

Temperature dynamics and water quality in distribution systems¹

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Quality assurance strategies for water distribution systems often include the application of chemical disinfectants to limit the growth and transmission of pathogens. Characteristics of water quality in individual systems, and the type of disinfectant employed, create significant complexity in understanding and quantifying the impact of disinfectants in different networks. An additional challenge is that disinfection by-products (DBPs), created through the breakdown of disinfectants, can be detrimental to human health. Therefore, it is necessary to maintain the correct level of disinfectant to control microbial pathogens while also limiting formation of DBPs to acceptable levels. Limiting formation of DBPs is an ongoing challenge for operators. This work examines the impact of ground surface temperature and changes in network operations on disinfectant breakdown. As drinking water utilities encourage customers to conserve water, water residence times within networks increase. Also, as surface temperatures increase, heat transfer into the drinking water in subsurface pipes can also increase. Here, we review the literature on ways in which temperature affects disinfection rates and the production of DBPs and select one pathway for more detailed assessment. Numerical modeling is used to examine the changes in DBP production as a function of residence time, ground surface temperature, and heat transfer through the soil to the pipe.

Introduction

Water delivered through the potable supply system is utilized for drinking, food preparation, and washing, among myriad other uses. To ensure the quality and safety of drinking water for human health, governments regulate water treatment and distribution. A common feature of regulations is the requirement to inactivate microbial pathogens by physical or chemical disinfection. Popular disinfection methods include applying ultra-violet light, ozone, chlorine, and chloramine. In particular, application of chlorine at water treatment facilities is one widely used approach to disinfection. As the chlorine reacts with other compounds, the residual disinfectant concentration decays over time. Reactions with other species, particularly with natural organic matter, can form disinfection by-products (DBPs). These compounds include trihalomethanes and haloacetic acids (also known as halogenated acetic acids, or HAAs). Total trihalomethanes (TTHMs) (the total concentration of chloroform, bromoform, bromodichloromethane, and dibromochloromethane) and HAAs are suspected carcinogens and regulated by the United States Environmental Protection Agency (US EPA). Current regulations limit the annual average concentration at a location to 80 $\mu\text{g/L}$ for TTHMs and 60 $\mu\text{g/L}$ for HAAs [1]. The chemical processes of disinfectant decay and formation of by-products depend on the temperature of the water.

The temperature of water in distribution systems has been studied recently by Blokker and Pieterse-Quirijns [2], who provide a model for the temperature of water in buried pipes. The model considers transfer of heat through the soil column to the pipe wall and then from the pipe wall into the flowing water. A key assumption is that the pipe wall, being in contact with the

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soil, is in thermal equilibrium with the soil column. They also developed an equation for temperature dynamics inside water pipes and tabulate some useful parameters related to temperature modeling.

The decay of chlorine, after it is applied as a disinfectant, has been studied in both laboratory and field settings. Rossman et al. develop a kinetic model for chlorine decay with terms for decay in the bulk flow and near the pipe wall [3]. The wall decay term accounts for radial diffusion of chlorine from the bulk flow. Clark suggests a second-order model for chlorine demand and DBP formation [4]. Amy et al. consider chlorine decay as a first order process that proceeds in two stages [5]. Their experiments found a fast decay of chlorine in the first five hours followed by a slower decay phase. More recently, Monteiro et al. have found that the slow chlorine decay phase is more sensitive to temperature [6]. Blokker et al. examined chlorine concentrations and water temperatures at the extremities of a distribution system under different demand models [7]. They found residual disinfectant concentrations to be more sensitive to the choice of the choice of chlorine model than demand model and that temperature played an important role.

Since the acknowledgement that DBPs are potentially harmful many researchers have studied DBP formation. Amy et al. consolidated a dataset concerning DBPs and developed multiple regression models for predictive purposes [5]. Later, Amy, working with Sohn et al., updated the multiple regression models to include corrections for pH and temperature, among other factors [8]. Sohn et al. also developed kinetic models for DBP formation, but showed that the kinetic models did not improve predictive ability compared to the updated multiple regression equations [8]. In addition to these two works, there are many other studies on DBP formation. A summary by Chowdhury et al. reviews 118 models from 48 scientific publications [9].

