, with a model regression coefficient of 0.65. Both the R^2 and Durbin–Watson statistics were found to be statistically significant. The Durbin–Watson value was 2.14, which falls within the acceptable range. Predicted THM concentrations were compared to actual concentrations measured during the sampling program. The results showed a good agreement between measured and calculated THM concentrations ($R^2 = 0.77$), indicating that the method presented in this paper can be effectively used to estimate THM concentrations throughout the system. The correlation and regression analyses used to examine the relationship between the independent variables and THM concentrations showed promising results, with strong relationships. Validation of the model revealed no significant differences between predicted and observed values, and the prediction error was low. The model developed in this study can be used to predict THM concentration levels in drinking water supplies under conditions typical of Bangladesh. It is noteworthy to mention that no previous attempts to assess, monitor, and predict THM concentrations in public drinking water have been reported for the country although a large fraction of the population consumes chlorinated public drinking

water. Until recently, there was no information available that pertained to the concentration level of THMs in drinking water, lest the development of a model thus making our research almost the first one of this kind.

Keywords **— Drinking water, Disinfection by-products, Multiple regression analysis, Model, THMs.**

I. INTRODUCTION

Disinfection of water is one of the most significant public health advancements of the twentieth century. It is an essential and indispensable process in water treatment for ensuring drinking water safety, as it inactivates pathogens. The disinfection process has been routinely practiced since the early 20th century to eliminate and inactivate pathogens in drinking water. In addition to removing pathogens, disinfectants also act as oxidants in water treatment. They are used for (a) removing taste and color, (b) oxidizing iron and manganese, (c) improving coagulation and filtration efficiency, (d) preventing algal growth in sedimentation basins and filters, and (e) preventing biological regrowth in the water distribution system [1].

Chlorine and its compounds are the most commonly used disinfectants for water treatment worldwide. Chlorine's popularity is attributed not only to its low cost but also to its strong oxidizing potential, which ensures a minimum level of residual chlorine throughout the distribution system, thereby protecting against microbial recontamination. In conventional water treatment, chlorine is added as elemental chlorine (chlorine gas), sodium hypochlorite solution (bleach), or dry calcium hypochlorite. When applied to water, each of these forms generates free chlorine, which destroys pathogenic (disease-causing) organisms [2].

Almost all drinking water treatment plants employ some type of chlorine-based process—either alone or in combination with other disinfectants such as ozone or ultraviolet (UV) radiation. Water utilities select disinfection methods based on site-specific needs and available resources. Although various disinfectants and disinfection strategies (chlorination, chloramination, chlorine dioxide, granular activated carbon with post-chlorination, ozonation, ultraviolet radiation) are used, chlorine remains the most effective and economical option [3, 4, 5].

Although chlorination has proven highly effective, it was later discovered that its use can lead to the formation of potentially carcinogenic halo-organic compounds, known as disinfection by-products (DBPs). To date, more than 700 DBPs have been identified, among which trihalomethanes (THMs) are the most commonly reported in drinking water [6]. The main THM species include chloroform ($CHCl_3$), bromodichloromethane ($CHBrCl_2$), dibromochloromethane ($CHBr_2Cl$), and bromoform ($CHBr_3$) [7].

Considering the potential health risks of THMs, many countries—such as the U.K., USA, Japan, France, and Australia—along with international agencies like the U.S. Environmental Protection Agency (USEPA) and the World Health Organization (WHO), have set regulatory limits for these compounds in drinking water. The USEPA established a maximum contaminant level (MCL) of 80 µg/L for total THMs [1]. Canada's guideline similarly limits total THMs to 80 µg/L [8], while most European countries have adopted an MCL of 100 µg/L [9]. In Bangladesh, there is no official standard for total THMs or their individual species; however, the limit for chloroform is set at 90 ppb [10].

Past studies have shown that THM levels in chlorinated water vary depending on precursor levels and several other factors such as pH, temperature, natural organic matter (NOM), ultraviolet absorbance at 254 nm (UV_{254}), bromide concentration, chlorine dosage, and reaction time [11]. Variations in these precursors and their concentrations significantly influence the formation and distribution of THM compounds in drinking water.

