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Real-time modeling of trihalomethane formation in a full-scale distribution system

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ABSTRACT

Using a combination of modeling and online water quality instrumentation, utilities can produce real-time predictions of trihalomethane (THM) formation in their distribution system. In this study, an empirical model was used to predict THM formation and embedded into a full-scale supervisory control and data acquisition (SCADA) system. Online water quality instrumentation provided input values to the THM model for total organic carbon (TOC), pH, and temperature. A hydraulic model was also embedded in SCADA, and provided residence time input values for the wholesale portion of the distribution system, which included large lateral pipelines, reservoirs, and pump forebays. Results from a 3-year evaluation showed that predicted THM concentrations were within 10 μg/L of the measured value 81% of the time. Real-time model predictions can provide an effective way to monitor the formation of THMs in a full-scale distribution system.

Key words | chlorination, disinfection byproduct (DBP), hydraulic model, online water quality instrumentation, predictive models, trihalomethane (THM)

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INTRODUCTION

Utilities that use free chlorine for secondary disinfection are often challenged with minimizing the formation of halogenated disinfection byproducts (DBPs). The United States Environmental Protection Agency (USEPA) has established a maximum contaminant level (MCL) of 80 μg/L for the sum of four trihalomethanes (TTHM) including chloroform, chlorodibromomethane (CDBM), bromodichloromethane (BDCM), and bromoform (USEPA 2006). Factors contributing to the formation of TTHMs include total organic carbon (TOC) concentration, bromide concentration, pH, temperature, chlorine dose, and hydraulic residence time (HRT) (Amy *et al.* 1987, 1998; Symons *et al.* 1993; Liang & Singer 2003). The process of evaluating THM formation and developing strategies to minimize formation is specific to both water quality and operational variables.

Numerous empirical models have been developed to predict THM formation using the six variables mentioned above. Comprehensive reviews have been performed evaluating their advantages, limitations, and overall applicability of each model to drinking water supply systems (Sadiq & Rodriguez 2004; Chowdhury *et al.* 2009). In one case study, historical data were reviewed to evaluate the accuracy of model predictions versus full-scale plant operating data (Westerhoff *et al.* 2000). The selected model proved to be quite accurate; however, limitations were identified such as determining changes in dissolved organic carbon (DOC) reactivity, accounting for booster chlorination, and accounting for temperature and hydraulic changes in pipelines and reservoirs.

Minimal research has been performed to develop real-time assessments of TTHM formation in the field. One analytical method has been developed for real-time analysis in the field using a capillary membrane sampling-flow injection analysis method (Emmert *et al.* 2004; Geme *et al.* 2005). Hydraulic models have been applied to calculate the water age when evaluating free chlorine decay (Grayman & Clark 1993). However, there have been no reported cases where a hydraulic model was interfaced with online water quality instrumentation to provide a real-time assessment of TTHM formation in a full-scale distribution system.

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In this study, an empirical TTHM model was incorporated into the supervisory control and data acquisition (SCADA) system of a full-scale distribution system to produce real-time TTHM predictions. The model was adapted from Amy *et al.* (1998), and a function of TOC, pH, temperature, bromide, chlorine dose, and time (Amy *et al.* 1998). Online water quality instrumentation was used to supply data for raw water TOC, finished water pH, and finished water temperature. The raw water bromide concentration was established as an input parameter, since the concentration in Lake Mead water is typically $91 \pm 8\ \mu g/L$. Operating data were collected for the chlorine dose and a hydraulic model was used to determine HRT. Comparisons were made between the predicted TTHM concentrations from the model and measured TTHM concentrations from laboratory analysis.

MATERIALS AND METHODS

Water treatment facility operation

The Southern Nevada Water Authority (SNWA) operates two surface water treatment plants in Las Vegas, NV. The 600-MGD Alfred Merritt Smith Water Treatment Facility (AMSWTF) and the 400-MGD River Mountains Water Treatment Facility (RMWTF) operate as direct filtration plants using raw water from Lake Mead (Figure 1). In July 2007, the addition of 0.5–0.9 mg/L of prechlorine was initiated to prevent quagga mussel proliferation in the raw water pipeline to the RMWTF. The goal was to maintain a 0.1 mg/L free chlorine residual at the point of entry into the treatment plant. Preozonation was used at both facilities using a dose between 1.0 and 2.5 mg/L. Bromate is minimized below the Stage 1 D/DBP Rule MCL of $10\ \mu g/L$ using ozone dose management at the AMSWTF, and chlorine-ammonia pretreatment at RMWTF (Wert *et al.* 2007). Residual ammonia is destroyed via breakpoint chlorination. Free chlorine and ferric chloride are applied at the rapid mix chamber. The filters consist of dual media containing sand and anthracite. The free chlorine residual produced at the rapid mix chamber is carried throughout the remainder of the treatment process. Therefore, the filters are not operated in biologically active mode. Additional free chlorine can be added prior to the clearwell to achieve the desired finished water free chlorine residual goal of 1.8 mg/L.

Both treatment facilities are equipped with a wide variety of online instrumentation. Online water quality instrumentation for pH, temperature, and TOC is available to provide input parameters into the TTHM model. Raw water TOC concentration is continuously monitored in raw water at the AMSWTF every 6 minutes using an online TOC analyzer (TOC 800, GE Analytical Instruments, Inc., Boulder, CO). The online TOC monitor is maintained quarterly by the manufacturer according to a service agreement, which involves replenishing chemical reagents, replacing the UV bulb, and replacing pump tubing. Finished water pH and temperature are also monitored with online instrumentation (Model P63, Great Lakes International, Milwaukee, WI). Online pH and temperature instruments are cleaned and calibrated every 6 months by SNWA treatment staff. The instruments are also logged into the SCADA system to facilitate extraction of the data. Hourly average data are extracted in Excel format.

