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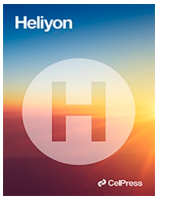

Research article

Combined application of EPANET and empirical model for possible formation of trihalomethanes in water distribution network of Chattogram city to identify potential carcinogenic health risk zone

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ABSTRACT

The study identifies potential carcinogenic health risk-zone of Chattogram city for the occurrence of trihalomethanes (THMs) at its water distribution network. The EPANET-THMs simulation model along with an empirical model have been adopted in the study to predict THMs content of supply water of the distribution network of the city's Karnaphuli service area. The empirical model has estimated THMs level of supply water based on influential water quality parameters, and few of these have been used as pre-set values for subsequent EPANET simulation. The simulation (R^2= 0.7) shows that THMs' concentrations throughout the network vary from 33 to 486 μg/L. Around 60% of total junctions showed THMs concentrations above 150 μg/L, while that is above 50 μg/L for most (99%) of the junctions. Residual Free chlorine, one of the pre-cursors for the THMs formation in distribution line, has also been simulated by EPANET considering varying applied chlorine dose at the water purification unit and wall (K_w) and bulk (K_b) decay constants. The simulated free residual chlorine peaks are found to be closer to the actual values with chlorine dose of 2 mg/L, and decay constants, $K_w = 1\ d^{-1}$ and $K_b = 1\ d^{-1}$. A mean lifetime total risk of cancer due to the presence of THMs has been found to be very high. Spatial distribution of carcinogenic risk shows that the central zone of the service area is the most vulnerable zone, followed by the western and northern zone. The first ever zone wise risk identification could be used as baseline data for operational and regulatory purposes and may raise awareness among the city's inhabitants. Furthermore, the application of EPANET in combination with an empirical model could be an effective tool for predicting THMs' concentration in water distribution networks in developing countries like Bangladesh to minimize the expenses of measuring THMs.

1. Introduction

Providing safe and adequate water is of great concern attaining sustainable goals, and disinfection by chlorination process has been

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used worldwide to make the water safe from microbial contamination. Disinfection-by-products (DBPs) are undesirably produced in disinfected water due to the chemical reactions between disinfectants and organic or inorganic precursors present in water. Trihalomethanes (THMs) and halo acetic acids (HAAs) are being observed mostly at the highest concentration during the chlorine-based the disinfection process [1,2]. These unintended halogenated DBPs have received considerable attention because of their carcinogenicity, genotoxicity and mutagenicity, and other potential adverse health effects from their long-term exposure [3–7]. Depending upon the presence of natural organic substances (e.g., humic compounds) and free residual chlorine, THMs can be produced at any point of the water distribution system. However, a least amount of free residual chlorine is to be maintained throughout the distribution network to keep water safe against pathogenic microbial contamination according to the World Health Organization (WHO). However, maintaining the recommended free residual chlorine in water distribution line against THMs formation, and monitoring of THMs in the water supply network is critical to minimize the adverse health effects from these by-products.

Extensive research till date has been conducted worldwide regarding DBPs in supply water, including their development, detrimental health effects, formation modelling, factors identification, risk assessment etc. [*inter alia* 8–13]. Like other developing countries, the research and knowledge regarding this critical problem are still at a rudimentary level in Bangladesh. Moreover, the country is struggling to supply safe drinking water to its people with limited and/or somewhat constrained resources. Therefore, awareness and monitoring of DBPs in supply water are required to be paid special attention in the country. Most developed countries have their own guidelines, standards, and regulations for DBPs in drinking water. The US EPA [14] has set its maximum allowable limit of 80 μg/L. Although there is a drinking water quality standard for trichloromethane ($CHCl_3$) which is 90 μg/L [15], standards for other species of DPBs are, however, missing in Bangladesh to comply with. Moreover, a comprehensive work is still lacking in the country regarding DBPs within water distribution networks and associated human health risks. Khan et al. [16] first studied the presence of THMs in textile effluent treated by chlorine, and later on, Suchana [17] evaluated THMs formation potential at six surface water treatment plants (WTPs) of Dhaka city. The study by Suchana [17] made an effort to incorporate the suppressive effect of ammonia based on few bench scale data by modifying the model formulated by Amy et al. [18]. Ahmed et al. [19] observed THMs in supply water of few sites of Dhaka city, and predicted cancer risk area of Dhaka city through spatial analysis. Based on influential water quality parameters of very little water samples, Khan et al. [16] predicted the existence of THMs in supply water of Chattogram city using different existing empirical models. The inhabitants of Chattogram city, are also anticipated to be at high carcinogenic risk because of the exposure to THMs in the city's supply water in that study. Besides, there is a lack of uniformity in ages and materials of pipelines of the city's distribution network. New pipelines have been installed at the existing network to expand the distribution facilities. Therefore, formation of THMs of supply water within the network may vary at different distribution zones with varying total organic carbon content and chlorine consumption within the pipe network. It is, therefore, a pressing demand to investigate the existence and development of DBPs within the supply network, and to identify the high-risk zones as well in the country.

Chattogram is the second largest and economic hub in the south-eastern part of the country. Chattogram Water Supply and Sewerage Authority (CWASA) is dealing with water supply and sewage disposal related services to the city's community. Although free residual chlorine in distribution line of the city is being monitored by CWASA on regular basis, concentration of THMs or other DBPs within the network is not taken into consideration to be monitored. Field level data of these compounds are, therefore, completely lacking. Monitoring of residual chlorine is, however, a crucial task up to the consumer's tap in order to ensure the safety of water, and measurement at the distribution line only is not adequate to depict the actual scenario [20]. Furthermore, measurement of THMs and its species is highly expensive, which involves sophisticated equipment such as Gas chromatography (GC)/GC-Mass spectrophotometry with toxic substances [7,21]. Therefore, a simple and economically affordable tool for predicting free residual chlorine and DBPs measurement is necessary to capture their occurrence scenario and risk level, especially in the context of developing countries like Bangladesh. In this connection, particular interest has been developed worldwide in the modeling of THMs considering various influencing factors as the other option of monitoring DBPs'in field [22–24]. However, the existing predictive models are mostly based on lab-scale researches while a very limited models have been formulated based on real water distribution sampling [25,26]. Empirical models have several positive aspects, such as providing a cost-effective approach to estimating THMs concentrations in the absence of actual data. Non-linear models have been widely used to predict THMs concentrations in drinking water, but in some cases their accuracy and usefulness have been debated in the literature. Ged et al. [25] evaluated the performance of 118 empirical models and found limitations in their predictive accuracy. However, it is important to consider that this study was based on a limited number of models and may not represent the entire field. Sathasivan et al. [27] also highlighted the limitations of empirical models in predicting THMs concentrations, particularly in the context of variations in raw water quality and chlorination conditions. These studies emphasize the need for careful evaluation and validation of non-linear models before their use in predicting THMs concentrations.

Concurrently many software packages have widely been used and accepted for the simulation of water quality behavior in the water distribution networks. EPANET is such a package, which conducts an extended duration simulation of both the hydraulic and water quality behavior within pressurized pipeline systems. The software is developed as a research tool for various applications in water supply systems analysis which includes sampling design, calibration of hydraulic model, analysis of chlorine residual, exposure assessment etc. [9,28]. EPANET has been extensively applied for residual chlorine simulation in distribution system in many studies [29–33]. However, it has not been applied that much to evaluate the THMs content in the supply water. García-Ávila et al. [34] demonstrated that in the corona pandemic season, residual chlorine modeling by EPANET could be an important tool to control residual chlorine content within the distribution network. Ahn et al. [35] also predicted residual chlorine and trihalomethanes (THMs) in a drinking water distribution system using EPANET 2.0. However, the study concludes that the predicted THMs values are lower than the existing target values.

