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SIMULATION OF THM SPECIES IN WATER DISTRIBUTION SYSTEMS

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Abstract—The Safe Drinking Water Act and its Amendments (SDWAA) may potentially limit each individual species of THM compounds in water distribution systems since the health risks associated with these species are not alike. A new approach to characterize and model the kinetics of THM species using nonlinear optimization was introduced in an earlier study. The approach combines site-specific water quality trends with stoichiometric expressions based on an average representative bromine content factor of the source. This paper incorporates the proposed kinetic approach in a full-dynamic water quality transport model. The model is capable of modeling chlorine, total THM, and the four THM species in water distribution systems subjected to different varying loading conditions. The model has been tested and verified by application to a portion of the Abu-Dhabi distribution system in the United Arab Emirates. High levels of bromoform and bromine incorporation factors were reported throughout the system. The quality trends of the bromide-rich desalinated water at the source were transmitted to different locations in the network using the proposed modeling approach. Overall agreement between the modeled and measured concentrations was reported. However, deviations at distant locations from the source indicate the degradation in the bromine incorporation factor under dynamic conditions and an increased tendency of the brominated THM compounds to hydrolyze. The model represents a useful and robust numerical tool to water utilities attempting to verify the SDWAA potential regulations regarding the THM species.

Key words—trihalomethane species, bromine content factor, quality modeling, water distribution systems

INTRODUCTION

New restrictive rules for filtration of surface water and maximum levels of total trihalomethanes in distribution systems are being imposed by The Safe Drinking Water Act and its Amendments (SDWAA). The new Disinfection/Disinfectants By Products (D/DBP) rule addresses the possibility of specifying maximum contaminant levels (MCL) for each individual THM species since their health risks differ significantly (Pontius, 1991, 1992). A study by the US National Cancer Institute in 1976 indicated that chloroform, a major component of THMs, is an animal carcinogen and eventually a suspected human carcinogen (Trussell and Umphres, 1978; Tuthill and Moore, 1980). Bromoform and bromodichloromethane were reported carcinogenic later (USEPA, 1990; Bull and Kopfler, 1991). Under the new D/DBP rule, MCL of THM is lowered to 0.08 ppm instead of the previous limit of 0.1 ppm. Since then, many incidents of violations have been reported by municipal water systems.

It is clear that properly developed quality models to simulate the temporal and spatial variations of different substances in distribution systems can potentially assist the utilities' operators in abiding with the new strict quality rules. A number of such models have emerged during the last decade. They were mainly developed to model the chlorine under different dynamic conditions. Other substances, characterized by reaction kinetics similar to chlorine, can also be tracked using these models. Two main approaches have been utilized in the quality models; the time-driven method and the event-driven method. The time-driven method is Eulerian in nature and moves the water between fixed-sized volume segments in pipes as the clock time advances in uniform increments. The event-driven method is Lagrangian in nature and moves variable-sized blocks or fronts through the network and

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updates the model conditions at the next event when a block or front reaches a junction node. EPANET (Rossman *et al.*, 1993) is a dynamic quality model employing the time-driven approach. The event-driven approach was first utilized by Liou and Kroon (1987) and was later incorporated in full dynamic models by Boulus (Boulus *et al.*, 1995). PICCOLO is another quality model, developed in France, that applies the event-driven approach (Jarrige, 1993). This paper employs the event-driven approach in modeling the substances required for estimating the four species of THM in distribution systems.

KINETICS OF THM AND THM SPECIES

A study conducted by the National Organics Reconnaisance Survey (Symons *et al.*, 1975) revealed that four THMs; chloroform, bromodichloroform, dibromochloroform, and bromoform, exist in chlorinated drinking water in the United States. The THM compounds develop in chlorinated water containing organic precursors, such as humic and fulvic acids. It has been reported that the relative contribution to the formation of THMs by the humic fraction is greater than that of the fulvic fraction since humic acids react more readily with chlorine (Babcock and Singer, 1979).