Wholesale delivery system

The wholesale water delivery system transports the finished drinking water to turnout locations, where the water is purchased from the wholesaler (SNWA) by a purveyor (e.g. Las

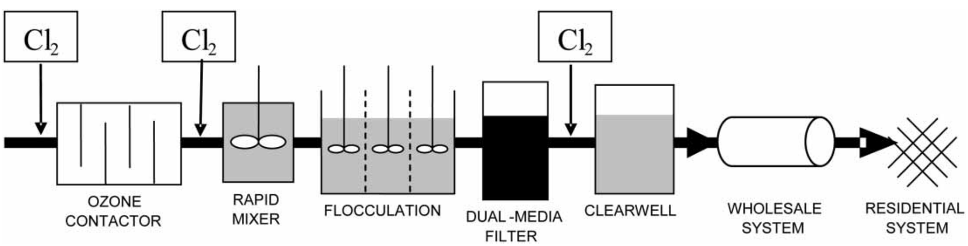

Figure 1 | Schematic of the drinking water treatment and transmission processes with chlorine application points identified.

Vegas Valley Water District, City of Henderson, etc.). The purveyor then distributes the drinking water to their residential customers through a metered service connection. However, there are no residential service connections within the wholesale delivery system. Sampling sites were selected to focus solely on the wholesale portion of the distribution system in order to simplify the approach and demonstrate the modeling concept prior to application under more complex hydraulic modeling scenarios.

In order to capture shorter residence times, the finished water from both AMSWTF (AMS-1) and RMWTF (RM-1) were included among the sampling sites. Seven additional sampling sites were selected at turnout locations, which have longer residence times. Two of the turnout locations (i.e. RM-2 and RM-3) were served primarily by the RMWTF (RM-1). Five of the turnout locations (i.e. AMS-2, AMS-3, AMS-4, AMS-5, and AMS-6) were served primarily by the AMSWTF (AMS-1). These nine locations were sampled quarterly for TTHMs to validate the accuracy of model predictions.

Hydraulic model

A hydraulic model was embedded into the full-scale SCADA system to produce real-time assessments of the HRT in the wholesale delivery portion of the SNWA distribution system. Focusing on the wholesale delivery portion of the system makes the hydraulic modeling effort much easier since it is inherently a skeletonized model and does not include any residential service connections.

There were 82 nodes incorporated into the hydraulic model for the wholesale distribution system, which accounts for pipeline volume in several transmission laterals, pumping forebays and reservoirs along each lateral. The HRT between each node was calculated based upon the measured flow rate (averaged over 15 minutes) and the volume of the pipeline. The model for a pipe segment (Figure 2(a)) was determined using the following series of equations:

$$q = (q_t + q_{t-1})/2$$
$$V_1 = q\Delta t$$
$$V_2 = V_p - V_1$$
$$\text{If } V_2 > 0, \text{then } A_2 = \left((V_2)\left(A_2^{t-1} + \Delta t\right) + (V_1)(A_1)\right)/V_p$$
$$\text{If } V_2 <= 0, \text{then } A_2 = A_1 + V_p/q$$

where q is the modeled flow through the pipe segment; q_t is the last 15 minute averaged flow through the pipe segment; q_{t-1} is q_t from 15 minutes ago; V_1 is the modeled volume of water flowing into the pipe segment over the last 15 minutes; Δt is the scan rate, 15 minutes; V_p is the volume of

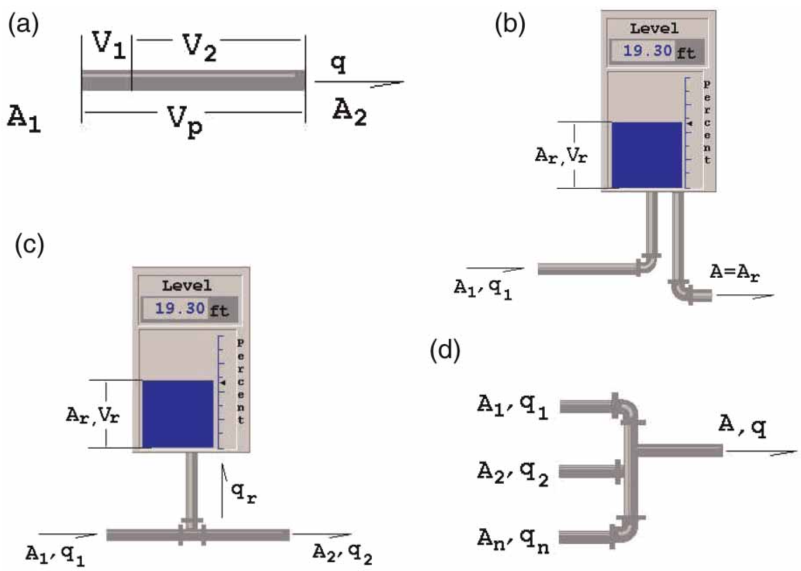

Figure 2 | Hydraulic model flow conditions: (a) pipe segment, (b) water age for a reservoir, where all flow goes through the reservoir, (c) water age for a reservoir, where net flow is calculated to the reservoir, and (d) water age for two or more streams being mixed.

the pipe segment; A_1 is the modeled water age at the inlet of the pipe segment (typically the calculated value of A_2 from the upstream node); A_2 is the modeled water age at the outlet of the pipe segment, the superscript t–1 signifies the value of A_2 calculated 15 minutes ago. The modeled water age is in hours, all measurement units are converted to yield the results in hours.