In this paper, we assemble models for temperature, chlorine decay, and DBP formation into a coupled model for application to water distribution systems. The model is then applied to an example system in order to study the influence of temperature on the processes of chlorine decay and DBP formation. The particular influence of temperature is also examined and an estimate of the heating time is provided. To the authors' knowledge this paper represents a first attempt to model temperature, chlorine decay, and DBP formation, together in a water distribution system. Validation by measurements in the field or laboratory is beyond the scope of this study and provides fertile territory for future research and development.

Model Development

This section assembles equations for temperature dependent chlorine decay and DBP formation in water distribution systems. The following quantities are tracked throughout the distribution system: water temperature in degrees Celsius; chlorine concentration in milligrams per liter; water age in hours; TTHM concentration in micrograms per liter; and, HAA6 concentration in micrograms per liter. Model equations are implemented in the software Environmental Protection Agency Network Model – Multi-species Extension (EPANET-MSX) for simulating multiple interacting water quality species in water piping systems [10]. Physical processes modeled by EPANET-MSX include advection, mixing, and reaction.

Temperature modeling

A recent study on the temperature of water flowing through distribution pipes examined both soil temperature and water temperature in a Dutch case study [2]. The authors found that the temperature of water in the pipes, T_{water} , was a function of pipe wall temperature, the water

temperature, properties of the pipe, fluid, and flow:

$$\frac{dT_{\text{water}}}{dt} = \frac{\alpha_{\text{water}}}{r^2 \left(\lambda_* + \frac{1}{Nu} \right)} (T_{\text{wall}} - T_{\text{water}})$$

The driving force for heat transfer is the difference between the pipe wall temperature T_{wall} , assumed constant, and the water temperature T_{water} . The term which multiplies the driving force is related to the properties of the pipe, fluid, and flow conditions. The thermal diffusion coefficient for water is $\alpha_{\text{water}} = \lambda/(\rho C_p)$ and depends on the thermal conductivity λ , density ρ , and heat capacity C_p . The pipe radius is r . The term $\lambda_* = \lambda_{\text{water}}/(10\lambda_{\text{pipe wall}})$ relates the thermal conductivity of the water and the pipe, and assumes the pipe wall thickness is 10% of the pipe diameter. The Nusselt number Nu describes the convective heat transfer and, for turbulent flow, is modeled as $Nu = 0.027Re^{0.8}Pr^{0.33}$. Here, Re is Reynold's number, and Pr is the Prandtl number.

Soil temperature damping depth

For buried water pipes, the temperature of the pipe wall can be assumed equal to the soil temperature because the soil and the pipe are permanently in contact. The soil temperature at a particular depth is related to the weather conditions at the land surface and depends on temperature, wind speed, and solar radiation, among other variables [2]. The soil column has a strong damping effect on surface temperature. The damping effect may be quantified by estimating the depth at which the amplitude of temperature oscillations falls below $1/e$; $d = \sqrt{2D/\omega}$. Using a thermal diffusivity $D = 6.67 \cdot 10^{-7}$ m²/s and oscillation period of 24 h, the damping depth is 13 cm. As most buried pipes are at least 100 cm deep, there is a justification for treating T_{wall} as constant for daily to weekly simulation horizons.

Characteristic Heating Time

An estimate of the time required for the difference in temperature between the pipe wall and flowing water to become small can be useful to quickly evaluate the time scales over which temperature dynamics occur. Following conventions in chemistry and circuits for first-order equations, the characteristic heating time can be defined as the inverse of the reaction rate.

$$t_{\text{heat}} = r^2(\lambda_* + 1/Nu)/\alpha_{\text{water}}$$

The characteristic time can be used as a threshold to determine whether temperature dynamics play an important role in a given system. When the residence time far exceeds T_{heat} , the water temperature will reach the wall temperature. In contrast, when the heating time is very large compared to the residence time, the temperature of the source water dominates the system. When the residence time is of the same order as the heating time, temperature dynamics may play an important role.