The concentration of THM precursors in surface water tends to be high and may further increase due to anthropogenic pollution. Therefore, it is essential to adapt existing water treatment processes to changing raw water conditions. A critical challenge is that THMs can form not only during treatment but also during water transport through distribution networks. In large cities, long transport distances and reduced water consumption increase the likelihood of THM formation, especially when additional chlorine is dosed at intermediate points to maintain disinfection residuals.

Thus, monitoring THM concentrations in drinking water is crucial for quality control and compliance with regulatory standards. However, precise monitoring is costly, and testing is often limited to a minimal number of locations. Developing predictive models for THM formation can reduce the need for expensive analyses while supporting effective quality control in water supplies. Such models can estimate THM concentrations based on raw water quality and operational parameters, enabling preventive actions by water utility managers. Predictive models also help assess the maximum allowable concentration of THMs and analyze cancer risks associated with them. Moreover, they can serve as decision-making tools for government officials evaluating the feasibility of stricter THM regulations [12]. Models are therefore valuable for improving public health risk management related to THMs, supported by toxicological and epidemiological studies [13]. They are also useful for developing preventive measures to minimize random events leading to water quality deterioration.

Numerous mathematical predictive models for THM formation have been proposed [14, 15]. Over the past decade, several empirical models with varying predictive capabilities have emerged [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30].

These models can be broadly categorized into two types: (a) empirical models, based on statistical relationships between THM concentration and influencing parameters, and (b) kinetic models, based on reaction mechanisms. Empirical models often employ linear, non-linear, or multivariate regression analyses using laboratory or field data [31]. Their applicability and reliability, however, vary widely due to differences in raw water characteristics compared to the synthetic waters used for model development [17]. Modeling efforts typically aim to relate THM concentrations with operational parameters that influence their formation [32, 33].

Some researchers have developed kinetic-based models describing chlorine reaction mechanisms [28, 34, 35], while others proposed empirical regression-based models linking operational and water quality parameters with THM concentrations [36, 37, 38, 39]. Due to the complexity of reactions between organic precursors and chlorine, most existing models rely on empirical equations rather than mechanistic kinetics. This complexity makes it difficult to develop universally applicable models suitable for diverse natural waters.

Although many THM models exist, the development of new ones remains valuable as scientific understanding evolves. Most current models use surrogate input parameters such as total organic carbon (TOC) or dissolved organic carbon (DOC) to represent NOM. While these provide general information about precursor concentrations, they do not describe organic characteristics unless combined with UV–visible absorbance data [40]. Therefore, the development of mathematical models for THM prediction continues to have significant practical importance—particularly for developing countries like ours.

Previous studies have shown that several factors—chlorine concentration, contact time, residual chlorine, bromide, ammonia, pH, temperature, and NOM type and content—affect THM formation. THM levels are usually highest at the farthest points of the distribution system, where water retention time is longest. Once formed, THMs are difficult to remove, though their formation can be mitigated by reducing or degrading precursors [41]. Although THMs have been studied globally since 1976, almost no comprehensive survey has been conducted in Bangladesh, except for a few academic studies, and none have developed a predictive THM model.

In recent years, THM research has increased in the USA and Europe, whereas in developing countries and parts of East Asia it remains limited, with many utilities relying on outdated WHO (1984) guidelines [42]. In Bangladesh, including Dhaka—the capital—chlorine is used as the primary disinfectant, following global practices. Since the inception of modern water supply systems in Bangladesh, chlorine has been used as the standard pre-oxidation and disinfection chemical.

Although THM concentrations in drinking water are generally low, the potential carcinogenic nature of these compounds warrants careful study. In Bangladesh, specific local conditions make such research particularly relevant: surface waters are turbid, contain high organic loads, and experience high temperatures, while chlorine remains the sole disinfectant. Industrial discharges near intake points have further degraded water quality, especially around the capital. These factors indicate a high potential for THM formation [43].