Even though it is well known that TTHM increases with time, information about the reaction mechanism of the formation of THM and its species is still limited. A linear relationship exists between chlorine consumption and the production of THMs with a reaction order greater or equal to unity (Kavanaugh *et al.*, 1980; Trussell and Umphres, 1978). Most dynamic quality models use simple limited *n*-th order kinetic relation for the THM formation. Clark *et al.* (1994) modeled TTHM in the North Main water distribution system as a conservative substance at the source. More recently, Clark (1998) proposed a linear relationship between THM formation and the chlorine demand based on second-order reaction kinetics for the chlorine.

THM evolution has been shown to be a function of many water quality parameters, including the total organic carbon, type of organic precursors, pH of chlorination, temperature, UV light absorbance, bromide level, and reaction time (Amy *et al.*, 1987). A multiple-parameter power formula was developed as a function of the above quality parameters using nonlinear regression procedure. A later study (Montgomery Watson, 1993) developed similar relations for each individual species of THM as a function of the same quality parameters. The study reported that three databases were used in developing and verifying these relations. The first is called "AWWA D/DBP TAW (Technical Advisory Workgroup)" where the data was collected by Montgomery Watson in a 1990 AWWA-sponsored project entitled "Disinfection/Disinfectants By-Products Database and Model Project". The second is called "AWWA D/DBP TAW COAGULATION DATABASE" where the data was collected during a 1991 AWWA-sponsored project entitled "Effect of Coagulation on the Formation of Disinfection By-Products". The third data base is called University of Arizona Database that was compiled in 1983 and 1984 including THM data from raw water chlorination experiments conducted on samples from nine different utilities across the country (Malcolm Pirnie, Inc. 1991). The quality parameters considered in the aforementioned relations have a different influence on TTHM evolution based on chlorine dosage and the bromide concentration with respect to the organic content of the water. Bromoform has been reported to always increase with time regardless of the chlorine dosage and the temperature levels.

A recent study (Elshorbagy, 2000) models the kinetics of the THM species under representative extreme conditions employing the site-specific quality trends with stoichiometric expressions based on an average representative bromine content factor (BIF). BIF is a measure of the brominated species content in TTHM that was earlier defined by Gould *et al.* (1981) as follows:

$$\mathrm{BIF} = \frac{\Sigma N[\mathrm{CHCl}_{(3-N)}\mathrm{Br}_N]}{\Sigma[\mathrm{CHCl}_{(3-N)}\mathrm{Br}_N]} \tag{1}$$

The developed kinetic approach is utilized in the current model and therefore its main steps are summarized here. An average BIF at the source is estimated first. Significant variations in BIF with time can be handled by considering constant average values of BIF discretized on a reasonable number of selected time increments. The following procedures are then implemented at each calculated time increment associated with a certain event in the quality model:

- Chlorine is modeled using a first-order decay equation

$$C_{(t+\Delta t)} = C_{(t)}\, \mathrm{e}^{(-k\Delta t)} \tag{2}$$

where k accounts for both bulk and wall decay coefficients as defined by Rossman *et al.* (1994). The molar concentrations of TTHM ([TTHM]) is modeled using a predictive regression equation based on chlorine demand as follows:

$$[\mathrm{TTHM}]_{(t+\Delta t)} = [\mathrm{TTHM}]_t + F^*(\mathrm{Cl}_{(t+\Delta t)} - \mathrm{Cl}_t) \tag{3}$$

- Bromoform is modeled using a first-order limited growth relation as follows:

$$\mathrm{Br} = (\mathrm{Br_p} - \mathrm{Br_o})[1 - \mathrm{e}^{-k_b t}] \tag{4}$$

- Calculate S_3 corresponding to bromoform where S_N (N = 0, 1, 2, 3) are distribution factors corresponding to the four THM species and defined by the equation:

$$S_N = \frac{[\mathrm{CHCl}_{(3-N)}\mathrm{Br}_N]}{[\mathrm{TTHM}]} \quad (N = 0,\ 1,\ 2,\ 3) \qquad (5)$$

• Obtain S_0, S_1, and S_2 by solving a nonlinear optimization problem whose objective function is given by:

Minimize

$$\lambda[S_0 + S_1 + S_2 + S_3 - 1]^2 + [S_1 + 2^*S_2 + 3^*S_3 - \mathrm{BIF}]^2 \qquad (6)$$

where λ is assigned a sufficiently large value.