Reservoirs and forebays were modeled similar to the pipelines, but the volume was calculated based on the reservoir level. This study assumed that the total flow goes through the reservoir, so only the flow into the reservoir was used to calculate the water age (Figure 2(b)):

$$V_1 = q_1 \Delta t$$
$$V_2 = V_r - V_1$$
$$A_r = \left((V_2)\left(A_r^{t-1} + \Delta t\right) + (V_1)(A_1)\right)/V_r$$

where q_1 is the modeled flow into the reservoir; V_1 is the modeled volume of water flowing into the reservoir over the last 15 minutes; V_r is the volume water stored in the reservoir; A_r is the modeled water age of the water stored in the reservoir. In this case, the water age in the reservoir is equal to the water age at the outlet of the reservoir.

In the wholesale portion of the distribution system, there are only a few places where flow reversal can occur. Flow reversal was only modeled where a reservoir sets off a lateral, or where a lateral branch is between a pump station and a reservoir (if the pump station is operating, then flow is from the pump station to the turnout, otherwise flow is from the reservoir to the turnout). Where a reservoir sets off the lateral, the net flow was used to calculate the water age in the reservoir (Figure 2(c)):

$$q_r = q_1 - q_2$$
$$V_1 = q_r \Delta t, \text{ if } V_1 < 0 \text{ then } V_1 = 0$$
$$V_2 = V_r - V_1$$
$$A_r = \left((V_2)\left(A_r^{t-1} + \Delta t\right) + (V_1)(A_1)\right)/V_r$$

where q_r is the modeled flow into the reservoir. A negative sign indicates flow is from the reservoir.

The water age at the outlet of the reservoir (A_2) may be the water age at the inlet ($A_2 = A_1$, if $q_1 > q_2$), or the water age of the reservoir ($A_2 = A_r$, if $q_1 = 0$), or the water age of the mixed stream of water from the inlet and water from the reservoir ($A_2 = ((A_1)(q_1)–(A_r)(q_r))/(q_1–q_r)$, if $q_r < 0$), where multiple streams mix the water age was modeled as follows (Figure 2(d)):

$$A = \sum (A_n)(q_n) / \sum q_n$$

Water age predictions were displayed in SCADA, and updated every 15 minutes. The water age data were logged in SCADA and are available in Excel format. There were no studies performed to compare the actual water age to the predicted water age.

TTHM formation model

Six TTHM formation models (Amy *et al.* 1998) were evaluated for accuracy with water quality data collected prior to ozone implementation (2000–2003). Of the models evaluated, one model was selected for further evaluation; Equation (1). The model was developed based upon raw/untreated water using DOC, free chlorine dose (Cl_2), bromide (Br), temperature, pH, and reaction time (Amy *et al.* 1998). The model was calibrated using several different raw waters, and is a function of the following independent variables and boundary conditions: DOC (1.2–10.6 mg/L), free chlorine dose (1.51–33.55 mg/L), bromide (7–600 μg/L), temperature (15–25 °C), pH (6.5–8.5), and HRT (2–168 h). The online instrumentation described above provided the input water quality values for the model. The hydraulic model described above was used for the time input parameter.

$$\text{TTHM} = 0.0412\ \text{TOC}^{1.098}\ \text{Cl}_2^{0.152}\ \text{Br}^{0.069}\ \text{Temp}^{0.609} \times \text{pH}^{1.601}\ \text{Time}^{0.263} \quad (1)$$

After a preliminary evaluation of the model using historical data, a few modifications were needed to improve the accuracy of the predictions prior to incorporating the model into SCADA. Since there is no online analyzer available to measure bromide, an average bromide concentration of 100 μg/L was incorporated into the numerical constant of the model. The constant bromide concentration changed the empirical constant from 0.0412 to 0.056 and eliminated the bromide term from Equation (1). Furthermore, the model overestimated TTHM concentration; therefore, a correction factor of 0.62 was incorporated into the numerical constant, which changed the constant from 0.056 to 0.035 resulting in Equation (2).

$$\text{TTHM} = 0.035\ \text{TOC}^{1.098}\ \text{Cl}_2^{0.152}\ \text{Temp}^{0.609}\ \text{pH}^{1.601}\ \text{Time}^{0.263} \quad (2)$$

TTHM predictions still appeared to be over predicted at locations with the greatest HRT. Since it was not practical to make site-specific adjustments within the SCADA system, a temperature criterion was established to make adjustments based on HRT information. If the HRT was greater than 25 h, then the finished water temperature was increased by 30% in model. This correction improved the model predictions in the SCADA system at locations with longer HRT. Additional research from SNWA showed that preozonation reduced TTHM formation by 10 μg/L (Wert & Rosario-Ortiz 2011). Therefore, predicted TTHM concentrations were reduced by 10 μg/L if ozone was online. A comparison between the accuracy of Equations (1) and (2) is shown in Figure 3.

The revised model shown in Equation (2) was embedded into the full-scale SCADA system to predict TTHM formation at nine locations over a 3-year study period (March 2006–May 2009). The hydraulic model described above was used to provide HRT information to the TTHM model every 15 minutes. Online water quality instrumentation described above was used for the input values for TOC, temperature, and pH. Data for each of the independent variables were stored in a database (or carousel) along with the collection time. When a model prediction was generated, the HRT would be used to go back in the database and extract archived data for DOC, free chlorine dose, pH, and temperature in order to generate the predicted TTHM concentration. For example, if the water age was found to be 44 h, then the archived data would be used from 44 h ago to serve as the input values to the model. Predicted TTHM concentrations were updated every 15 minutes in SCADA, which produces a real-time assessment of TTHM formation in the distribution system.