In this context, this research aims to identify a potential risk zone by predicting the trihalomethanes (THMs) in supply water of Chattogram city throughout its distribution line. The EPANET-THMs simulation model and an empirical model, the AMY98 [18] model

have been adopted in the study. Water quality parameters were investigated from the distribution network of the Karnaphuli Service Area (KSA) of the city, and the presence of THMs has been predicted by the model based on the investigated parameters. EPANET simulation model for THMs has then been applied for the overall distribution network with pre-set values for different junctions taken from the model prediction. Additionally, coupling of simulation models with optimization techniques has been tried as well in this study to assess the free residual chlorine content in the water distribution line of CWASA. Potential carcinogenic risks through multi exposure pathway of supplied water due to the formation of THMs in the studied area of the city are also evaluated. It is expected that the first ever zone-wise predicted data for the occurrence of THMs and relevant human health risk of Chattogram city in an alternative way would be a beneficial tool for further investigation and policy making.

2. Study area

The existing water supply network of CWASA comprises 564 km of transmission and distribution pipelines which supply water to major four areas of the city. Among the four service areas of CWASA, the Karnaphuli service area (KSA) is selected in this study. The type of water supply system practiced in the study area was an intermittent system. KSA receives water from Sheikh Hasina Water Treatment Plant (SHWTP) of capacity 286,000 m^3/d, and it is located about 30 km away from SHWTP. Moreover, the area consists of northern, central, and western areas of the city geographically and are served by two reservoirs and two elevated tanks. The Northern, central and western regions are covered by Nasirabad reservoir and elevated tank, Battali hill reservoir and Halishahar elevated tank, respectively. A total of 38 random sampling points has been selected from the distribution line for water quality analysis, of which 10 from Northern, 10 from central, 6 from eastern and 10 from the western part of KSA (Fig. 1).

3. Material and methods

3.1. Characterization of supply water

The collected water samples were characterized for their few quality parameters following standards procedures (APHA, 2005), and the results were adopted in model equation. The samples were taken from consumer's tap joined to the distribution network. Water samples were collected randomly, without considering the time of supply or the water age in the pipeline. Due to resource constraints, it was challenging to collect the samples at specific times that correspond to the age of the water in the pipeline. Therefore, the timing of sample collection was not identified.

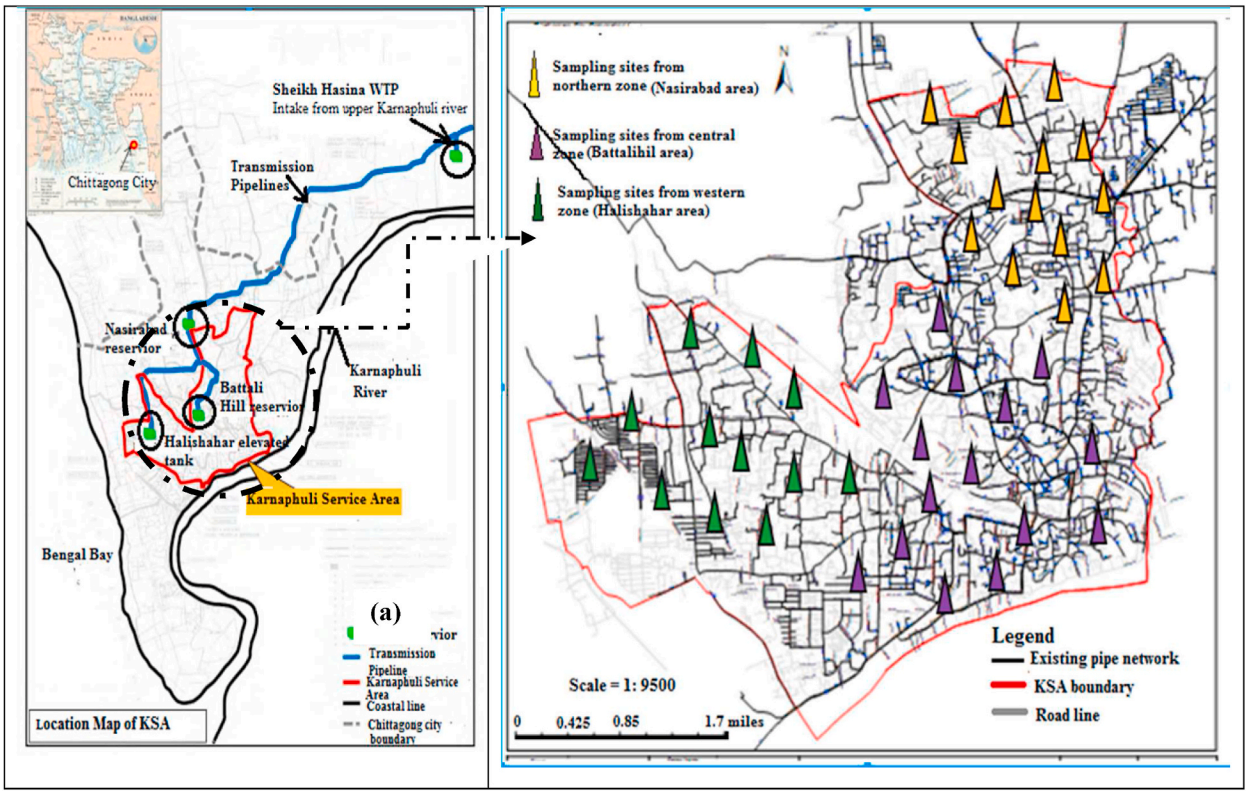

Fig. 1. Location map of study area a) Karnaphuli service area (KSA) b) Sampling points.

The water samples were collected after allowing the water to run for at least 2 min for avoiding any external contamination. The bottles were then kept in an incubator for maintaining a constant temperature if it was essential. DR 6000 HACH spectrophotometer was used for free chlorine and UV_{254} measurement. Total organic carbon (TOC) were measured by Shimadzu TOC-5000 analyzer. Approximately 2.5 mg/L of chlorine dose is used the SHWTP, and it is taken as the applied dose in the model equation. Chlorine contact time was assumed as 6 h considering the elapsed time between chamber of chlorine contact and the point of consumer tap.

3.2. Hydraulic modeling and THMs' simulation by EPANET 2.0

The basic hydraulic model of KSA was developed by EPANET 2.0 software represented as a series of links and nodes (Fig. 2) as proper hydraulic modeling is a prerequisite to simulate water quality parameters [36]. Input data for simulation (reservoirs' volume, tank elevation height, demand pattern etc.) are collected from the authority of CWASA. The developed hydraulic model suits a combined system of gravity and pumped distribution, consisting of a looped network with two elevated tanks, two reservoirs and 88 nodes and 152 pipes. The model simulation was performed considering a 24 h water requirement pattern, and for an extended period of 10 days. Water quality of all external inflows such as source chlorination, THMs concentration at initial node were specified at the start of the simulation and yield coefficient was kept a value of 0.2 (see Table 1).