Chlorine decay in pipes

Many water treatment facilities inject chlorine to disinfect the water supply before it is distributed. In the distribution system, the concentration of chlorine decays due to demand in the bulk flow and demand at the pipe wall. The conventional approach to modeling chlorine decay treats bulk and wall decay as first order effects, depending directly on the concentration of chlorine in the bulk flow. Some studies [11, 12] have found better agreement with experimental

data using a two-stage model for chlorine decay that uses additional parameters. Although many researchers have proposed methods to parameterize chlorine decay, the parameters remain difficult to assess without laboratory studies. Considering this complexity, and to limit the number of parameters to be selected for this study, the following first order model of Rossman et al. [3] was adopted.

$$\frac{dC}{dt} = -k_b C - \frac{2k_w k_f C}{R(k_w + k_f)}$$

The bulk decay coefficient k_b (1/min) is modeled as a function of the temperature and total organic carbon concentration TOC according to the relation of Kiene et al. [13].

$$k_b = 1.8 \cdot 10^6 [TOC] \exp\left(-\frac{6080}{T}\right)$$

The expression is valid for $1 < TOC < 3$ mg/L and $5 < T < 25$ °C. In this work, TOC is treated as equal to dissolved organic carbon (following Sohn et al. [8]) and is further assumed to be in excess. Thus, TOC is treated as a parameter of the model and not tracked as a water quality species. The wall decay rate is $k_f = Sh(D/d)$, where the Sherwood number is modeled under turbulent flow conditions as $Sh = 0.0149Re^{0.88}(\nu/D)^{\frac{1}{3}}$. The molecular diffusivity of chlorine in water is D ; the pipe diameter is d ; and the kinematic viscosity of water is ν . It is noted that D and ν are also functions of temperature, but are treated as constant for the purposes of chlorine decay modeling in this study.

Formation of disinfection by products

Since the identification of DBPs as a potential health concern, many models to describe the formation of DBPs have been developed. The largest database on which the models are based was published by the US EPA and models were developed by Amy et al. [5]. These models took the form of multiple regression equations rather than kinetic expressions. Later, Sohn et al. [8] updated these models to correct for changes in temperature and pH, and they also developed kinetic expressions. In comparing the kinetic and multiple regression models, it was found that the models were essentially equivalent. Because applying the kinetic models requires more parameters and has a less obvious dependence on temperature, the following multiple regression models developed Amy et al [1] are used, with the temperature and pH corrections developed by Sohn et al. [8] used here.

$$TTHM = 3.296(DOC)^{0.801}(Cl_2)^{0.261}(Br^-)^{0.223}(time)^{0.264}1.156^{pH-7.5}1.0263^{T-20}$$

$$HAA6 = 5.22(DOC)^{0.585}(Cl_2)^{0.565}(Br^-)^{0.031}(time)^{0.178}0.932^{pH-7.5}1.021^{T-20}$$

The concentration of TTHMs and HAA6, both in micrograms per liter, depend on several variables: dissolved organic carbon (DOC) in milligrams per liter, which is related to the level of natural organic matter; chlorine (Cl_2) dose in milligrams per liter; bromide (Br) concentration in micrograms per liter; reaction time in hours; water temperature in degrees Celsius; and pH. Note that the chlorine dose is the concentration applied at the treatment plant and not the concentration at a particular point in the distribution system. Implementation of these equations uses a step function based on the local chlorine concentration, so that no DBPs appear if chlorine is completely absent at a node. Therefore, the expressions for TTHM and HAAs are coupled to the expression for chlorine decay only for presence or absence but not chlorine level.

Water Age

In order to compute the TTHM or HAA concentration at a point in the distribution system the reaction time since the application of chlorine dose is needed. Water age A is modeled as a zero-order reaction with rate constant 1; i.e., $dA/dt=1$.

Case Study Scenarios

Qualitative and quantitative aspects of the characteristic heating time and temperature, chlorine, and DBP model are illustrated through example applications.

Characteristic heating time

Values of characteristic heating time across several variables are of interest to quickly assess the magnitude of temperature dynamics expected for a particular system. To address this, characteristic heating times are calculated for the pipe materials unlined cast iron and polyvinylchloride (PVC). Times are given for a range of diameter, water temperature, and flow velocity. Interactions between these variables can be complex. Conductive and convective mechanisms of heat transfer sometimes conflict. Parameters, which themselves depend on temperature, appear several places in the expressions. Accordingly, the calculations carried out for this study treat the density, kinematic viscosity, specific heat, and thermal conductivity of water as functions of temperature.