Due to the number of corrections made to this model, further evaluations have been performed by SNWA to develop site-specific empirical models for TTHMs and haloacetic acids (HAAs). If a utility chooses to pursue this modeling effort, it is recommended to develop a site-specific model or validate an existing model for their specific range of water quality conditions. As more data are collected, refinements can be made to enhance the accuracy of these predictive models.

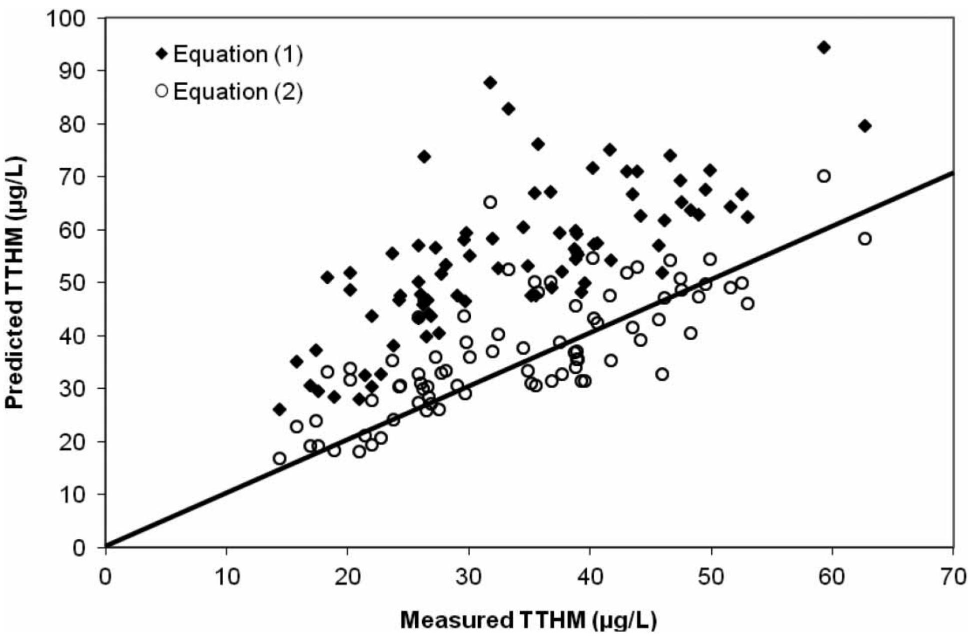

Figure 3 | Comparison of predicted and measured TTHM values using Equations (1) and (2). (*Note*: Line of equality shown for reference.)

RESULTS

Accuracy of online water quality instrumentation

The TTHM model can only produce accurate predictions if the online water quality instrumentation is producing accurate results. Water quality comparisons were made to compare online instrumentation values to grab sample data collected by laboratory staff. Figure 4 shows daily average data for the following water quality parameters: raw water TOC, finished water pH, and finished water temperature.

Online TOC measurements indicated that there were time periods when an instrument malfunction caused the TOC concentration to exceed the reported grab sample concentration. Possible explanations why these deviations occurred may include a plant shutdown, loss of sample flow for cleaning and maintenance, or depletion of chemical reagents. These TOC data points illustrate that anomalies can happen, and must be considered when using this approach. After October 2007, both measurements appeared to coincide very well with one another.

Finished water pH and temperature showed excellent correlation between the online and grab sample measurements. Grab sample temperature readings were ~0.5 °C greater than the online measurement during the summer months, likely due to the ambient air temperature conditions at the time of analysis in the field. The temperature readings were very similar during the winter months when ambient air temperatures were not a factor. The raw water bromide concentration slowly declined from 0.095 to 0.082 mg/L during the 3-year period. These results may indicate that the model may be over-predicting TTHM formation, since the input concentration of bromide of 0.100 mg/L remained constant during the 3-year period.

Hydraulic residence time

Daily average HRT information for the nine sites studied is shown in Figure 5. The results show that HRT increased in the winter months and decreased in the summer months. Table 1 summarizes the minimum, maximum, average, standard deviation, and median HRT for the nine sites investigated. The average HRT of these sites varied between 2 and 44 h.

Free chlorine decomposition

The free chlorine dose applied at both plants varied between 2.6 and 4.8 mg/L. The chlorine dosages were used in SCADA to generate the predicted TTHM concentrations. Sites served by the RMWTF used the chlorine dose applied at RMWTF, while sites served by AMSWTF used the chlorine dose applied at the AMSWTF. During July 2007, a treatment change was made in raw water pipeline serving the RMWTF (RM-1, RM-2, and RM-3). Prechlorination was initiated using a dose of 0.8 mg/L in order to prevent quagga mussel attachment in the pipeline. As a result, the 10 μg/L reduction due to preozonation was eliminated at sites RM-1, RM-2, and RM-3, and predicted TTHM values were adjusted accordingly.

TTHM model comparison

The TTHM model input parameters have been discussed in the previous sections. The accuracy of the TTHM model was compared to laboratory compliance monitoring at nine sites described previously. Results from the finished water of both treatment facilities (AMS-1 and RM-1) are shown in Figure 6. These results show that the predicted TTHM concentrations were close to the measured TTHM concentrations. However, the measured TTHM concentration increased by 10 μg/L at RM-1 between July 2007 and October 2007. The increase corresponds to the start-up of prechlorination for quagga mussel control at the intake serving the RMWTF, which began in late July. Prechlorination negated the 10 μg/L reduction in TTHM formation due to ozonation (Wert & Rosario-Ortiz 2011), which was accounted for in the model predictions.