- A set of simple non-equality relationships among the distribution factors (S_0, S_1, S_2, and S_3) may be incorporated in the optimization problem as linear constraints. This set describes and characterizes the quality trend of the water in terms of its THM speciation. The set is determined through studying the quality of produced water at the source and inspecting a sufficient amount of measurements of THM species.
- The weight concentrations of chloroform, bromodichloromethane, and dibromochloromethane are calculated from equation (5).

It should be noted that the above equations need five regression coefficients to be defined earlier by establishing relevant quality relations at the source. These are: the chlorine decay coefficient k of equation (2); the TTHM and chlorine demand proportionality coefficient F of equation (3); and the bromoform growth coefficients k_b, Br_p, and Br_o of equation (4).

SYSTEM-SIMULATION MODEL

Modeling the four THM species in water distribution systems using the aforementioned kinetic approach requires the following modeling components:

- Modeling of chlorine concentrations.
- Modeling of total THM molar concentrations.
- Modeling of bromoform concentrations.

QUALNET is a dynamic quality model that has been used before in modeling the chlorine in a brushy-plain distribution system (Elshorbagy and Lansey, 1994). It employs an event-driven approach in moving the clock time and tracks the quality fronts through the pipe network. KYPIPE, the University of Kentucky hydraulic simulation model (Wood, 1980), is utilized by QUALNET in calculating the velocities and other hydraulic parameters. QUALNET is incorporated in the current developed model to model the chlorine and other substances after being modified to account for the relevant kinetic relations, i.e. equation (3) for (TTHM) and equation (4) for bromoform. The distribution factors S_0, S_1, and S_2 are obtained at each time increment by invoking a nonlinear optimizer to solve the problem given in equation (6) including any considered constraints explained earlier. (6)

Since the time increments associated with modeling different substances are related to events and decays of these substances, the problem involves two different time increments associated with the chlorine and bromoform solvers. To accommodate these time increments in modeling the THM species, two approaches can be followed. The first approach solves for S_0, S_1, and S_2 at a time increment naturally obtained from one solver after having the other solver producing its solution by the end of that increment. The second approach allows the two solvers to solve for chlorine [TTHM], and bromoform using their natural time increments up to another specified time increment "TSPEC", at which S_0, S_1, and S_2 are obtained. This approach means that a time-driven method is used to change the clock time associated with S_0, S_1, and S_2 calculations while chlorine, [TTHM] and bromoform are still calculated during the duration, TSPEC, based on an event-driven approach. All events of [TTHM] and bromoform can still be captured in this case during the simulation period. The later approach was selected to model the four species after assuring that the simulation accuracy is unaffected while the size of calculations (for S_0, S_1, and S_2) can still be controlled. The flowchart shown in Fig. 1 illustrates the sequence of the modeling approach. The nonlinear optimization problem is solved using the GRG2 model (Lasdon and Waren, 1978) that employs a generalized reduced gradient Lagrangian method. THMSPEC is a Fortran code utilizing the summarized approach in modeling different THM species at different nodes of water distribution systems.

APPLICATION SYSTEM

Abu-Dhabi is the capital city of United Arab Emirates (UAE) with a population of about 500,000. The city lies on an island inside the Arabian Gulf with an average daily water consumption of about 70 million gallons (318,000 m^3). The main source of water supply is desalinated seawater as is the case with most cities in the gulf area. About 85% of the total demand (60 MGD) is produced from the Um-Al-Nar (UAN) desalination plant which is located outside the island (Fig. 2). The rest of the demand (10 MGD) is produced from the Abu-Dhabi Power and Desalination plant (ADPD) which is located on the island. Water is transmitted from UAN through three pressure ring-mains directly to the distribution system and through one trunk-main to two pumping units (Unit I and Unit II) which are located on the island. Unit I also receives ADPD's water through two trunk-mains (Fig. 2).