It is noteworthy that, until recently, no attempts had been made to assess, monitor, or predict THM concentrations in Bangladesh's public drinking water systems, despite widespread consumption of chlorinated water. Hence, this research represents one of the first studies of its kind in the country.

In Bangladesh, chlorine is widely used as a disinfectant for drinking water, consistent with global practices. Considering the potential health risks posed by THMs resulting from chlorination, and given the limited access to advanced, costly analytical instruments across the country, this study aims to develop a predictive model for THM formation using both field and laboratory data. The model applies a multiple linear regression (MLR) approach to predict THM concentrations in a drinking water supply system that draws raw water from the nearby Sitalakhya River.

II. METHODOLOGY

A. Study Area

The study area is Dhaka the capital city of Bangladesh with a population of more than fifteen million located in the central part of Bangladesh. The city has a distinct monsoonal season, with an annual average temperature of 26°C and monthly means varying between 19°C in January and 29°C in May, sometimes reaching to 40°C. Approximately 87% of the annual average rainfall of 2,123 millimeters occurs between May and October. Dhaka is located at 23°42′N 90°22′E, on the banks of the Buriganga river and surrounded by other peripheral rivers. The largest treatment plant of the country is situated beside the river Sitalakhya in the eastern periphery of Dhaka city at Latitude N 23° 43' 11.25" and Longitude E 90° 26' 14.25" [44]. The water from this plant was collected and used for this study (Figure 1). Water samples were collected from three different points over the plant, which supplies water to nearly four million people. River Sitalakhya is the source utilized for fresh water in Dhaka. The Dhaka WTP with a design capacity of 450,000 m³/d receives water from Sitalakhya river. It consists of two separate units, each unit treating 250,000 m³/d, respectively. Each unit is of conventional design: major features include pretreatment, coagulation, flocculation, sedimentation and filtration. The prechlorination is applied just before the coagulation channels and the postchlorination is applied at the entry of the storage reservoir before the input of finished water in the distribution system.

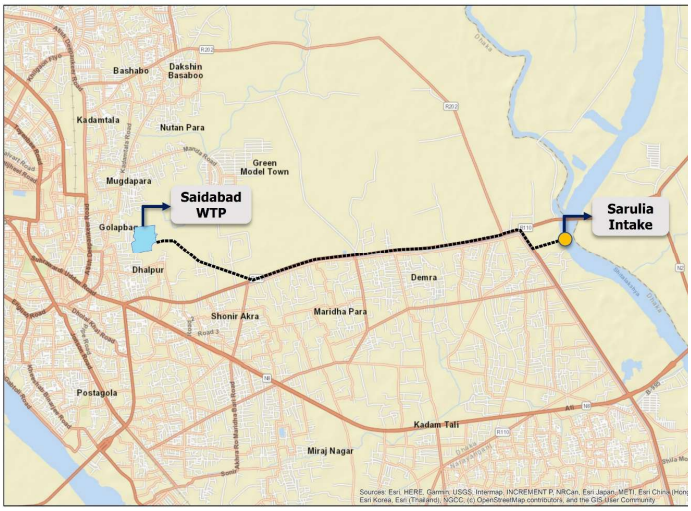


Fig. 1: Location of Dhaka Treatment Plant and Sitalakhya River

B. Samples

All data for this study were obtained from Dhaka WTP of the capital city, Bangladesh. Sampling was carried out across 2018 to 2020 in twelve occasions covering the dry and wet seasons of the year. Duplicate samples for THMs measurement were collected from each sampling location in 40-ml glass bottles and were capped with PTFE-faced silica septum (Pierce 13075), including samples containing raw water. Sample bottles were carefully filled just to overflowing, without passing air bubbles through sample or trapping air bubbles in sealed bottle. The bottles were prepared by washing with soap and water, rinsing with tap water, ultrapure water (Millipore: Milli-Ro 5 plus and Milli Q plus 185), acetone (Mallinckrodt Chemical Works St. Louis) and placing in an oven at 150°C for 2 h. HCl (4 drops 6 N/40 ml) was added to each raw water sample to prevent biodegradation and dehydrohalogenation, while sodium thiosulfate (3 mg/40 ml) was also added to each sampling bottle as a reducing agent [45]. After sampling, the bottles stored in the dark at temperatures between 0 and 4°C, were carried by air to Mytilene for analysis in the quality control Laboratory at the Dhaka WTP.

