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Exploring integrated impact of temperature and flow velocity on chlorine decay for a pilot-scale water distribution system

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ABSTRACT

The reduction rate of residual chlorine concentration in water distribution systems depends on water quality and system parameters. Temperature is the one of the important factors affecting the rate of chlorine decay, and flow velocity further affects chlorine variation along the distribution pipeline. In this study, we explored the combined impact of temperature and flow velocity on chlorine decay rate in water distribution systems. A pilot-scale water distribution system was designed and fabricated to obtain time series of residual chlorine concentration under various temperature and flow velocity conditions. The parameters of kinetic reaction models were calibrated using genetic algorithm for further generalization of kinetic coefficient prediction. The impact of flow velocity was incorporated into the Reynolds number and integrated into a combined equation to show the relationship of temperature to decay coefficients. The decay rate obtained from the combined equation shows good agreement between simulation and experimental verification.

Keywords: Chlorine decay; Genetic algorithm (GA); Temperature; Flow velocity

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1. Introduction

Chlorine compounds are frequently added to drinking water at the end of the treatment process as a secondary disinfectant to maintain an adequate residual disinfectant concentration along the full length of a water distribution system. Because chlorine is a non-selective oxidizing agent, the concentration of chlorine decreases as the water moves through the pipeline network.

The chemical reaction rate tends to increase with temperature, and modifications of the Arrhenius equation are widely accepted into equations used to describe the relationship between reaction rate and temperature [1–5]. AWWARF [1] proposed an equation for chlorine decay rate taking into account the total organic carbon concentration, the initial concentration of chlorine, the number of rechlorinations, and the temperature [5]. The impact of temperature upon chlorine decay has usually been expressed using an equation which combines a pre-exponential term and exponential term [2]. The pre-exponential terms of the equation is considered to be constant and expresses the properties of the chemical reaction that are associated with water quality parameters.

The chlorine decay rate in a pipeline is also closely related system parameters. The impact of flow conditions such as flow velocity, flow rate, and pressure variation within the system have been explored in a number of studies. Menaia et al. [6] studied rates of chlorine decay under various flow velocities and found a positive correlation. A similar result was found by Mutoti et al. [7]. Kim et al. [8] found a linear relationship between Reynolds number (Re) and chlorine decay rate. Kim and Kim [9] and Kim et al. [10] further explored the impact of transient flow on chlorine decay and found that the transient events attenuated the decay rate of chlorine.

Chlorine compounds in the water distribution system interact with various water and system parameters. Despite

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the numerous studies on the factors affecting chlorine decay, the combined impact of water quality and system parameters on chlorine decay rate has not been rigorously investigated. In this paper, we explored the combined impact of temperature and flow velocity in pipeline systems. In order to achieve this goal, we designed and fabricated a pilot-scale water distribution system. The concentration of residual chlorine was measured under various temperature and flow velocity conditions. We proposed a combined equation for chlorine decay rate incorporating both temperature and flow velocity based on experimental data. Both the calibration of kinetic coefficients and the validation of the proposed model with unused data sets showed good agreement between predictions and experimental observations.

2. Methods and materials

2.1. Experimental setup

A pilot-scale pipeline system was fabricated to monitor variations in residual chlorine concentration under various conditions. Fig. 1 shows a schematic diagram of the experimental system. The reservoir was a cylindrical water tank with a diameter of 0.9 m and a capacity of 600 L. The pipeline system was connected to a centrifugal pump located at the upstream end of the pipeline. A flow control valve was installed at the outlet of the pump to adjust the flow rate of the system. The pipe coil was made with polyethylene (PE) and had a total length of 100 m, an internal diameter of 0.025 m, and a thickness of 0.0029 m. The pipe coil was submerged in a constant-temperature water bath of volume of 800 L. During this study, the water bath temperature range used was 10–35°C, to simulate a range of possible temperatures in a pipeline system. Chlorine and temperature sensors were located at the middle of the pipeline, and a data acquisition system collected residual chlorine concentration and temperature at a sampling rate of 1 Hz. The chlorine sensor had a measurement range of 0.02–2 ppm with an accuracy in ±0.02 ppm (Prominent Inc., Germany). The measurement range of the temperature sensor was 0–100°C.

2.2. Chlorine decay models

Chlorine compounds are strong non-selective oxidants, and it is difficult to model the distinct reaction between chlorine and different reduction agents. Therefore, the rate of chlorine decay has been approximated by fundamental kinetic equations. Haas and Karra [11] proposed kinetic models for chlorine decay using several equations. These chlorine decay models are summarized in Table 1.