EPANET simulation with operating conditions (Table 2) has been applied to the basic hydraulic model to predict the occurrence of THMs throughout the distribution line of KSA. EPANET requires input data in a specific format. The input file contains information on the network topology, including the location and properties of pipes, nodes, and tanks. It also includes details on the physical and chemical properties of network elements, such as pipe diameter, length, roughness, elevation, demand, and hydraulic variables. The input file also specifies the chlorine injection rates and decay coefficients. The user can modify the input file using a text editor or a graphical user interface software. The simulation is run using the hydraulic solver in EPANET, and the results are saved in a text or binary file for further analysis. The initial input of THMs' for the simulation has been taken from the estimated value of THMs using an empirical model developed by Amy et al. [18], (Eq. (1)). The authors conducted another study [16] in which the total THMs content and its species have been predicted based on water quality analysis at a few points of the area by applying three different empirical models proposed by Amy et al., [18]; Rathbun [36] and Malcolmprine [37]. The study evaluated the associated cancer risk due to the exposure of THMs using the highest predicted values of THMs and its species by AMY 98 model, and hence this model has been applied

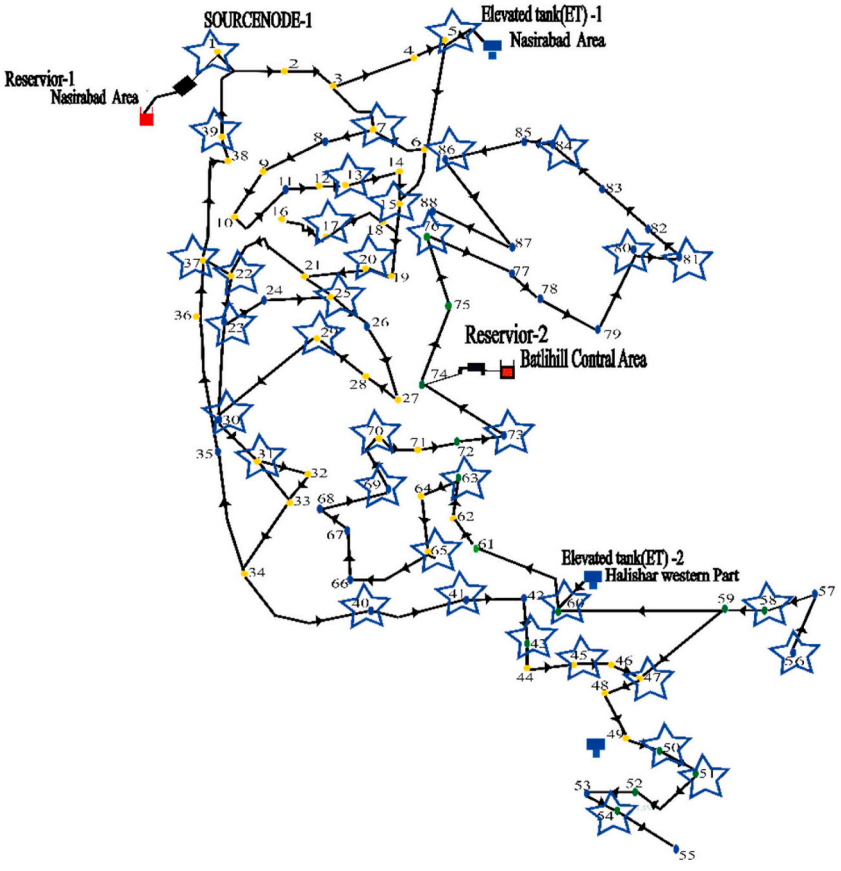

Fig. 2. The network of KSA and its critical nodes developed in EPANET 2.0. ☆ Denotes the sampling points.

Table 1
The boundary conditions for the THMs of AMY98 models.

Parameters	Range
Dissolved Organic Carbon, [DOC], mg/L	1.2–10.6
Applied Chlorine, [Cl_2], mg/L	1.51-33.55
Concentration of Bromide [Br-], μg/L	7–600
Incubation Temperature (Temp), °C	15–25
pH	6.5–8.5
Reaction time (t), hour	2–168

Table 2
Input values for chlorine simulation in EPANET.

Considered cases	Different Conditions	Effluent's chlorine conc. (mg/L)	Chlorine bulk decay, k_b (d^{-1})	Chlorine wall decay, k_w (d^{-1})
Case I	Condition 1	2	1	0
	Condition 2	2	0	1
	Condition 3	2	1	1
Case II	Condition 1	3	1	0
	Condition 2	3	0	1
	Condition 3	3	1	1
Case III	Condition 1	4	1	0
	Condition 2	4	0	1
	Condition3	4	1	1

with more data in this study. The current study evaluates the total THMs concentration from the measured water quality parameters at 38 sampling points by AMY98 model, and a total of 10 estimated values of THMs from this model have been used as preset values for EPANET simulation at 10 nodal points. The remaining points were used to compare with the EPANET simulation. As the residence time of chlorine is the maximum in the reservoir, most of the THMs are assumed to be formed within the source prior to be pumped to the distribution system for the ease of simulation. The reservoir is the location where water is stored prior to distribution, and therefore, it has a longer residence time than the downstream pipes.

$$[\mathrm{THMs}] = 10^{-1.385}[\mathrm{DOC}]^{1.098}[\mathrm{Cl_2}]^{0.152}[\mathrm{Br^-}]^{0.068}\mathrm{Temp}^{0.609}\mathrm{pH}^{1.601}\ t^{0.263} \quad \text{Eq.(1)}$$

3.3. Free residual chlorine simulation

Simulation of free chlorine has been performed using three cases of different doses of chlorine, injected at the source tank, which are 2, 3 and 4.0 mg/L, and for considering different values of bulk decay coefficients (K_b) and the coefficients of pipe wall (K_w). It is noteworthy to mention that the source of chlorine concentration for the study area comes from both the treatment plant and the chlorine boosting station located in the city. The chlorine concentration at the source ranged from 2 to 4 mg/l. The frequency of injection for booster stations can range from several times a day to once every few days. Based on existing practices, a typical concentration of 0.5–1.0 mg/L for chlorine and an injection frequency of 2–3 times per day were considered for the booster stations. EPANET TTHM formation model and EPANET first-order chlorine decay model are two distinct models utilized in water quality simulations. The first-order chlorine decay model is used to simulate the decline of chlorine concentration in a water distribution system. This model assumes that the rate of chlorine decay is proportional to the residual chlorine concentration, and that the rate constant of decay remains constant over time. However, it does not consider the formation of disinfection byproducts (DBPs), such as trihalomethanes (THMs). In contrast, the EPANET TTHM formation model is a more intricate model that considers the formation of THMs, which are formed when chlorine reacts with natural organic matter present in the water. This model takes into account the kinetics of THM formation and incorporates factors such as temperature, pH, and chlorine dosage. It predicts the formation and distribution of THMs in the water distribution system.

Most of the pipes in the distribution area have been installed long time before, and some were the latest imbedded in 2015–2020. Therefore, the value of K_w was put 0 or 1 for the pipes in CWASA's distribution system in different considered cases [28]. A K_b of 0 per day means that the concentration of chlorine in the water will not be affected by the presence of bulk organic matter in the system. In other words, the concentration of chlorine will only be affected by the first-order decay rate and the wall decay coefficient. A K_w of 1 per day means that the concentration of chlorine will decrease by an additional 1 mg/L for every square meter of pipe surface area through which the water passes. The following lines describes the steps to simulate free chlorine for different doses of chlorine, injected at the source tank, and for different values of bulk decay coefficients (K_b) and pipe wall coefficients (K_w). A new project was created in EPANET and the network was set up by defining nodes, pipes, tanks, and other relevant components. The source tank was defined and the desired doses of chlorine was set as input parameters. The bulk decay coefficient (K_b) and pipe wall coefficient (K_w) were defined as input parameters for the simulation. The simulation is run for each of the three different doses of chlorine and the resulting free chlorine concentrations were recorded at different points in the network. The results of the simulation were compared for the different

doses of chlorine and different values of K_b and K_w to identify any trends or patterns. After analyzing the results conclusions were drawn about the effectiveness of different doses of chlorine and different values of K_b and K_w in maintaining desired free chlorine concentrations in the distribution system.

However, the value of K_b and K_w were taken by trial and an improvement method using observed data. Different conditions of the simulation have been presented in Table 2.

The EPANET input file includes two additional lines that specify decay coefficients for chlorine in the water supply system. In EPANET input file, the "Bulk Chlorine 1.0" line specifies that the bulk decay coefficient for chlorine in the system is 1 per mg/L per day, meaning that for every milligram per liter of bulk organic matter, the concentration of chlorine in the water will decrease by an additional 1 mg/L per day. The "Wall Chlorine 0.0" line specifies that the wall decay coefficient for chlorine in the pipes is 0.0 per mg/m^2 per day, meaning that there is no additional decay due to wall effects in the pipes.