C. Analytical Procedure

All samples were analyzed according to the respective procedure described in standard methods [45] and reported in previous works. Especially, liquid–liquid extraction and gas chromatography were used to measure the concentration of THMs in the water samples. The bromide ion concentrations in the raw and finished water were determined with the phenol red colorimetric method [45]. The detection limit of bromide is 0.1 mg/l [45]. Typical data including, water temperature, pH, chlorine dose and free residual chlorine were collected in the plant.

D. Data Set

The variables examined and used for the model development in the present work were TOC, DOC, UV254, COD, SUVA, temperature, pH, chlorine dose, residual free chlorine, bromide, chlorine contact time and ammonia nitrogen. The concentrations of THMs are expressed as µg/L, the temperature as °C, time in hours, the concentrations of COD, TOC, DOC, NH_3, chlorine dose, residual free chlorine and Bromide as mg/L, while UV254 as cm^{-1}, and SUVA as L/mg.m. The development of the models was based on the THMs concentrations from the finished water, pretreated & raw water of the plant, similarly all other parameters concentrations were used from the respective waters. The concentrations of Bromide in the water were not included, since they were approaching beyond detection limit. The sum of prechlorination and postchlorination was used for the chlorine dose in case of treated water, as the reaction is continued with the addition of chlorine during the latter step, contributing to the further formation of THMs.

E. Data Analysis

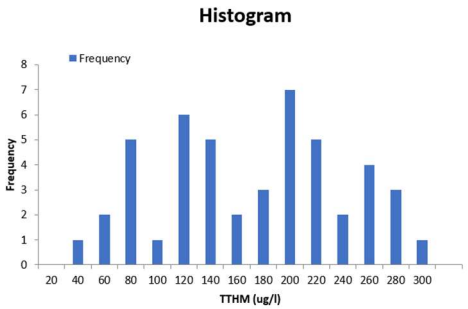
The relationships between the variables were examined by simple correlation [46]. Multiple regression analysis was applied as a means for evaluating statistically significant variables of the system [47]. The level of significance (α) for the inclusion of a variable in the model was 0.05. The t-criterion was used to eliminate statistically insignificant variables and for the coefficient bj of the j variable, H_0: bj = 0 and Ha: bj ≠ 0, this t statistic can be formed as [46], t = bj/Sbj, where Sbj is the standard deviation of the respective coefficient bj; if n is the total number of observations, k the number of independent variables used to describe the dependent variable in the model, then the criterion for the rejection of H_0 in favour of Ha is $|t| > t(n-k-1, \alpha/2)$, indicating that the specific variable is statistically different from zero and should be incorporated in the regression model.

Prior to the regression analysis, the database was subdivided into two parts, the major parts for model development and the rest for model validation, respectively. The bigger sample was the basis for the development of the mathematical equations, while the smaller one was used for the validation of these models.

III. RESULTS AND DISCUSSIONS

A. Development of THM Model

Statistical analysis is elaborated to develop the necessary models. Initially, the dependable variables are tested for normality using the Data analysis tool pack from where the description statistics and histogram was tested to check the goodness-of-fit to the normal distribution at significance level 0.05 (Fig. 2). It can be seen that the mean & median values of the data are almost equal (162.20, 169.05 respectively), the kurtosis & skewness are almost zero (-0.96 & -0.07 respectively) which along with the histogram confirm the normality of the data. Then, the Pearson correlation matrix is used to examine the relationships between the variables.