In the mid 1960s, a simple water distribution system, directly fed from the water production plants, began to serve Abu-Dhabi city. Since then, the population, and, consequently, the water demand, have grown rapidly bringing about the construction of pumping Units I and II in addition to many other water projects.

To carry out the current quality verification on the city's distribution system, accurate and careful hydraulic calibration is first required. A large number of pipes and nodes, in addition to the presence of storage tanks in the system, increase the level of uncertainty in estimating the required parameters and usually lead to poor hydraulic calibration. This can eventually produce erroneous quality results. Since the main goal is to verify the proposed approach of simulating the kinetics of THM species in real systems, it was sought to minimize the major sources of errors that may affect the quality results. Therefore, a portion of the Abu-Dhabi distribution system, free of tanks, and with a reasonable number of pipes and nodes was selected for the verification procedure. A previous hydraulic study (Al-Nassay and Rabiah, 1998) showed that the portion of the network to the right of section 1-1 (Fig. 2) is mostly fed from UAN during the entire 24-h duration of a typical operation. Note that the inflows reported at node 76 were smaller than the respective nodal demands. That portion was selected for the current application with 48 pipes and 38 nodes (Fig. 3).

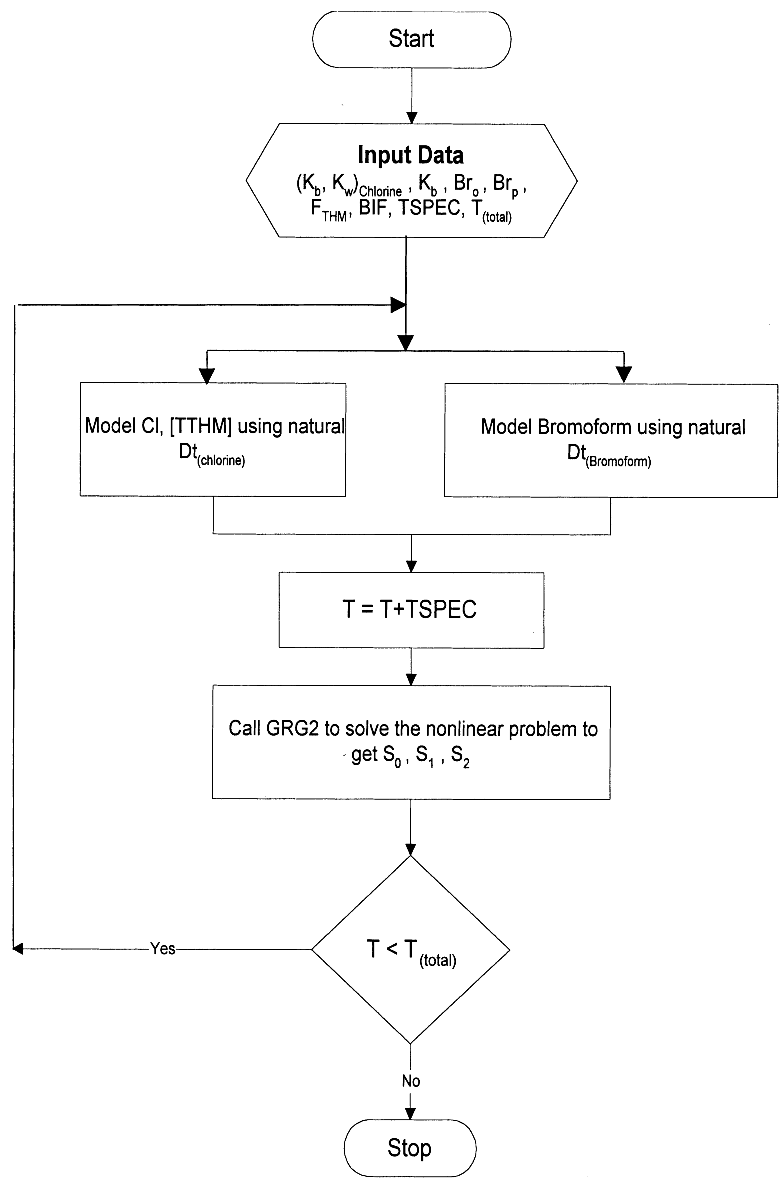

Fig. 1. Main components used in modeling the THM species.