3.4. Cancer risk assessment and its spatial distribution in the study area

Cancer risk assessment of THMs was conducted following the method prescribed by the United States Environmental Protection Agency (USEPA) [38] for muti-pathway exposure. The guidelines of USEPA [39–41] have been adopted to assess the risk for dermal, inhalation and oral ingestion through chronic daily intake (CDI) and the respective slope factor (SF) [42]. The necessary input parameters for the human risk analysis have been summarized in Table 3. The study conducted by Khan et al. [16] demonstrates that the major compound of THMs of CWASA's supply water is chloroform ($CHCl_3$) and other THMs' compounds such as dibromochloromethane (DBCM), bromo dichloromethane (BDCM), bromoform (BF) form in a negligible amount. It is noteworthy to mention that risk assessment analysis has been calculated for chloroform ($CHCl_3$) as it is the dominant THMs' compound. CDI for each exposure pathway has been estimated using the following equations (Eq. 2 to 5) according to USEPA [40].

$$\text{CDI ingestion } (\text{mg}/\text{kg}-\text{day}) = \frac{C \times Ir \times Ef \times Ed \times Cf}{Bw \times At} \tag{2}$$

$$\text{CDIdermal } (\text{mg}/\text{kg}-\text{day}) = \frac{C \times Sa \times F \times Pc \times Et \times Ef \times Ed \times Cf}{Bw \times At} \tag{3}$$

$$\text{CDIinhalation } (\text{mg}/\text{kg}-\text{day}) = \frac{Cair \times Ir \times Ef \times Ed \times Cf}{Bw \times At} \tag{4}$$

$$\text{Total cancer risk} = \text{CDI}_{\text{ingestion}} \times \text{SF}_{\text{oral}} + \text{CDI}_{\text{Inhalation}} \times \text{SF}_{\text{Inhalation}} + \text{CDI}_{\text{Dermal}} \times \text{SF}_{\text{Dermal}} \tag{5}$$

SF is the carcinogenic slope factor ([mg/kg/day] $-^1$) for the mentioned three exposure pathways.

Two resistance theory by Little, [44]; Gratt, [52]) was used for the calculation of inhalation exposure. Two resistance theories have been adopted to calculate the content of THMs' species in air, C_{air} [54], and the equations are as $C_{air}=(C_{initial} + C)/2$, where $C_{initial}$ denotes the initial concentration of THMs' while C_t implies its concentration at any time t. It has been assumed in this study that $C_0 = 0$, and C_t has been calculated by the following equations (Eqs. (6)–(9)) according to Little, [44].

$$C = \frac{[1 - \exp(-bt)] \times a}{b} \tag{6}$$

Table 3
Input parameters and abbreviations for multi-exposure risk assessment.

Notation	Input parameters	Units	Values	References
Bw	Body weight	Kg	70	[43]
C	THM concentration of supplied water	mg/L	Findings of the study (as per Fig. 6)	This study
C_{air}	THMs' concentration in air	mg/L	Derived by little's Model	[44]
Cf	Conversion factor	L/m^{-3}	0.001	
Ef	Exposure frequency	$days/year^{-1}$	365	[45]
Et	Exposure time	min/day^{-1}	35	[45]
Ed	Exposure duration	Year	70	[43]
F	Fraction of skin in contact with water	%	90	[43]
H	Henry's law constant at 40 °C		0.25(chloroform);	[46]
Ir	Ingestion rate	$L\ day^{-1}$	4.01	[43]
$K_{oL}A$	Overall mass transfer coefficient	$L\ min^{-1}$	Chliorform 7.4;	[44]
Pc	Permeability Coefficient	cm/h^{-1}	Chloroform 6.8×10^{-3}	[47]
Q_G	Air flow rate	$L\ min^{-1}$	50	[44]
Q_L	Water flow rate	$L\ min^{-1}$	5	[44]
Sa	Skin surface area	m^2	1.8	[48]
SF_{oral}	Carcinogenic slope factor (oral)	$(mg.kg^{-1}day^{-1})^{-1}$	Chloroform 6.10×10^{-2}	[49]
SF_{der}	Carcinogenic slope factor (dermal)	$(mg.kg^{-1}day^{-1})^{-1}$	Chloroform 3.05×10^{-2}	[49,50]
SF_{inh}	Carcinogenic slope factor (inhalation)	$(mg.kg^{-1}day^{-1})^{-1}$	Chloroform 8.05×10^{-2}	[47,51]
Vr	Ventilation rate	$m^3\ h^{-1}$	0.83	[43]
V_s	Bathroom volume	m^3	10	[44]

$$b = \frac{[(Q_L/H) \times (1 - \exp(-N) + Q_G)]}{Vs} \tag{7}$$

$$a = \frac{[(Q_L.C_W).(1 - \exp(-N))]}{V_S} \tag{8}$$

$$N = \left[\frac{K_{OL}A}{Q_L}\right] \tag{9}$$

Here N means a dimensionless coefficient, Q_L = Water flow rate in liter per minute, t = time of contact, and a and b are factors.

Spatial distribution of risk level has been performed using inverse distance weighting (IDW) method with Arc GIS10.5 to identify potential risk zone of the study area. The (IDW) was used to simulate the risk estimates for the prediction of any unsampled site [53]. The attribute value for a point is the weighted mean of the investigated values in the vicinity and the weight is inversely proportional to the distance between the anticipated and investigated locations.

4. Results and Discussions

4.1. Characterization of supply water of the study area

EPANET simulation for THMs formation has been performed using a few preset values of THMs, which were derived by the model AMY98. Therefore, the necessary water quality parameters for the model were investigated in the study and the statistical summary of which is shown in Table 4. The pH value of the studied water samples are observed to be in range of 6.25–7.46, and that of temperature was from 21.4 to 30.5 °C. The variation of pH might be ascribed to the varied chlorine dose applied at treatment plant and the booster station located at northern Nasirabad. The value of pH decreases with the increased hypochlorous acid concentration resulted from the reaction of chlorine and water. Therefore, increased chlorine dose decreases pH value, and the water specimens taken from the point immediately after the Nasirabad booster station showed pH value below 7. On the other hand, the varying temperature might be ascribed to the fact of different collection dates. There is a positive correlation between pH and temperature and the formation of THMs, and their formation was found to be increased from 30% to 50% with the increase of pH from 6 to 11 [22] The other most important parameter total organic carbon (TOC) found in the distribution line, which is mainly due to biofilm of the pipe line was also assessed in the study. The major transmission and distribution pipelines in the city were installed in 1966, and till date new pipelines are connected to the existing network on an ad-hoc basis to supply water immediately to the consumer. Basically, three categories of pipe materials are there in the in existing system which are ductile iron (DI), asbestos cement (AC) and polyvinyl chloride (PVC) pipes with different ages. The TOC content of the supplied water was also observed in variable concentration, which might be due to the varying pipe material used in the distribution system.

4.2. Evaluation of residual chlorine and existence of THMs in supply water of the KSA

Free residual chlorine within the supply network has been simulated by EPANET for three conditions as mentioned in earlier section. The observed value of free chlorine within the study area ranged from 0.02 to 0.17 mg/L. The simulated values have been found to be very close to the actual values with good correlation for CASE I ($K_b = 1$ and $K_w = 1$) shown in Figs. 3 and 4. The world health organization (WHO) set the limit for free residual chlorine as 0.2 mg/L to keep the water safe from any microbial recontamination within the distribution network. Mensha et al. [54], analyzed decay of residual chlorine within Juja water distribution network in China by EPANET, and showed that a minimum and proper level of residual chlorine was maintained all over the distribution system by adjusting the initial chlorine dose. It is observed in the current study that an initial chlorine dose of 3 mg/L ($K_b = 1$ and $K_w = 1$) is appropriate for sustaining a residual content close to 0.2 mg/L all over the network. On the other hand, an primary chlorine dose of 4 mg/L (case III) causes high level of free chlorine for all of the nodes to be above 0.2 mg/L.