Three locations in the distribution system were selected among the seven turnout locations to illustrate the measured and predicted TTHM concentrations in Figure 7. The three sites were selected based upon their HRT: AMS-4 (17 h), AMS-5 (26 h), and AMS-6 (44 h). Results showed that the SCADA-predicted TTHM concentrations were similar to the measured TTHM concentration. SCADA predictions

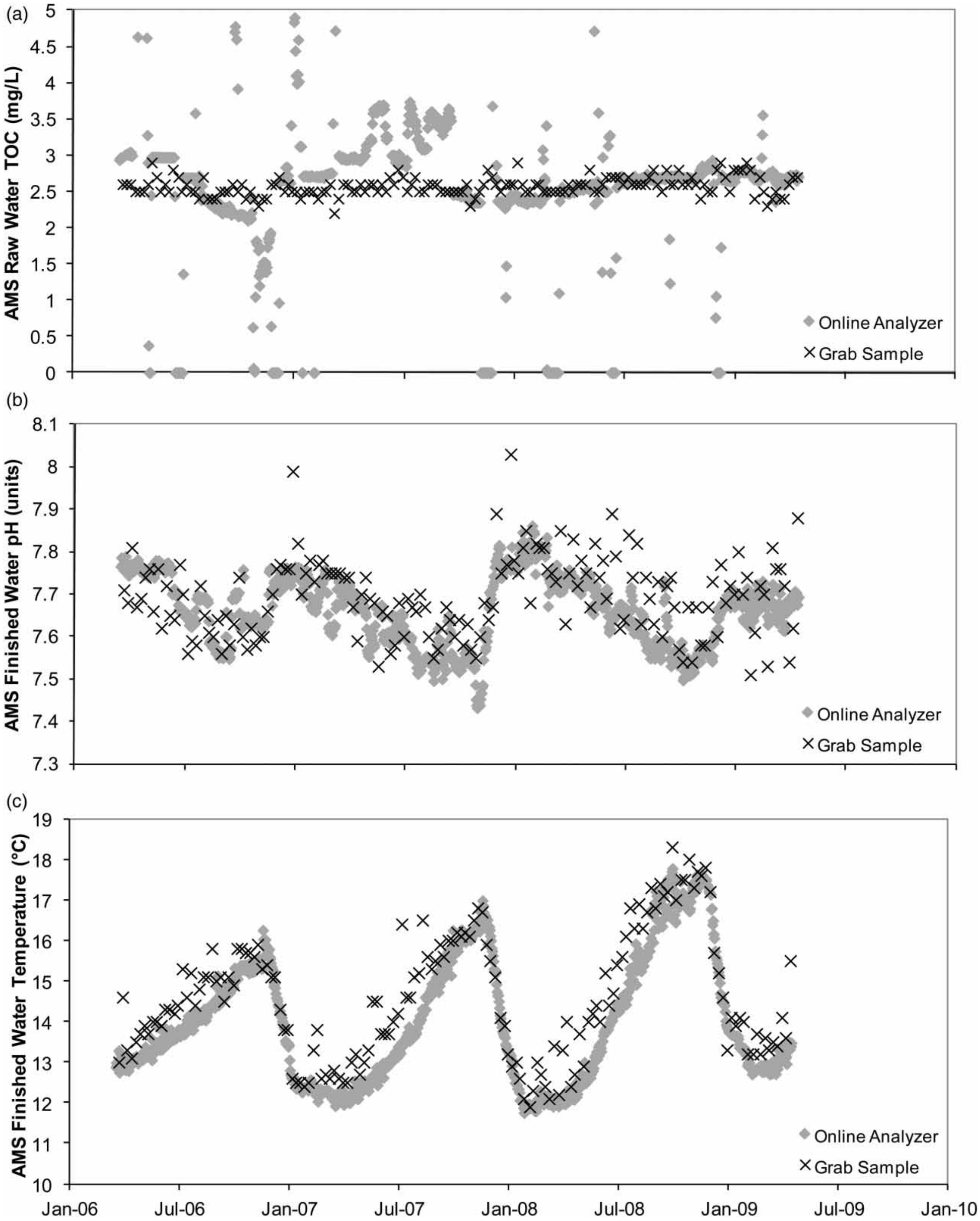

Figure 4 | Comparison of daily average online water quality instrumentation and weekly grab sample analysis: (a) TOC, (b) pH, and (c) temperature.

also appeared to be sensitive to the TOC changes shown in Figure 4 using online instrumentation between January and October 2007. These results further illustrate the importance of online instrumentation accuracy.

Accuracy of TTHM model

All of the above data points were compared to evaluate the overall accuracy of the TTHM model. TTHMs were shown