Summary Statistics	
Mean	162.20
Standard Error	10.08
Median	169.05
Mode	75
Standard Deviation	69.11
Sample Variance	4776.30
Kurtosis	-0.97
Skewness	-0.08
Range	260
Minimum	24
Maximum	284
Sum	7623.3
Count	47

Fig. 2: Summary statistics and histogram of the dependent variable

To perform a linear regression, the total trihalomethanes (TTHMs) concentration (Y), is assumed to be a linear function of the inputs, X. The unknown parameters to be determined, a_i are the coefficients, as given in (1):

$$Y = a_0 + a_1X_1 + a_2X_2 + ... + a_nX_n \quad (1)$$

where n is the number of inputs used. The coefficients are chosen to minimize the sum of the squared differences between the predicted and actual values of Y. Multiple regression analysis is used to evaluate the statistically significant variables at a level of significance α. The models are tested using ANOVA tests to check if the residuals of the models follow the normal distribution, and the mean value of the residuals is zero. To check autocorrelation, the Durbin Watson estimate is calculated. R^2 values are also gathered to check how well the model fits the data. Finally, the developed models are used for the validation of the results, comparing observed and predicted data.

For development of the model, multiple linear regression analysis of THM data was carried out. Based on the data, multiple regression analysis was applied at significance level α, which was 0.05. Throughout the process of model development, several linear regression analyses were performed. The inclusion of each variable in the proposed model was based on the t-criterion. Methodological details about the model development are extensively discussed in past studies. Multiple regression analysis tool from Excel/Minitab was used. For the WTP, all variables are initially used as independent variables (inputs). As a number of independent variables are not statistically significant ($p > 0.05$), they are excluded one-by-one from the model development process.

Temperature, pH, initial chlorine dose (mg/L), residual chlorine (mg/L), residence time, COD (mg/L), TOC (mg/L), DOC (mg/L), SUVA, Bromide ion (mg/L), UV_{254} and ammonia–N (mg/L), total THMs (µg/L) were designated as independent variable and THMs as dependent variable.

Table I presents the total number of values (N), average (AV), standard deviation (SD), minimum (MIN), and maximum (MAX) values of the parameters studied.

TABLE I TOTAL NUMBER, AVERAGE, STANDARD DEVIATION, MINIMUM AND MAXIMUM VALUES OF THE PARAMETERS

Parameters	Sample numbers	Average	Standard Deviation	Minimum	Maximum
THMs (µg/L)	47	162.20	69.11	24	284
COD (mg/L)	47	15.43	6.63	0	24
TOC (mg/L)	47	15.67	2.61	13.44	22.63
DOC (mg/L)	47	2.09	2.26	0.06	8.2
UV254 (cm^{-1})	47	0.1031	0.0564	0.0342	0.1894
SUVA (L/mg m)	47	12.89	11.12	1.03	22.63
Chlorine dose (mg/L)	47	21.17	13.27	6	50
Residual chlorine (mg/L)	47	1.25	1.78	0	7.6
pH	47	7.5	0.59	6.75	9.55
Bromide (mg/L)	47	0.05	7.01 E-18	0.05	0.05
Ammonia – N (mg/L)	47	1.88	1.87	0	10
Temperature (°C)	47	27.92	2.18	23	30.8
Contact time (Hrs)	47	12.96	13.49	0.5	48

Various combinations of these independent variables were tested to find out the best suitable model predicting the formation of THM. Finally, COD, UV254, chlorine dose and ammonia nitrogen are found to be statistically significant ($p < 0.05$). Finally, the developed model is: The best suited linear model for predicting THM concentration are shown by Eqs. (1).

$$THM = a - b(UV_{254}) + c(Cl_2 \text{ dose}) + d(COD) - e(NH_3\text{-}N)$$

where chlorine dose (Cl_2) in mg/L, COD is the chemical oxygen demand expressed in milligrams per liter, UV_{254} is the ultra violet absorbance expressed in per centimeter, NH_3-N is the ammonia-N expressed in milligrams per liter and a, b, c, d, and e are the estimated values of statistical coefficients. The summary of THMs models is shown in Table II.