It has been observed that there is a significant effect of K_b on the residual chlorine content, and a reduction in K_b from 1 to 0 reduces the chlorine content by 25%. The effect of K_w is, however, found very less in case of chlorine residual changes in the distribution network. It is found by Monteiro et al. [31] that a variation of 30% in K_w decreases the simulated value by 10% only. Rahman [33], conducted a study within the water distribution network of Dhaka city of Bangladesh by EPANET and demonstrated that a negligible concentration of free residual chlorine is found at the nodal points located far away from chlorination point. Gradual decay of free

Table 4
Statistical summary of the characteristics of water of the study area.

Parameters	Minimum	Maximum	Mean	Standard deviation
pH	6.25	7.46	7.042	0.297
Temperature (^{0}C)	21.4	30.5	28.27	2.7681
UV_{254}(cm^{-1})	0.01	0.1	0.05	0.0023
TOC (mg/L)	0.78	5.86	2.526	1.509
Br^-(mg/L)	0.002	0.1	0.045	0.0132

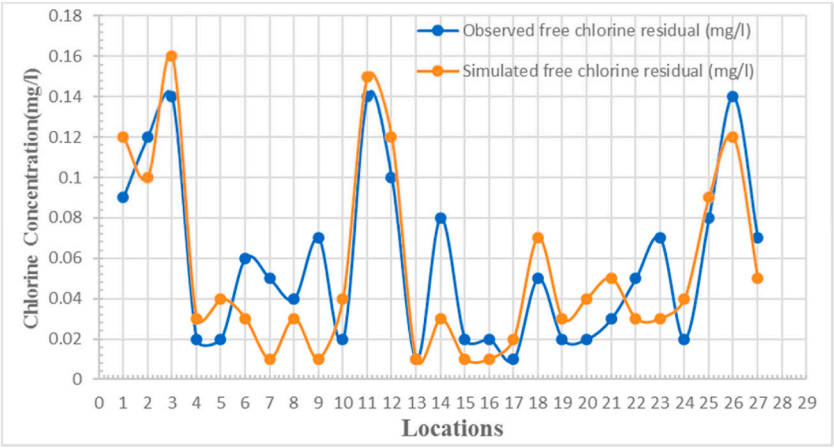

Fig. 3. Comparison of simulated and observed chlorine concentration (Case I Condition 1; source chlorination, 2 mg/L, $K_w = 1\ d^{-1}$ and $K_b = 1\ d^{-1}$).

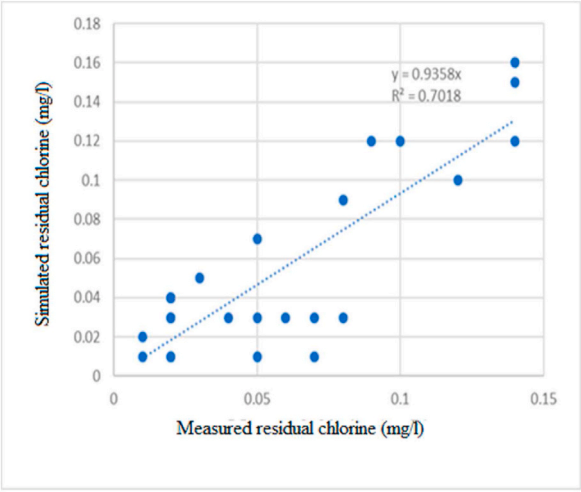

Fig. 4. Correlation between computed and measured chlorine concentration.

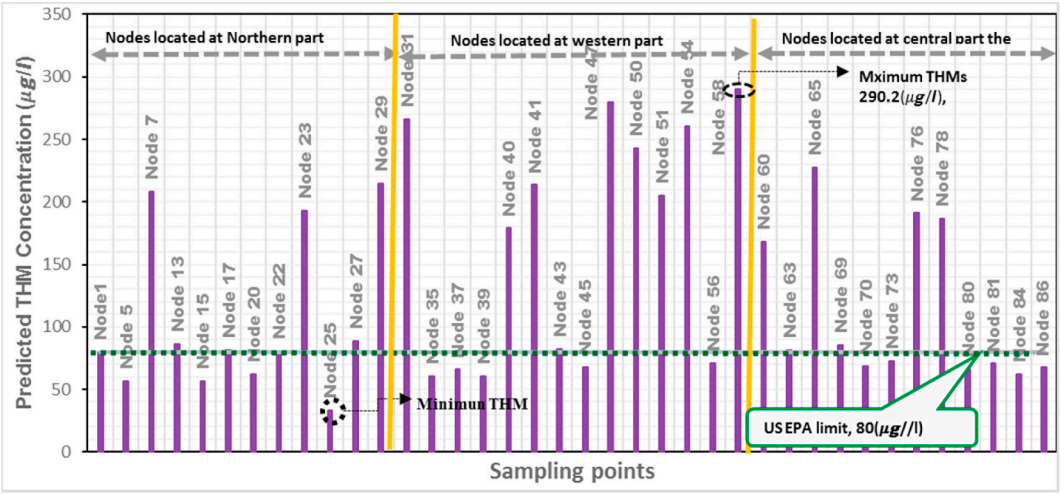

Fig. 5. Predicted concentration of total THMs at different sampling points by AMY98 model.

residual chlorine within the distribution network is also observed by the current study.

(Case I: Condition1; source chlorination, 2 mg/L, $K_w = 1\ d^{-1}$ and $K_b = 1\ d^{-1}$).

The predicted concentrations of total THMs at 38 measurement points of the service area by AMY98 model are shown in Fig. 5. The predicted concentration of THMs for northern, central and western part are 56–214 μg/L, 60–290 μg/L and 68–227 μg/L respectively. The predicted THMs concentration of different part of the study area are classified in Fig. 5 and the highest THMs concentration is predicted for node 58 located at west Halishahar area in the western part of the KSA. Water is being supplied to the consumers of this area from an elevated tank (ET) of capacity 2,400 m^3, which is 9 km away from Nasirabad reservoir. Therefore, a long retention time might be ascribed for the possible formation for by-products compounds in this area.

A total of 88 nodal points were simulated by EPANET for the production of THMs in the water supply network and the predicted value was in range of 33–486 μg/L approximately shown in Fig. 6. As mentioned earlier the THMs concentrations entering the network (79.43 μg/L) from its source node (Node 1) is taken from the AMY98 model prediction along with other preset values for 10 nodal points which have been marked in Fig. 7.

It has been observed in the simulation study that about 27% of the total 88 nodal points shows the THMs' concentrations are 150 μg/L -or less, and almost 99% of that shows the values are greater than 50 μg/L. Moreover, the initial concentration (79.3 μg/L) of THMs in the distribution network has been increased to 485.5 μg/L the location of which is at the longest residence time. An approximate representation of the distribution of THMs' concentration is shown by a histogram shown in Fig. 7. The highest peak of the histogram corresponds to the concentration range 220–240 μg/L with a maximum number of nodes 13. A probability curve is superimposed on the histogram which describes the frequency of the number of nodes over the mean value of THMs (272.27 μg/L).

The simulated values by EPANET and the predicted values by AMY98 have been compared and shown in Fig. 8 (a, b) and it shows a good predictability with R^2 value 0.8254. The variations in the two values might be due to the cumulative value at the junction points of more than one nodes in EPANET. While computing the THMs growth within the pipelines, the two major aspects are considered in EPANET as shown in Fig. 9. EPANET predicts the THMs concentration as a function of free chlorine whereas AMY98 model is formulated incorporating 7 influencing parameters. The results of the model are influenced by the measured water quality parameters especially pH and TOC. However, a good correlation indicates that EPANET in combination with AMY98 model could be an effective tool for forecasting THMs' formation within the any water distribution network (see Fig. 10).