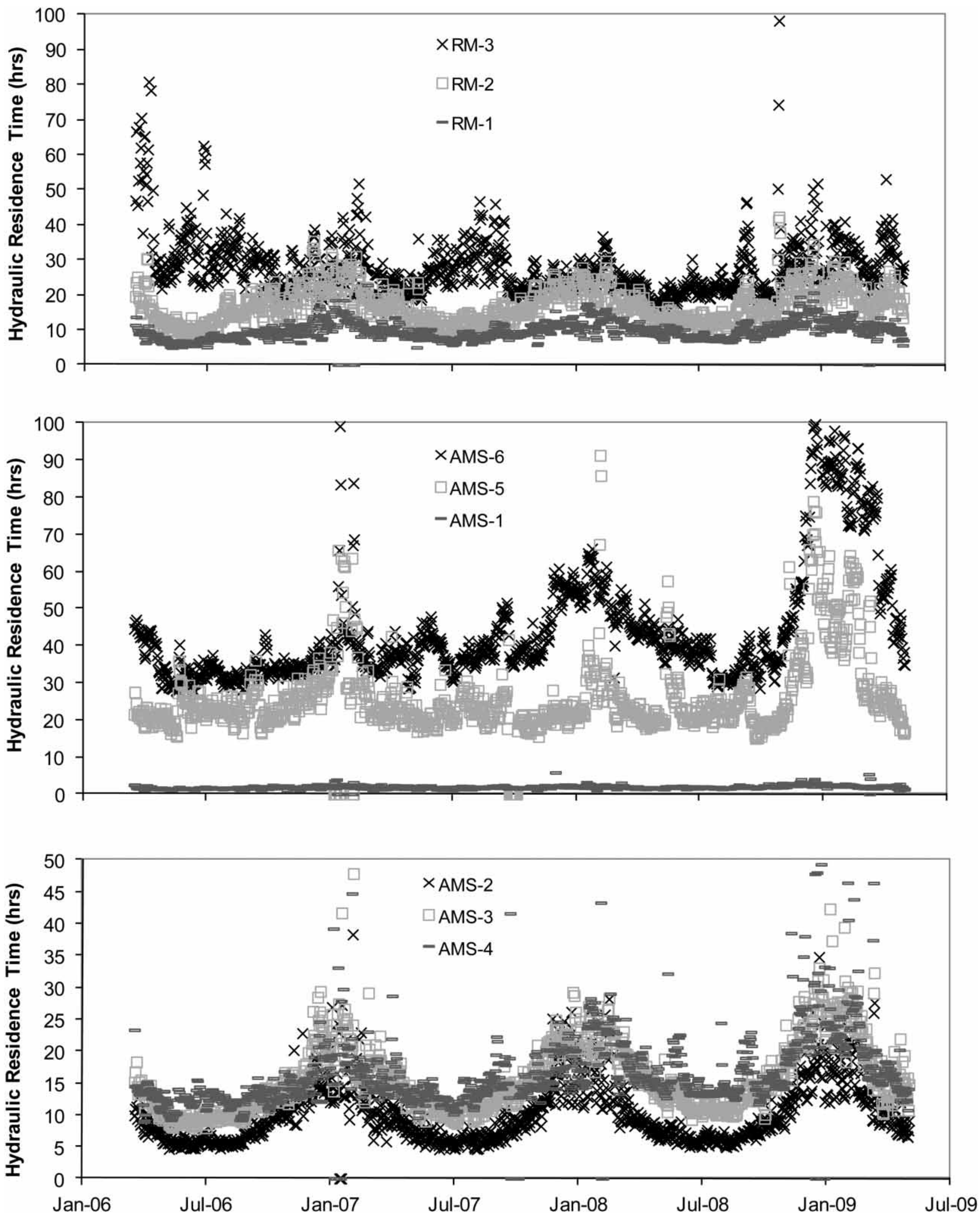

Figure 5 | Summary of model predicted HRT at site locations served by AMSWTF and RMWTF.

to vary between 8 and 55 μg/L, and the distribution of data points was well distributed over this range. Water quality conditions also varied during this year period: TOC (2.1–2.8 mg/L), pH (7.5–8.0), temperature (11.9–18.3 °C), HRT (1.9–44 h), and chlorine dose (3–5 mg/L). The difference between measured TTHMs and predicted TTHM was calculated, and the relative frequency of error is shown in the histograms in Figure 8. At AMSWTF ($n = 122$), 55% of the

Table 1 | Summary of HRT information in the wholesale delivery system

	Hydraulic residence time (h)				
Location	**Minimum**	**Maximum**	**Average**	**Standard deviation**	**Median**
RM-1	4.9	23	9.7	2.4	9.3
RM-2	7.0	42	17	5.0	16
RM-3	14	115	28	9.3	26
AMS-1	1.0	6	1.9	0.4	1.8
AMS-2	4.6	69	10	5.4	8.8
AMS-3	7.8	88	16	7.3	15
AMS-4	8.9	72	17	6.2	15
AMS-5	15	91	26	11	23
AMS-6	28	108	44	16	39

predicted TTHM concentrations were within 5 μg/L of the measured value, and 81% of the predicted TTHM concentrations were within 10 μg/L of the measured value. At RMWTF ($n = 50$), 43% of the predicted TTHM concentrations were within 5 μg/L of the measured value, and 76% of the predicted TTHM concentrations were within 10 μg/L of the measured value. When considering the entire data set ($n = 172$), 52% of the predicted TTHM concentrations were within 5 μg/L of the measured value, and 81% of the predicted TTHM concentrations were within 10 μg/L of the measured value. These results show that the TTHM model produced accurate predictions given that five variables were used in the model, each with associated variability and error.