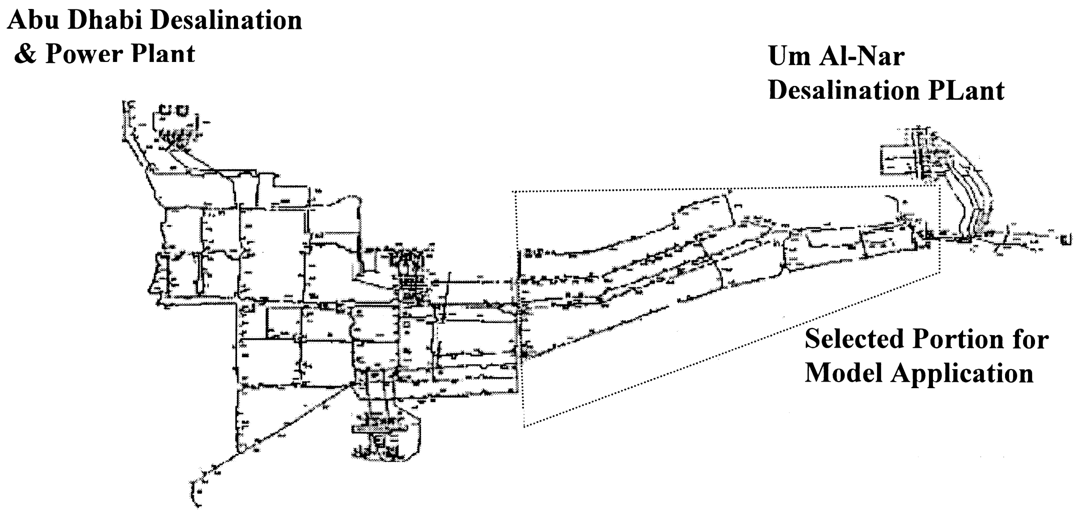

Fig. 2. Abu-Dhabi water distribution system.

The flows coming out from that portion through nodes 70, 72, 74, 76, and 78 during the 24-h simulation period were obtained from the aforementioned hydraulic study conducted on the entire network (Al-Nassay and Rabiah, 1998). These flows were included in the external demands of their respective nodes for the current application.

HYDRAULIC CALIBRATION

Information related to the pumping conditions at the UAN desalination plant is not readily available due to strict security measures applied in the region. To avoid this limitation, measurements of flow and pressure at pipes 1 and 3 were taken on an hourly basis using installed current meters and pressure gages to define the inflow conditions to the system. Close readings were averaged up so that a total of seven periods were found adequate to represent the variable hydraulic conditions during one day. Table 1 lists the source averaged pressures and flows along with the global demand coefficients and flows of the peripheral end nodes at the seven considered periods. Seven artificial reservoirs were used to simulate the inflow conditions with water levels set according to the pressures of the considered seven periods. Each reservoir was connected to nodes 2 and 4 setting the connecting pipes open during the period associated with that reservoir. For example, the pipes connected to the first reservoir were set open during the first 5 h and were closed during the rest of the day, while pipes connected to the second reservoir were set open from 17:00 to 20:00 and were closed otherwise. The estimated demands of different nodes, obtained from the Water and Electricity Department in Abu-Dhabi, were adjusted in each period until their summation matched the inflow to the system as reported from the inflow measurements. Another calibration procedure was carried out to adjust the roughness parameters of different pipes (Hazen-Williams coefficients) by checking the solved flows and pressures against measured values at some selected locations.