4.3. Assessing the predictability of total THMs by EPANET

The performance of the developed total THMs simulation model (Model parameters: source chlorination = 2 mg/L, $K_w = 1\ d^{-1}$ and $K_b = 1\ d^{-1}$ with a yield co-efficient = 0.2**)** was evaluated using few actual data of total THMs which were measured later on by the authors for another study [55]. The model showed moderate accuracy, with an R^2 value of 0.70 and an RMSE of 9.61 μg/L. The % Error was 9.23% indicating that the model predictions were within a reasonable range of the measured values. While the model could benefit from further refinement, these results suggest that it could be a useful tool for predicting TTHM levels in the studied water distribution system.

4.4. Carcinogenic risk assessment and its spatial distribution

An average lifetime total carcinogenic risk due to the existence of THMs in supply water of the study area has been found as 5.39×10^{-4} which is almost 100 times higher than 1×10^{-6}, prescribed by USEPA guidelines. Oral ingestion has contributed the maximum

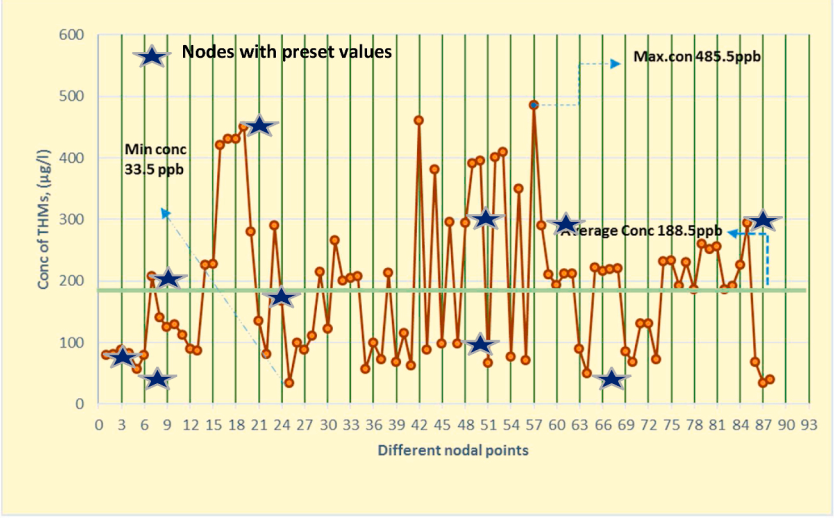

Fig. 6. THMs' simulation results at various nodal points.

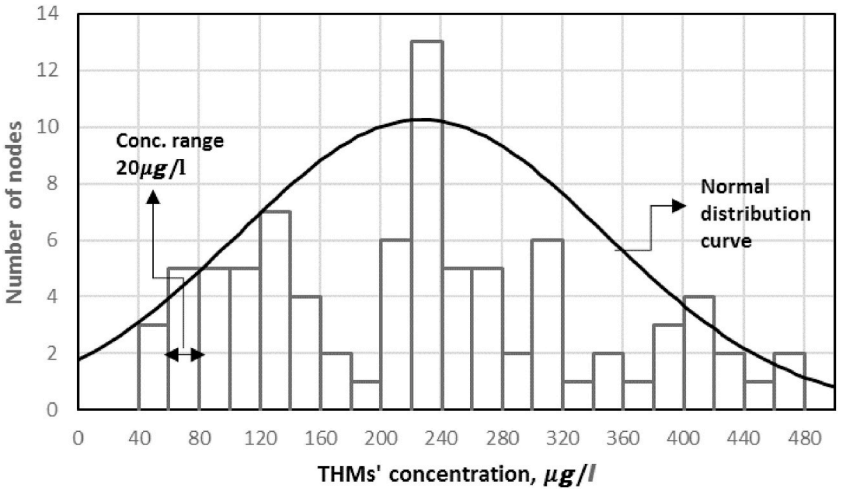

Fig. 7. Histogram of THMs' concentration predicted by EPANET throughout the studied network.

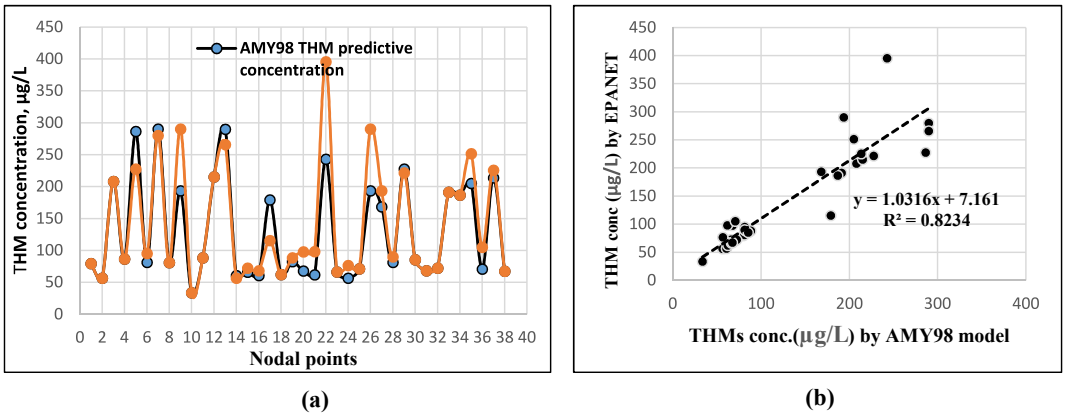

Fig. 8. a) Comparison of predicted THMs' conc. by AMY98 and EPANET; b) Correlation between predicted THMs' conc. by AMY98 and EPANET.

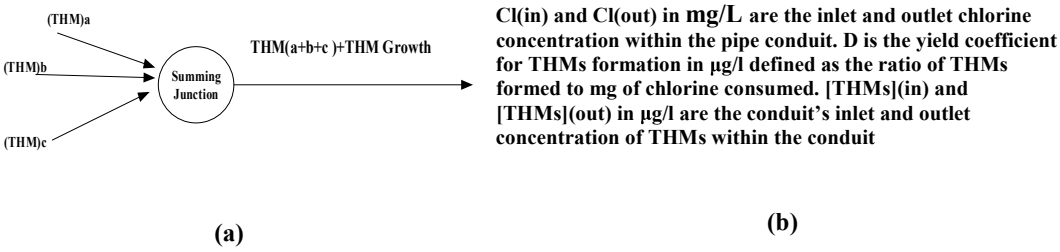

Fig. 9. THMs growth mechanism in EPANET a) Cumulative concentration at junction node b) Equation of THM Growth with free residual Cl concentration.

cancer risk followed by dermal and inhalation. The box plots in Fig. 11 (a, b, and c) show the five-number summary of the risk data, which includes the minimum, first quartile, median, third quartile, and maximum risk value. An average lifetime cancer risk for oral ingestion, inhalation and dermal of THMs compounds from the supply water was found as 1.706×10^{-4}, 7.509×10^{-6} and 2.07×10^{-7}, respectively. Therefore, risk for the dermal route was found to be below the prescribed risk level. The chronic daily intake (CDI) values of different pathways are mainly attributable for varying risk levels. The calculated CDI values from three routes followed the order $CDI_{oral} > CDI_{inhalation} > CDI_{dermal}$. The findings of risk levels follow a similar trend with the reported results of the risk study

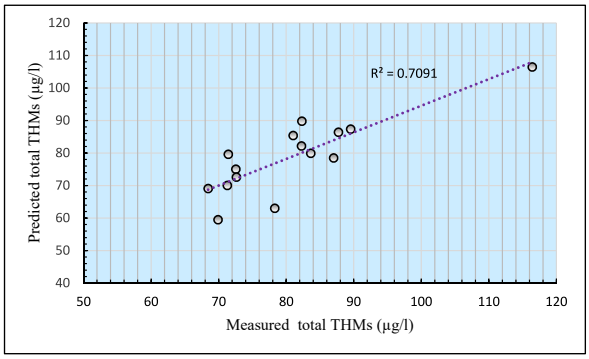

Fig. 10. Comparison of measured total THMs with predicted value in (µg/l).