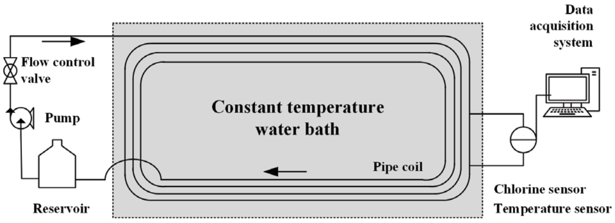

Fig. 1. Schematic diagram of the pilot-scale water distribution system.

We calibrated the parameters of the kinetic models using data sets collected from our experiment, which minimized the difference between the experimental results and the model-predicted results, using the genetic algorithm (GA). The fitness function of the algorithm can be written as follows:

$$f_{\text{obj}} = \sqrt{\left\{\sum_{i=1}^{n}\left[C_{\exp}(i) - C_{\text{model}}(i,k,n,\ldots)\right]^2\right\} \Big/ n} \quad (1)$$

where f_{obj} is the objective function of the GA, i is the index, n is the total number of samples, $C_{\exp}$ and C_{model} are the residual chlorine concentrations (mg/L) of the ith sample from the experiment and from the model, respectively, and k is decay constant.

3. Result and discussion

The residual chlorine concentration in the pilot-scale water distribution system was measured under various temperature and flow rate conditions. Table 2 shows the experimental conditions for six experimental data sets for chlorine decay.

Table 1
Kinetic model for chlorine decay

Kinetic model	Governing equation	Parameters
First order	$C = C_0\exp(-kt)$	k
nth order	$C = \left[(n-1)kt + \left(\frac{1}{C_0}\right)^{(n-1)}\right]^{-\frac{1}{n-1}}$	k, n
Limited first order	$C = C_* + (C_0 - C_*)\exp(-kt)$	k
Limited nth order	$C = C_* + \left[(n-1)kt + \left(\frac{1}{C_0 - C_*}\right)^{(n-1)}\right]^{-\frac{1}{n-1}}$	k, n
Parallel first order	$C = wC_0\exp(-k_1t) + (1-w)C_0\exp(-k_2t)$	k_1, k_2, w

Note: t is time, C is residual chlorine concentration at time t, C_0 represents initial chlorine concentration, k, k_1, and k_2 are rates of chlorine decay, n is the order of the reaction, and C_* represents the concentration of the stable chlorine compound.

Table 2
Experimental conditions for six chlorine decay data sets

Index	Flow rate (Q), L/s	Temperature (average ± standard deviation), °C
A18	0.5986	18.1 ± 0.1
A23	0.5986	23.0 ± 0.1
B18	0.5442	18.2 ± 0.1
B23	0.5442	23.0 ± 0.1
C18	0.3039	18.3 ± 0.1
C23	0.3039	23.0 ± 0.1

The initial concentration of the chlorine in the system was set to 0.9 ppm, and residual chlorine concentrations were collected over the course of 1.2 d. A total of 105,001 residual chlorine concentrations were collected for each data set. A moving average method was applied to the raw data to eliminate the noise from the measurement device. Fig. 2 presents raw and filtered (moving average) data. There was no significant difference in decay behavior between raw data and filtered data.

3.1. Chlorine decay under various temperature and flow rate conditions.

Fig. 3 shows the temporal variations in residual chlorine concentration under various temperature and flow rate conditions. Higher water temperature resulted in a higher rate of the chlorine decay for all flow rates.

Tables 3–5 show the calibrated parameters of first-, second-, third-, fourth-, and fifth-order chlorine decay models and the corresponding coefficients of determination in terms of root mean square error (RMSE) and R^2 for flow rates of 0.5986 L/s, 0.5442 L/s, and 0.3039 L/s, respectively.

Table 3 shows that decay coefficient tends to increase in higher order of kinetic models in an identical condition of flow and temperature. The optimized decay constants in lower temperature were lower than those of higher temperature for all kinetic models. The third-, fourth-, and fifth-order models show good agreement between experimental data and model prediction. The calibration result for different flow rates also showed similar results (Tables 4 and 5). Comparison among Tables 3–5 at identical temperatures showed that flow rate and optimum decay constant are related to flow velocity. In fact, the positive linear relationship between chlorine decay rate and Reynolds number (Re) has previously been reported [8].