Characteristic heating times for water flowing through unlined cast iron and polyvinylchloride (PVC) pipe materials were tabulated over several pipe diameters, water temperatures, and flow velocities (**Table 1**). The values considered were diameters of 100, 300, and 600 mm; water temperatures of 5, 15 and 25 °C; and flow velocities of 0.1, 0.5 and 1 m/s.

Temperature, chlorine, DBP model

A case-study system of a simple pipeline serves to illustrate properties of the temperature-chlorine-DBP model. The case-study system transmits water from a reservoir through a PVC pipeline of length 5 km and diameter 300 mm. Demand for water through the pipeline averages 20 L/s but varies between 9 and 29 L/s in a weeklong pattern having diurnal variations. The simulation runs over a one week period (168 h) using a hydraulic and water quality time step of five minutes.

The system is considered for winter and summer temperature scenarios. In winter, the source water has a temperature of 5 °C, and the soil and pipe wall have a temperature of 10 °C. The summer scenario considers source water at 25 °C and the soil and pipe wall at 20 °C. Levels of pH, dissolved organic carbon, and bromide were the same for both scenarios, and based on values reported by Amy et. al. (Table 3.2) for California State Project water after coagulation with iron [5]. Chlorine doses of 1.5 mg/L in winter and 6 mg/L in summer were selected to give residual concentrations around 1 mg/L at the end of the pipeline. Parameter values for the scenarios are summarized in **Table 2**.

Simulations assumed water in the 5km pipeline had an initial water temperature equal to the pipe wall temperature. Initial chlorine concentrations in the pipeline were 0 mg/L, and initial TTHM and HAA6 concentrations were 0 µg/L.

Results and discussion

Characteristic heating time

Characteristic heating times for water flowing through unlined cast iron and polyvinylchloride (PVC) pipe materials were tabulated over several pipe diameters, water temperatures, and flow velocities (Table 1). For the parameter values considered, characteristic heating times are dominated by pipe material and size, with flow velocity and water temperature playing a smaller role. Unlined cast iron, a material that conducts heat easily, had characteristic times of less than 1 hour. In contrast, PVC pipes had heating times ranging from 2 hours for 100 mm pipes and up to 65 hours for 600 mm pipes. Comparing within flow velocities, smaller pipes have more surface area relative to the water volume and so experience shorter heating times. The connection with surface area is emphasized by the r^2 term in the characteristic heating time equation. The relationship between velocity and heating time is governed by convective effects as summarized by the Nusselt number. Higher velocities have a higher Reynolds number, and so a higher Nusselt number indicating more convective heat transfer and so lower heating times. In the range of Table 1, water temperature had only a small effect on heating time. Higher water temperatures had a lower heating time because the thermal conductivity increases with temperature, while the kinematic viscosity decreases. The decrease in kinematic viscosity raises the Reynolds and Nusselt numbers. Thus, a higher water temperature will have more conduction and more convection.

The tabulated values of characteristic heating time can help identify cases where temperature dynamics play an important role. For pipes that conduct heat easily, the water temperature shortly becomes the pipe (ground) temperature. For pipes that are more insulating, the heat transfer dynamics are slower and so water may have a different temperature in different parts of the system.

Temperature, chlorine & DBP model

The characteristic heating times from Table 1 can be used to give a preliminary assessment of temperature effects for this case. The flow rate of 20 L/s corresponds to a velocity of 0.28 m/s and travel time through the pipeline of 5 hours. From Table 1, the characteristic heating time is 16 hours (i.e., it will take 16 hours for the temperature difference to fall to $1/e$ of its original value). As the residence time is of similar order as the heating time, temperature changes are expected during the simulation horizon.