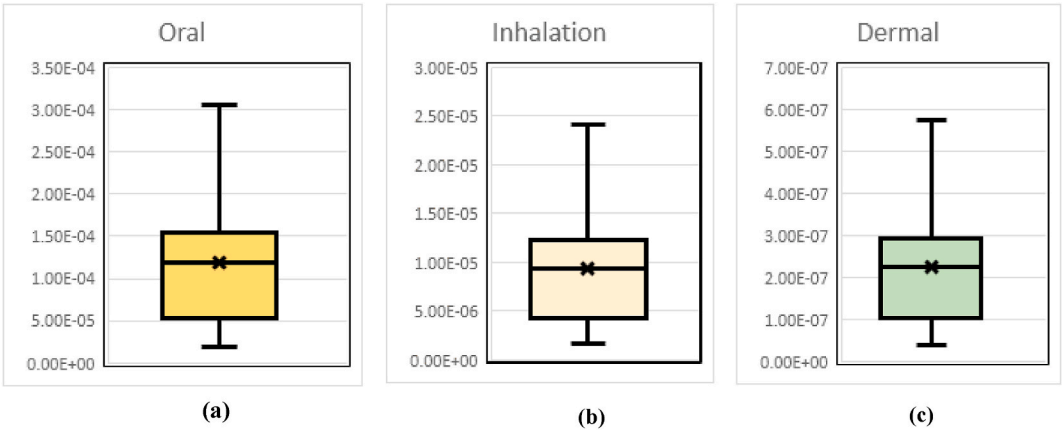

Fig. 11. Box plot of cancer risk level showing maximum, minimum and median of risk values (a) Oral risk level (b)Inhalation risk level (c) Dermal risk level.

conducted in Canada, China and India [5,7,56,57].

The authors conducted another study [16] based on only 11 nodes of the study area, and found the risk from various routes as 2.51 $\times 10^{-4}$. The variations in the risk level between the two studies are ascribed as the variation of the number of data points. The present study overcomes the limitations of the previous one by considering more study points. The findings of both studies, however, indicate that the supply of water in Chattogram is susceptible to posing a cancer risk to human health which may cause numerous diseases among the exposed community. However, few factors such as variability, frequency and duration of exposure, permeability of THMs through the skin, frequency of shower, human bodyweight and average lifetime, etc., are not considered in this study during the cancer risk estimation, which might be crucial improving the overall risk assessment.

The cancer risk (CR) classes developed by Chowdhury et al. [56] and Legay et al. [58] have been followed in this study. These studies categorized four classes of cancer risk level based on risk value: unacceptable risk ($CR = 10^{-4}$), negligible risk ($CR < 10^{-6}$), acceptable low risk ($1 \times 10^{-6} \leq CR < 5.1 \times 10^{-5}$) and acceptable high risk ($5.1 \times 10^{-5} \leq CR < 10^{-4}$). As mentioned before.

KSA is sub-divided into 10 sectors named as A to I (Table 5). Table 5 shows CR of different sectors for average total risk. As seen sectors D, E and F of central zone and I from western zone are identified as the potential risk sectors. The difference between THMs concentrations in different region is the main fact for varying risk level. As expected, regions which receive water with high THMs concentration shows higher risk value.

The spatial distribution of estimated cancer risk across the KSA is shown in Fig. 12 (a, b, c and d). As seen the left region is the northern zone of a service area covering points 1 to 25, while the right region is western zone with points 61 to 90. The central zone covers the rest of the sampling points. The central zone is identified as the highest risk zone for total cancer risk, which is presented in the red color, followed by the western and northern zone (Fig. 12a). This zone is highly vulnerable regarding the cancer risk among the dwellers comparing to another zone. Risk through oral ingestion exceeds the USEPA limit (10^{-6}) in all of the three zones of KSA. A similar pattern of distribution is therefore seen for oral ingestion as this route is the major contributor of total cancer (Fig. 12b). In all regions, risk through dermal absorption is found within the USEPA safe limit. The risk level for inhalation exposure exceeds the minimum risk level for some areas from central and western zones.

The variation of risk level for different zone as visualized by the spatial distribution may be described as follows. Chlorine boosting is done at the Nasirabad boosting station and the northern zone of KSA receives supply water immediately after the boosting.

Table 5
Sector wise risk evaluation.

Major parts of KSA	Sectors	Average oral risk value	Average inhalation risk value	Average Dermal risk value	Average Total risk value	Risk Level
Northern part of KSA	A	5.13×10^{-5}	4.12×10^{-6}	9.77×10^{-8}	5.55×10^{-5}	Acceptable high risk
	B	7.55×10^{-5}	6.02×10^{-6}	1.43×10^{-7}	8.17×10^{-5}	Acceptable high risk
	C	7.10×10^{-5}	5.67×10^{-6}	1.35×10^{-7}	7.68×10^{-5}	Acceptable risk
Central part of KSA	D	1.51×10^{-4}	1.20×10^{-5}	2.84×10^{-7}	1.63×10^{-4}	High risk
	E	2.50×10^{-4}	1.98×10^{-5}	4.70×10^{-7}	2.70×10^{-4}	High risk
	F	1.06×10^{-4}	8.39×10^{-6}	2.00×10^{-7}	1.14×10^{-4}	High risk
	G	4.57×10^{-5}	3.68×10^{-6}	8.75×10^{-8}	4.95×10^{-5}	Acceptable low risk
Western part of KSA	H	9.33×10^{-5}	7.42×10^{-6}	1.76×10^{-7}	4.95×10^{-5}	Acceptable low risk
	I	1.40×10^{-4}	1.11×10^{-5}	2.64×10^{-7}	1.52×10^{-4}	High risk
	J	7.58×10^{-5}	6.05×10^{-6}	1.44×10^{-7}	8.20×10^{-5}	Acceptable high risk

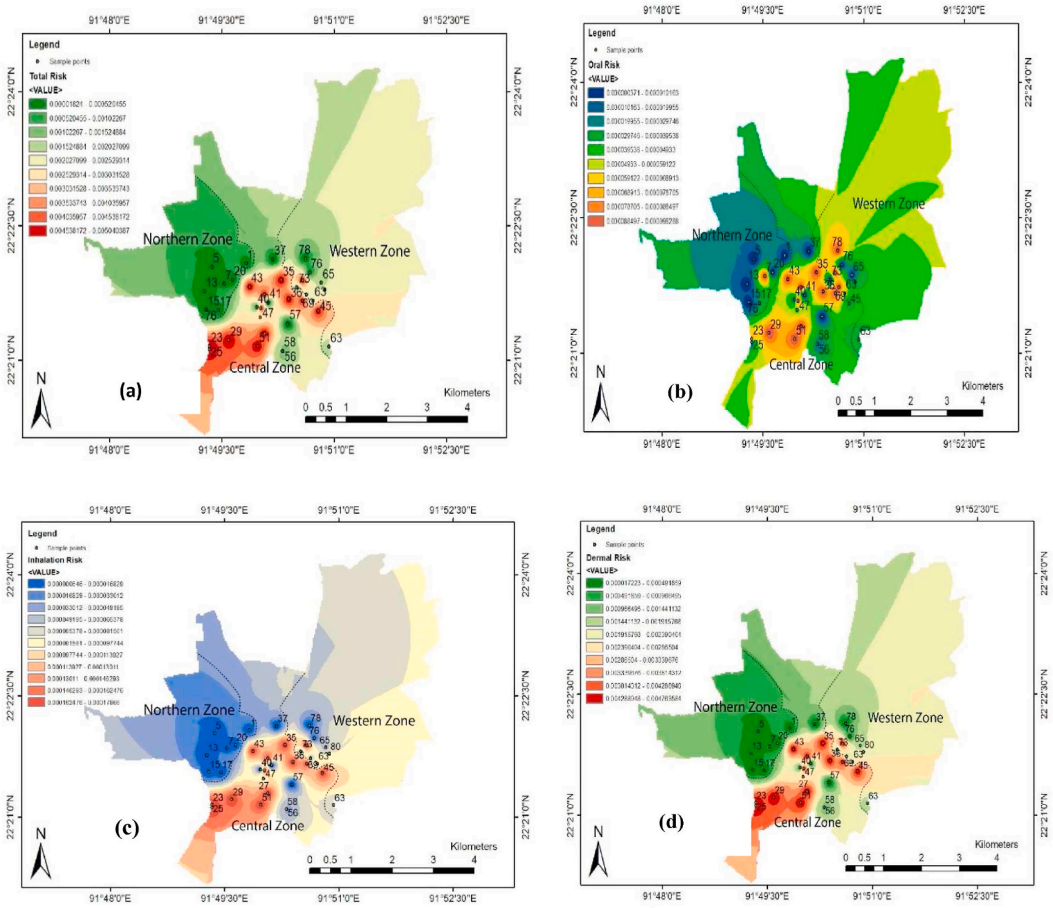

Fig. 12. Spatial distribution of cancer risk in selected regions a) Total Risk b) Oral Risk c) Inhalation Risk d) Dermal Risk.