TABLE II THM FORMATION MODEL SUMMARY

Serial number	Parameters	Values
1	Coefficient of correlation (r)	0.647485
2	Coefficient of determination (R^2)	0.419236
3	Adjusted R^2	0.363926
4	Std. error of the estimate	55.11877
5	Durbin-Watson	2.14
6	Statistical coefficients	
	a	85.92362

	b	-500.289
	c	1.929311
	d	6.697541
	e	-8.72204

The summary of THMs models is shown in Table II. Analysis of the models revealed that Cl_2 dose, COD, NH_3-N and UV_{254} are statistically significant as compared to other parameters. COD was found most influencing parameter responsible for THM formation followed by UV_{254}, chlorine dose and ammonia-N. In terms of coefficient of correlation (r), it appears that the correlation coefficient value of 0.65 is important. The R^2 and Durbin–Watson estimate were also statistically significant. The value of Durbin–Watson is preferred to be between 1.5 and 2.5 for statistically best fit model [48].

B. Model Validation and Discussion

The purpose of validation is to measure how well the model fit the experimental data. In order to validate these models, the THMs concentration was predicted using Eqs. (1) for an independent set of data and compared with the experimental data (Fig. 3). The validation statistics of this model are given in Table III.

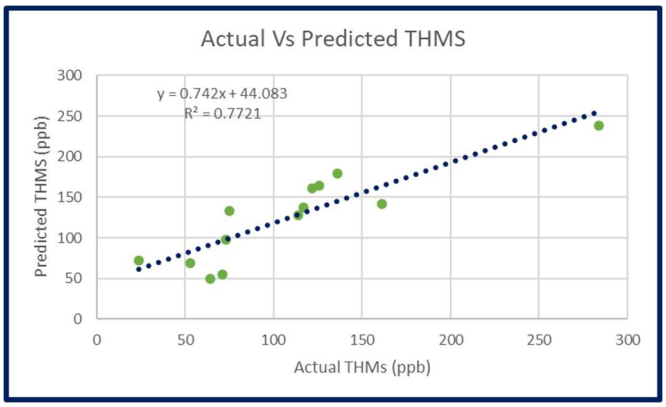


Fig. 3: Correlation between the experimental and prediction values

A t test was performed to determine the biasness of the model. The t values for these models were less than the t critical value, and the p values were also greater than 0.05. This indicated that the model biasness is insignificant. The analysis of the model revealed that the model can be used for the prediction of THMs. The coefficient of correlation for this model was higher than those reported by Abdullah et al. [49]. Uyak et al. [48] also reported that multiple regression model seems to be promising for the prediction of THMs in field conditions. However, these predictive models are site specific and applicable to similar geo-climatic conditions. Several models have been reported in different countries but after many trials, no valid results could be obtained [50, 16]. In Bangladesh, no such attempts were made to develop these models for prediction of THMs. Indeed, studies on THM in drinking water in Bangladesh is rare.

IV. CONCLUSIONS

This study revealed the presence of very low concentration of THMs (less than 80 µg/L) in drinking water. Seasonal variation of THMs revealed highest levels in autumn followed by summer. COD, UV254, Cl_2 dose, and ammonia–nitrogen are the most influencing parameter responsible for THM formation. The correlation and regression analysis for examining the relationship between the independent variables with THM showed promise and the relation appeared to be good. Validation of the model revealed that there were no significant differences and the error of prediction was low. The model described above can be used for predicting THM concentration levels in drinking water supplies for Bangladesh conditions.

The development of the models was based on the THMs concentrations from the finished water, pretreated & raw water of the plant, similarly all other parameters concentrations were used from the respective waters.

In order to predict the formation of THM in the treated water, a mathematical model was developed using multi linear regression (MLR) approach. THM was designated as the dependent variable, and the water quality parameters such as pH, temperature, COD, TOC, UV254, ammonia, bromide, residence time, and residual chlorine were defined as independent variables.

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