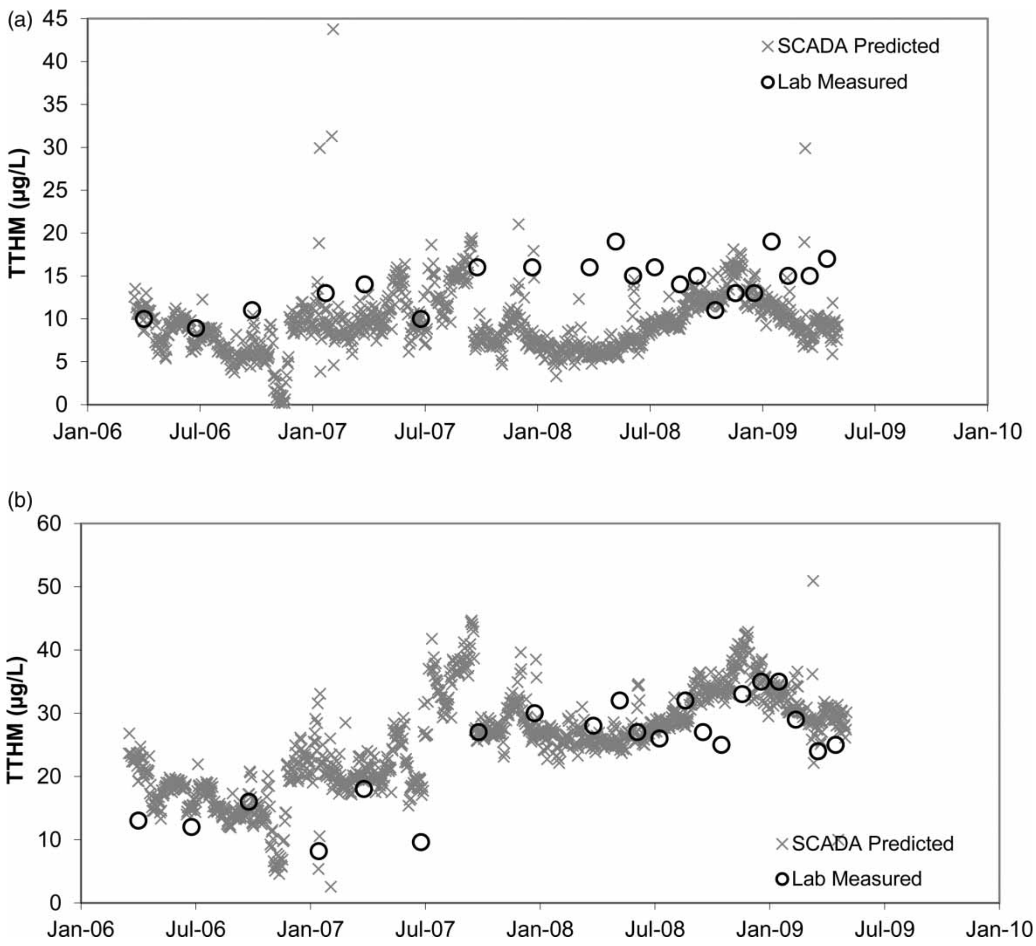

Figure 6 | TTHM comparison in the finished water at both water treatment facilities: (a) AMS-1 and (b) RM-1 (*Note*: Prechlorination began in July 2007 for the control of quagga mussels at site RM-1).