Therefore, due to breakpoint chlorination fact, free chorine is found in a negligible amount in the pipe lines of northern zone to form THMs since free chlorine is considered to be the main driver of THMs formation [59]. The findings of the study also identified the sectors of this zone is as low risk area. The central area supplies water to its consumers from elevated tank (ET) which is 9 km away from the Nasirabad reservoir. Therefore, a long retention time is there for by-products formation. This zone is the most vulnerable zone as found by the current study (Fig. 12). On the other hand, in western part availability of free chlorine is less as no boosting is done in between northern and western zone. Sectors of this area shows acceptable low risk value. Fig. 13(a) and (b) show the identified

high-risk area for each of the three exposure and ingestion scenarios separately.

5. THM monitoring in developing countries: role of models and software tools

The process of monitoring disinfection byproducts (DBPs) in drinking water is demanding and requires expensive equipment such as gas chromatography (GC) and GC/mass spectrometry (MS), as well as complex sample preparation techniques. This has been highlighted in previous studies such as Arbuckle Tye et al. [59], Li et al. [60], and Li and Mitch [61]. These challenges include the high cost of analysis equipment, limited resources, and lack of access to specialized laboratories. To address these challenges, various models have been developed to estimate the formation of DBPs, including THMs. This study aimed to use an empirical model combined with EPANET to predict THMs in water supply systems in Chittagong, Bangladesh. Despite the absence of THMs measurement facilities in the area, the methodology adopted in the study may provide a solution for water utilities in resource-constrained settings to assess and manage potential risks associated with THMs in drinking water. While direct THMs measurements are ideal, this approach offers a viable alternative for developing countries facing similar resource constraints.

6. Limitations of the study

The study has been conducted based on a few water quality parameters which are influential for THMs formation. The work would be great if the actual measurement of THMs in supply water could be made. However, pipe material and pipe length, which also have great effect on THMs, have not been considered in the study. On the other hand, water stability is a critical factor in the formation of disinfection byproducts (DBPs), including THMs which is a measure of how well the water resists changes in its quality or characteristics, such as pH, alkalinity, and dissolved organic matter. When water is unstable, it can lead to rapid changes in these characteristics, which can result in increased formation of DBPs during disinfection. Therefore, it is important to consider water stability in the design and operation of water treatment and distribution systems to predict the formation of DBPs and protect public health. Moreover, chlorine simulation has been performed taking the value of K_b and K_w from literature. However, the use of EPANET MSX is a viable option for including the degradation of DBPs in the distribution system (Monteiro et al., 2013). The probable scenario of THMs has been tried to capture, which would be beneficial for raising awareness regarding monitoring and setting standards for the compounds for securing water safety.

7. Conclusion

THMs are the dominant group of possible disinfection byproducts formed in chlorinated supply water and induce the highest cancer risk from different exposure pathways. The objective of the study is to identify the potential risk zone of Chattogram city due to the probable occurrence of THMs in the supply water of the city. In this regard, free residual chlorine is simulated and the THMs concentrations are predicted within the distribution network by applying EPANET simulation in combination with AMY98 model. Free chlorine simulation under varying chlorination conditions shows that source chlorination of 3 mg/L is appropriate with $K_b = 1\ d^{-1}$ and $K_w = 1\ d^{-1}$ to maintain 0.2 mg/L within the network as per WHO guidelines. On the other hand, from simulated THMs' concentrations, it is noteiced that the estimated concentration of THMs' for 80% of the total nodal points of the network is higher than that of the USEPA limit (80 μg/L). An average estimated lifetime cancer risk based on the anticipated level of THMs in supply water was observed to be 5.37×10^{-4}, that is over 100 times greater than the acceptable risk level recommended by USEPA. The spatial-based analysis identifies the Battali hill area as a high-risk region of high cancer, followed by Halishahar and Nasirabad. The high-risk zones are the

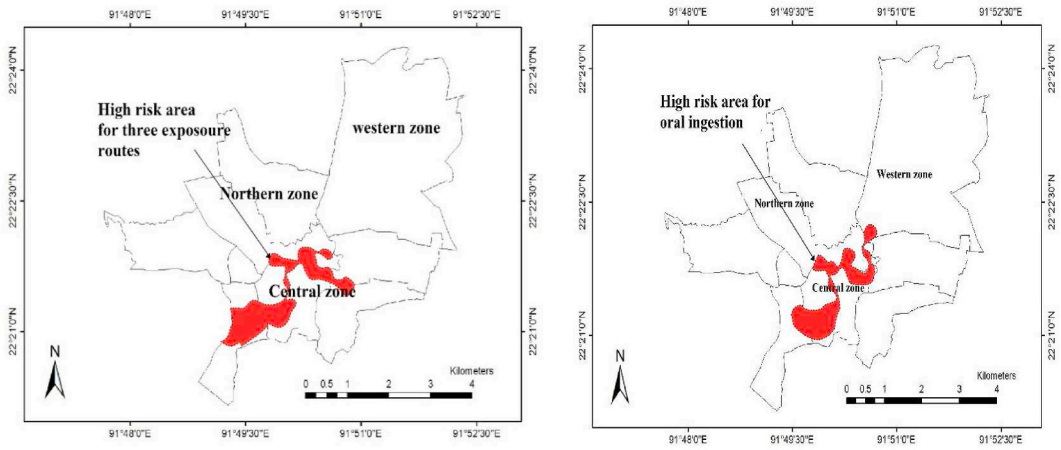

Fig. 13. Identified high risk area.

areas where there are enhanced chlorination and junction of distribution pipes. The findings of the study clearly show that community water supplies in the city are susceptible to create a cancer risk due to the probable occurrence of THMs. The findings, however, highlight the necessity for monitoring the actual value of THMs along the distribution system of the city. Zone wise risk identification is of great importance for operational and regulatory purpose and to help operators in managing chlorine residuals and THMs throughout the network. Additionally, the applied combined method can be used as an effective alternative of field level investigation of THMs with minimal measurement of water quality data. The proposed method might be adopted by other developing countries as THMs measurement involves sophisticated instrumentation with expert handling. The study may, therefore, be useful to upgrade the water safety of the city and also provide in any epidemiological study to evaluate peoples' exposure to potentially harmful DBPs.

CRediT authorship contribution statement

Mst. Dr. Farzana Rahman Zuthi, Farjana Khan and Md. Sazzad Zahid Sajol: Conceived and designed the experiments, performed the experiments, contributed analysis tools data and wrote the paper. Maisha Kabir, M. Ethtesham Kaiser, S. M. Farzin Hasan and M. Safiur Rahman: Analyzed and interpreted the data; contributed materials, and wrote the paper.

Data availability statement

The authors of this study can provide the data supporting their findings upon a reasonable request. The additional supporting information already includes the specific research methods mentioned in the article as well as the original images of the results.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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