Simulation results for the point at the end of the case-study pipeline in winter appear in **Figure 1**. Water age results confirm an average travel time of about five hours. The time for the first water to arrive from the source is nearer to seven hours, owing to lower velocities early in the simulation. Once water from the source arrives, temperature drops from an initial value of 10 °C to between 6-7 °C. Water temperatures remain 1-1.5 °C warmer than the source water as the ground provides a warming effect. The chlorine dose of 1.5 mg/L (Table 2) results in residual concentrations of 0.75 – 1 mg/L. TTHM values averaged 31 µg/L while HAA6 levels were around 13 µg/L, both well below regulatory levels.

Simulations for the summer scenario (**Figure 2**) showed the same results for water age and velocity but different trends in temperature and species concentrations. In summer, the ground serves to cool the source water by 1-1.5 °C. The 1-1.5 degree change with respect to source temperature occurs because the difference between soil and source temperature was 5 °C in both

cases. Given that average water temperatures are warmer by 17-18 degrees, a higher chlorine dose is needed in the summer to maintain residual concentrations. Residual chlorine averaged 0.9 mg/L based on a dose of 6 mg/L. As expected, DBP formation was also higher in summer. TTHM levels averaged 70 µg/L, near the regulatory level of 80 µg/L. Concentrations of HAA6 averaged 41 µg/L. Comparing to the winter scenario, increasing the chlorine dose by a factor of four yielded a similar chlorine concentration. However, TTHM levels increased by 2.3 times and HAA6 increased by 3.2 times.

Conclusion

This paper has assembled and applied a model for the effects of water temperature and residence time on chlorine decay and DBP formation. A characteristic heating time for water pipes was also proposed and sampled over a range of parameters typical of water distribution systems.

The characteristic heating time provides an idea of time scales applicable to temperature dynamics. Choice of pipe material has a strong effect on heating times. Replacement of unlined cast iron pipes with PVC (plastic) pipe increases the heating time by as much as two orders of magnitude. Even with increased insulation, heating times are still lower than residence times for small diameter pipes.

Water temperature has a strong effect on DBP production. The scenarios examined here show an approximate increase in DBP production of 2 to 3 times for the summer conditions relative to winter conditions where chlorine is dosed to achieve similar residual concentrations.

The models selected and implemented aimed at an approximate understanding of temperature effects. In particular, this paper has treated the pipe wall temperature as constant and equal to the soil temperature. In the case of exposed pipes on the land surface, wall temperature will depend on the local air temperature, wind speed, and solar radiation, among other factors. The temperature model applied here remains valid as long as the net effect of these processes results in a wall temperature that is constant over the simulation horizon. More sophisticated models could be applied where adequate data for setting parameter values is available.

Although the case-studies presented here considered a single pipe, implementation of the models in EPANET-MSX opens the possibility to consider more complex networks. In particular, the model applied here could be used to highlight areas within a network where water quality needs to be better managed.

With the changes currently being observed in the climate, larger differences between soil temperature and source water temperature may arise due to warming at the land surface and or usage of water from different sources. For example, distributing water from deeper intake points on reservoirs or from different depths in the ground could change the temperature of water supplied to the piping network. Whether the source water temperature has a material effect on the temperature at the tap depends most strongly on pipe material. Pipes with low thermal conductivity provide some opportunity for utilities to influence temperature in the system.

As new regulations of DBPs come into enforcement it will be important to have the tools for understanding DBP formation as applied to distribution systems. We hope that the work of this paper can be used to provide a first assessment of the impact of temperature on DBPs in the distribution system. Future work may consider using a kinetic rather than empirical model for DBP formation.

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Table 1. Characteristic heating time in hours for water flowing through unlined cast iron and polyvinylchloride (PVC) pipes. The cast iron columns refer to unlined cast iron.

<i>Pipe Diameter</i>	<i>Water Temperature °C</i>	<i>Water Velocity in Cast Iron</i>			<i>Water Velocity in PVC</i>		
		<i>0.1 m/s</i>	<i>0.5 m/s</i>	<i>1 m/s</i>	<i>0.1 m/s</i>	<i>0.5 m/s</i>	<i>1 m/s</i>
100 mm	5	0.08	0.03	0.02	1.9	1.8	1.8
	15	0.07	0.02	0.02	1.9	1.8	1.8
	25	0.06	0.02	0.01	1.9	1.8	1.8
300 mm	5	0.33	0.12	0.09	16.7	16.5	16.5
	15	0.29	0.11	0.08	16.6	16.4	16.4
	25	0.25	0.10	0.08	16.5	16.3	16.3
600 mm	5	0.83	0.35	0.28	66.3	65.8	65.8
	15	0.73	0.33	0.26	65.9	65.5	65.4
	25	0.66	0.31	0.25	65.6	65.3	65.2