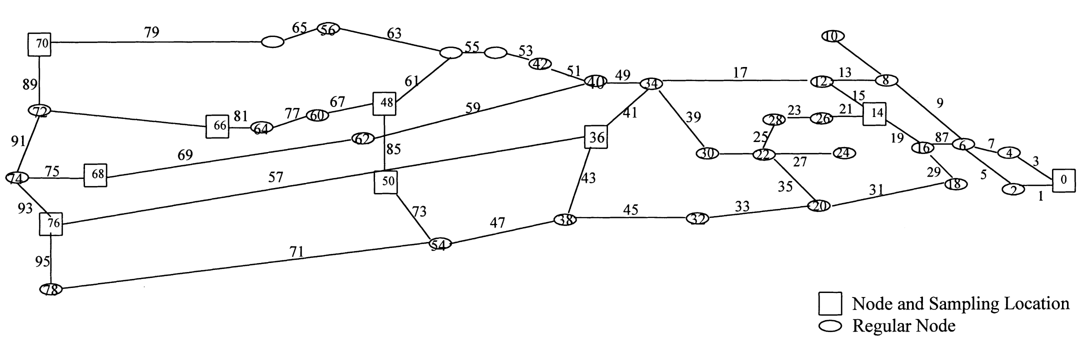

Fig. 3. The selected portion of the Abu-Dhabi water distribution system for model application.

Table 1. Inflow and outflow hydraulic conditions

Period No.	1	2	3	4	5	6	7
Duration	(12:00–17:00)	(17:00–20:00)	(20:00–24:00)	(24:00–2:00)	(2:00–7:00)	(7:00–11:00)	(11:00–12:00)
Source inflow (l/s)	1202	1741	1444	1264	772	1148	1609
Source pressure (m)	29.5	40	35	43	28.5	39	34.5
Global dem. coefficient	1	1.48	1.21	1.06	0.52	0.94	1.35
Outflow at node 70	165.4	225.7	191.8	174.3	92.4	181.5	211.8
Outflow at node 72	86.3	121.7	106.5	87.5	182.3	81.4	114.7
Outflow at node 74	23.7	31.2	28.4	24.4	14.3	20.6	29.6
Outflow at node 76	−13.6	−16.2	−17.4	−18.4	−22.7	−19.1	−16.5
Outflow at node 78	130.6	180.6	154.7	137.5	84.6	122.6	176.4

SAMPLING AND QUALITY CALIBRATION

Nine sampling points were selected in the application portion of the network for quality verification purposes (Fig. 3). A 24-h sampling program was conducted on these sampling points. Measurements of chlorine and THM species were taken at six different hours (14:00, 17:00, 20:00, 24:00, 8:00, and 11:00). Site 1 is located so close to the desalination plant that it was considered as a source for the modeled portion and its reported measured substances were dealt with as source concentrations. Table 2 lists the measurements of different substances at sampling site 1 along with the calculated BIF and the obtained chlorine bulk decay coefficients. Residual chlorine concentrations were slightly varying during the 24-h simulation period (0.59–0.63 ppm). An average constant value of 0.61 ppm was considered at the source. Samples of water were taken at the six considered hours and analyzed for the chlorine bulk decay coefficients. The results are listed in the table and an average value of 0.95 was again assumed constant during the simulation period.

The THM compounds were analyzed in a gas chromatograph (GC) with an electron capture detector (ECD) using a Fused-Silica Chrompack capillary column. The liquid–liquid extraction procedure was first applied to all samples using *n*-pentane organic solvent. The results show that the source water in the given system is dominated by brominated THM compounds, mainly THM4 (Bromoform), and opposite to common cases covered in the literature. This may be explained and attributed to the nature of the sea water that is originally rich in bromide content. An average constant value of 2.25 was assigned to BIF during the entire 24-h period of simulation. Other quality parameters, defined in the modeling approach, are obtained from laboratory-controlled experiments and regression procedure. These parameters are: F [equation (2)] = 0.582 and Br_o, Br_p, and k_{br} [equation (3)] are 26.1 ppb, 81.2 ppb and 0.116 1/day, respectively.