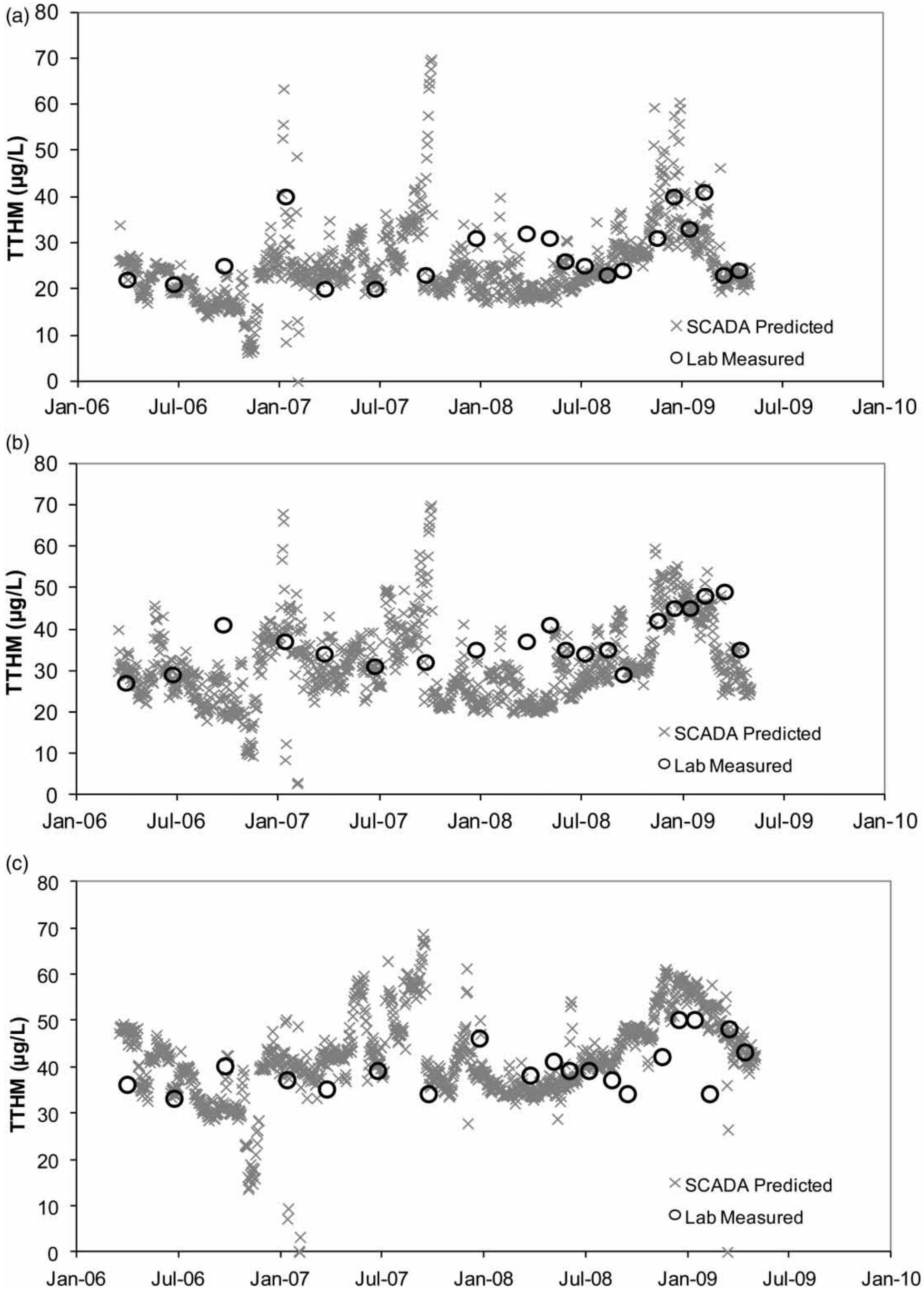

Figure 7 | TTHM comparison at three turnout locations in the distribution system: (a) AMS-4, (b) AMS-5, and (c) AMS-6.

Upon completion of the 3-year data collection period, some sensitivity analysis was performed to quantify the contribution of each independent variable to the model predictions. The 10th and 90th percentile data points were calculated for TOC (2.32, 3.54 mg/L), finished water pH (7.54, 7.76), finished water temperature (12.1, 16.4 °C), HRT (2.4, 37 h), and chlorine dose (2.93, 4.24 mg/L). These percentile values were then raised to their respective power shown in Equation (2). Under the water quality conditions observed in the study, the changes in water age,

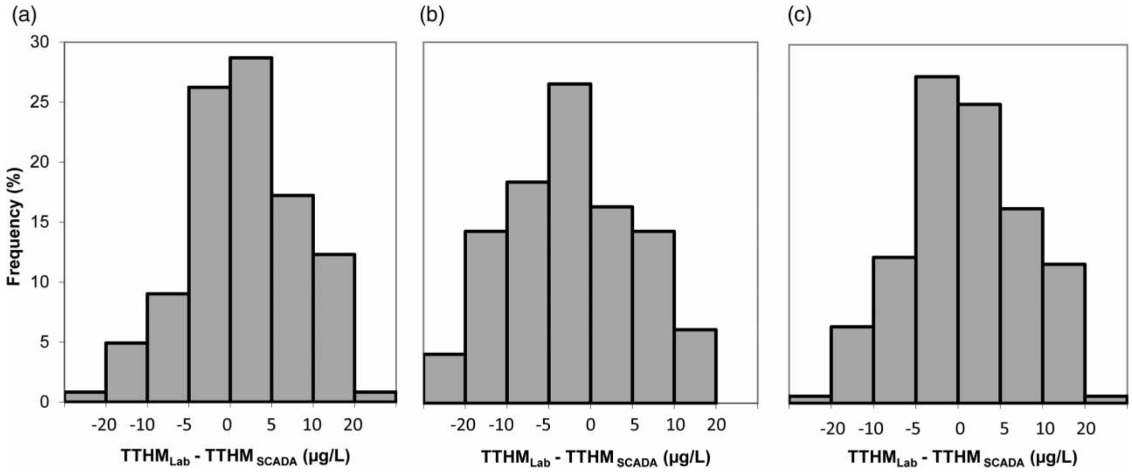

Figure 8 | Histograms indicating the accuracy of the TTHM model: (a) Sites served by AMSWTF ($n = 122$), (b) Sites served by RMWTF ($n = 50$), and (c) All sites studied ($n = 172$).

TOC, and temperature had the greatest impact by changing the predicted values as much as 52, 37, and 17%, respectively. The fluctuations in chlorine dose and pH changed the model predictions by 5.5 and 4.5%, respectively.

Practical implications

Real-time modeling provides utilities with another tool to further optimize their treatment process to meet DBP regulations. Although precursor removal is not practiced at this facility, the modeling effort does provide insight as to the temporal variability in DBP formation. The model can also be used to identify when THMs reach their peak formation, which allows treatment plant staff to better understand these seasonal fluctuations and identify a method to reduce their concentration either within the treatment process or by minimizing HRT in the distribution system. Once a model has been identified to be accurate using a historical water quality database, a utility can incorporate the model into the SCADA system. Periodically, data reports can be reviewed to identify periods of high formation potential.

Treatment process changes and their impact on the model must also be considered to maintain the accuracy of the model predictions. The modeling approach may not be applicable in waters with highly variable bromide concentrations, since bromide is typically not measured using online instrumentation. Other restrictions include the effects of rechlorination, changing distribution system hydraulics and HRT, and blending alternative water sources within the distribution system. When implemented and maintained properly, real-time modeling can provide useful information with minimal cost or maintenance associated with online analyzers.

This evaluation was performed in a wholesale delivery system to demonstrate the concept in a simple network of pipelines and reservoirs. Further evaluation would involve extending these models further out into the distribution system with residential service connections. Hydraulic modeling was recommended as a method to comply with the Initial Distribution System Evaluation (IDSE) requirement of the Stage 2 Disinfectants and Disinfection Byproducts Rule. If these hydraulic models can be embedded into the SCADA system, then an approach such as this would have greater application potential. The work contained in this manuscript shows promise, but is highly dependent upon accurate hydraulic modeling and online water quality instrumentation.

CONCLUSIONS

TTHM concentration predictions were made in SCADA every 15 minutes using input values from online water instrumentation, process control information, and HRT information obtained from a hydraulic model. The predicted TTHM concentrations were within 10 μg/L of the measured value 81% of the time over a range of water quality conditions. However, the model predictions were susceptible to treatment process and water quality changes that hindered model accuracy. However, this research showed that predictive models can be applied successfully to provide utilities with real-time information regarding DBP formation in the distribution system.

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