Table 2. Model parameters for scenarios

<i>Parameter</i>	<i>Winter Scenario</i>	<i>Summer Scenario</i>
Soil temperature, °C	10	20
Water source temperature, °C	5	25
<i>Parameters at source water temperature</i>		
Thermal conductivity of water, W/m K	0.565	0.585
Density of water, kg/m ³	1000	999
Kinematic viscosity of water, m ² /s	$1.52 \cdot 10^{-6}$	$1.15 \cdot 10^{-6}$
Specific heat of water, J / kg K	4202	4185.5
Molecular diffusivity of chlorine, m ² /s	$6.91 \cdot 10^{-10}$	$9.45 \cdot 10^{-10}$
<i>Temperature independent parameters</i>		
Thermal conductivity of pipe, W/m K	0.16	0.16
Kinetic coefficient for wall decay of Cl, m/s	$2.5 \cdot 10^{-5}$	$2.5 \cdot 10^{-5}$
Dissolved organic carbon, mg/L	2.58	2.58
Chlorine dose, mg/L	1.5	6
Bromide concentration in water, µg/L	308	308
pH	7.8	7.8

Figure 1. Simulation results at the end of the pipeline for the winter scenario.

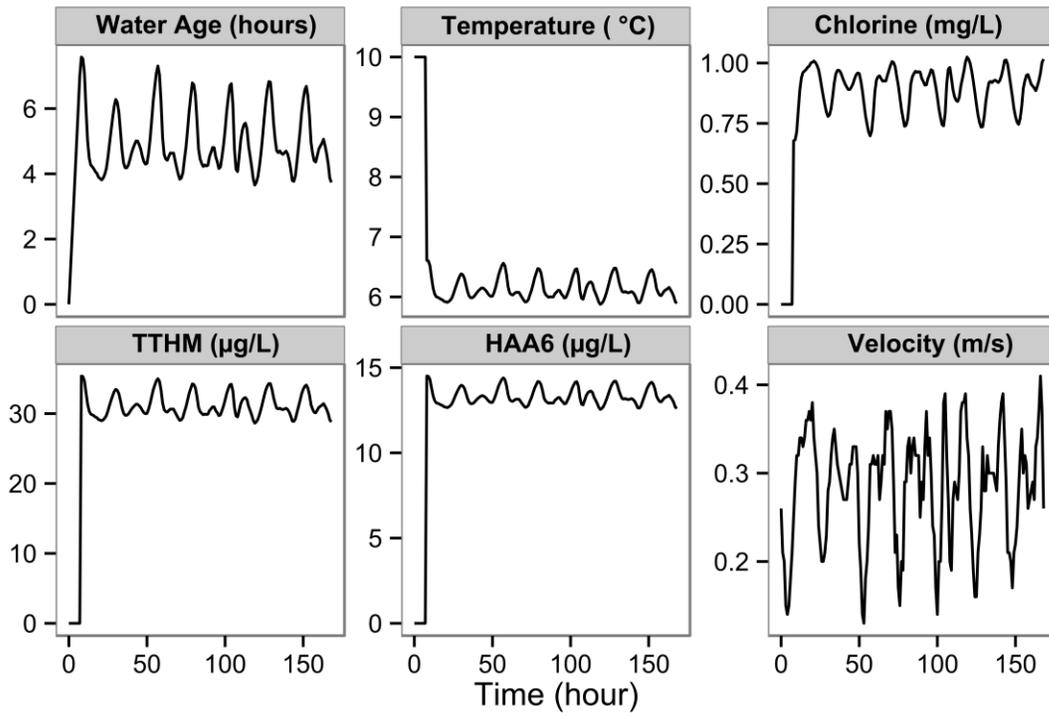


Figure 2. Simulation results at the end of the pipeline for the summer scenario.