Inspection of the distribution factors S_0, S_1, S_2, and S_3 at the entrance location showed that all measurements can be characterized by the following relations:

$$S_3 > S_2 \tag{7}$$

$$S_2 > S_1 \tag{8}$$

$$S_2 > S_0 \tag{9}$$

The above relations were utilized as linear constraints in the nonlinear optimization problem [equation (5)] to solve for S_0, S_1, and S_2. Since S_0 and S_1 are only bounded from above in the previous constraints, the solution may produce zero values for these variables in some instants. A better description of the source quality can further restrict the problem and eliminate the zero-value solutions. This description can relate the lower bounds of S_0 and S_1 to S_3 since S_3 is a known value in the nonlinear optimization problem. It has to be noticed that this situation does not exist in the more common conditions when the chlorinated THM species dominate the THM compounds.

Table 2. Quality analysis at sampling site (1)

Time	14:00	17:00	20:00	24:00	8:00	11:00
THM1, ppb (chloroform)	2.1	2.7	2.2	1.9	2.1	1.6
THM2, ppb (bromodichloromethane)	3.0	4.1	3.3	3.1	3.4	2.4
THM3, ppb (dibromochloromethane)	3.9	6.1	7.3	5.3	6.1	11.1
THM4, ppb (bromoform)	26.1	28.4	26.6	22.1	23.2	17.1
Total THM, ppb	35.1	41.3	39.4	32.4	34.8	32.5
[TTHM], mmol/l	0.158	0.189	0.179	0.148	0.159	0.150
BIF	2.31	2.22	2.27	2.25	2.23	2.17
Res. chlorine, ppm	0.60	0.59	0.60	0.61	0.63	0.62
Chlorine bulk decay coefficient (1/day)	1.02	0.96	0.91	0.94	0.98	0.92
Bromide (ppm)	0.67	0.71	0.68	0.78	0.73	0.81
TOC (ppm)	0.0505	0.0402	0.0371	0.0539	0.0606	0.0576

RESULTS AND DISCUSSION

All obtained parameters and relations were fed to the THMSPEC to model the THM species in the selected portion of the Abu-Dhabi distribution system under the considered hydraulic conditions. A 5-min increment of TSPEC was used during the 24-h period of simulation. A value of 1000 assigned to λ in equation (5) was found to be adequate to produce stabilized solution.

The concentrations of THM species measured at selected sampling points were plotted against the modeled values (Fig. 4). The results reflect some deviation between the measured and modeled values at some hours, especially for the distant nodes from the source (nodes 70, 76). These deviations can be generally attributed to the uncertainties present in many parameters required for the model and in the hydraulic calibration required for the considered portion of the distribution system. Another expla-

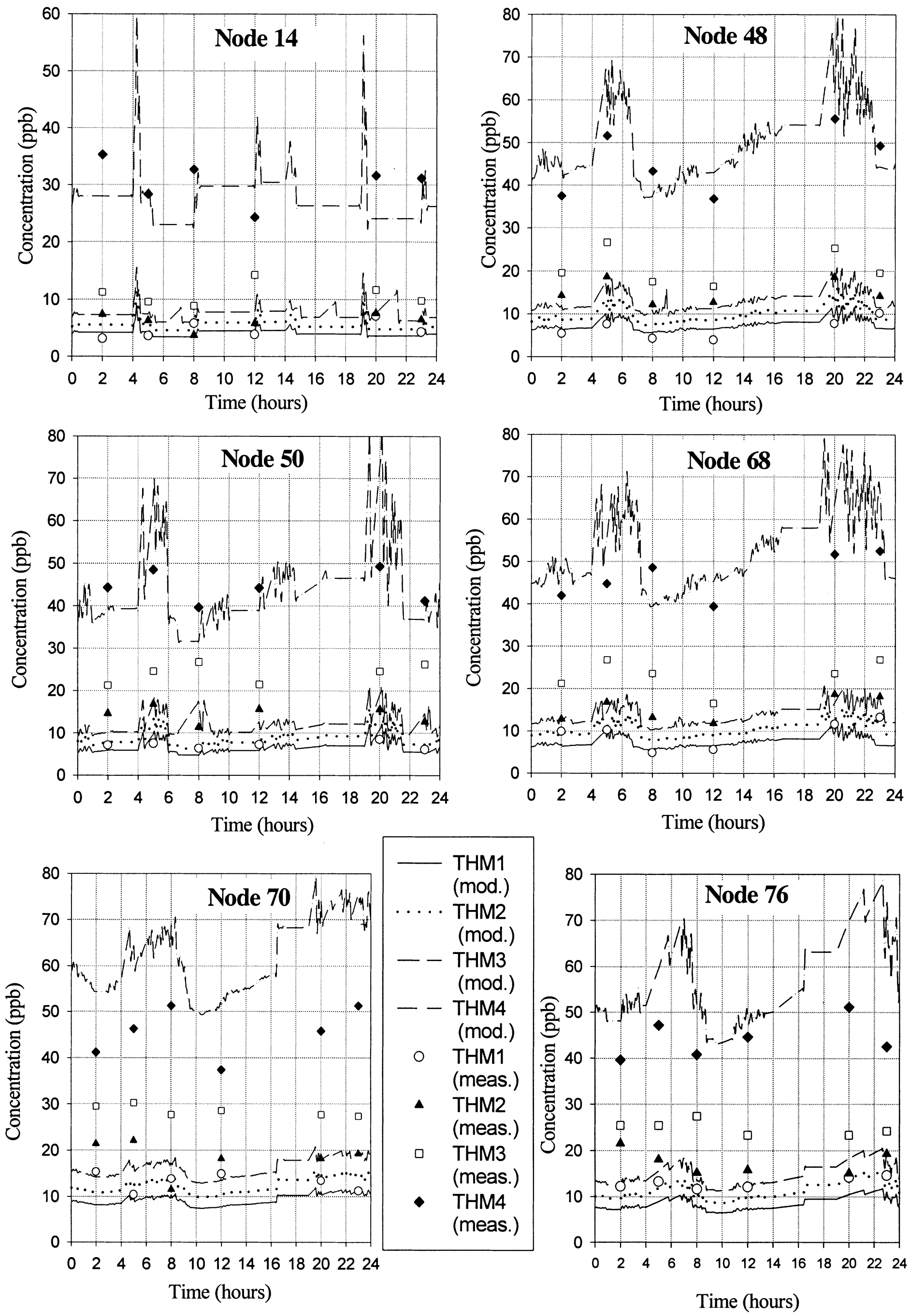

Fig. 4. Modeled and measured THM species.

Table 3. Distribution of Bromine Incorporation Factor at the sampling nodes

Time	14:00	17:00	20:00	12:00	8:00	11:00	Time-weighted average
Node 14	2.16	2.06	2.04	1.99	2.04	2.05	1.97
Node 36	2.06	2.08	1.98	2.17	1.98	2.00	1.95
Node 48	1.92	1.93	2.07	2.01	1.95	1.87	1.88
Node 50	1.93	1.92	1.96	1.9	1.91	1.96	1.85
Node 66	1.82	1.8	2.07	1.97	1.8	1.77	1.78
Node 68	1.72	1.77	1.75	1.78	1.88	1.8	1.73
Node 70	1.6	1.77	1.8	1.59	1.71	1.81	1.64
Node 76	1.65	1.72	1.74	1.75	1.76	1.63	1.65

nation is derived from the relatively low BIF value associated with the measured THM species of the nodes away from the source compared to the average considered value (1.64 and 1.65 at nodes 70 and 76 compared to the used average BIF of 2.25, see Table 3). This suggests that BIF decreases with time, i.e. the THM brominated compounds tend to hydrolyze when subjected to dynamic conditions. This can be clearly noticed in Fig. 4 (nodes 70 and 76) where the measured THM4 is much less than the modeled one, whereas the measured THM1, THM2, and THM3 are considerably larger than the modeled ones. However, more investigation and study are still required to substantiate that founding.

Overall reasonable agreement at many hours during the simulation period can still be observed. Given the complexity of the whole process and the involvement of many parameters in the process, the model can serve as a powerful numerical tool to predict the propagation of THM compounds in water distribution systems. Further development and refinements are still needed to handle other systems like those having multiple sources.

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