3.2. A combined equation

Modifications of the Arrhenius equation had been widely used to predict the rate of reaction at different temperatures. The equation can be written as follows:

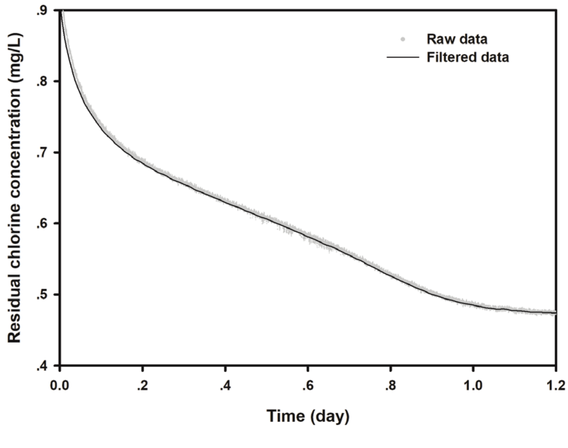

Fig. 2. Comparison of raw and filtered data using moving averages.

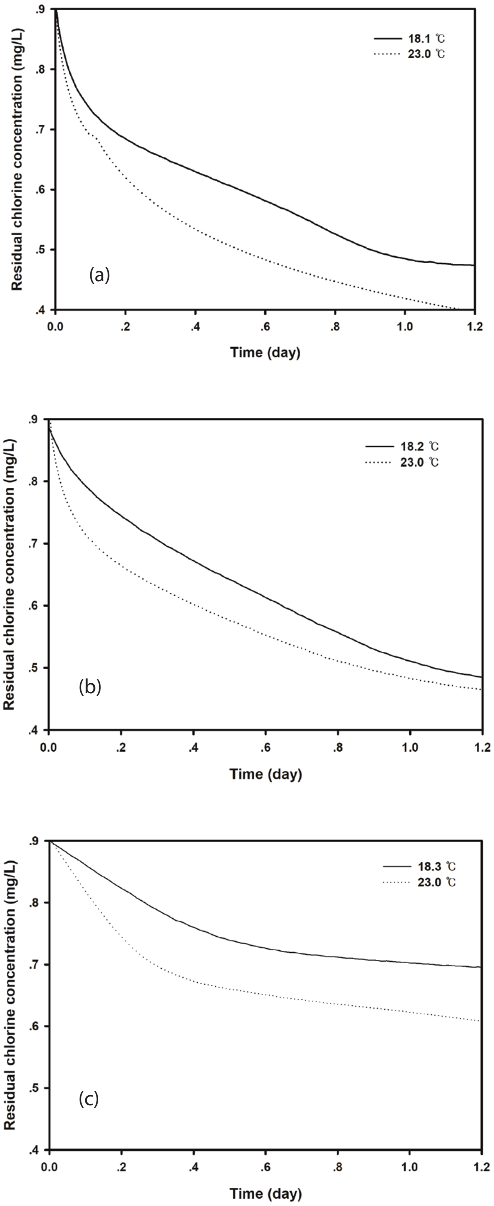

Fig. 3. Temporal variation of residual chlorine concentration under various temperature and flow rate: (a) Q = 0.5986 L/s, (b) Q = 0.5442 L/s, and (c) Q = 0.3039 L/s.

Table 3
Summary of the calibrated decay rate and corresponding determination constants (RMSE, R^2) under various temperature conditions with a flow rate of 0.5986 L/s

Condition	A18			A23.0		
	k	RMSE	R^2	k	RMSE	R^2
First	0.70	0.1418	0.61	0.95	0.1878	0.44
Second	1.07	0.1025	0.80	1.59	0.1233	0.76
Third	1.61	0.0719	0.90	2.64	0.0722	0.92
Fourth	2.40	0.0507	0.95	4.36	0.0334	0.98
Fifth	3.60	0.0416	0.97	7.18	0.0204	0.99

Table 4
Summary of the calibrated decay rate and corresponding determination constants (RMSE, R^2) under various temperature conditions with a flow rate of 0.5442 L/s

Condition	B18			B23		
	k	RMSE	R^2	k	RMSE	R^2
First	0.59	0.0633	0.93	0.77	0.1778	0.35
Second	0.85	0.0333	0.98	1.19	0.1298	0.65
Third	1.23	0.0195	0.99	1.83	0.0904	0.83
Fourth	1.78	0.0315	0.98	2.79	0.0589	0.93
Fifth	2.55	0.0491	0.96	4.26	0.0364	0.97

Table 5
Summary of the calibrated decay rate and corresponding determination constants (RMSE, R^2) under various temperature conditions with a flow rate of 0.3039 L/s

Condition	C18			C23		
	k	RMSE	R^2	k	RMSE	R^2
First	0.28	0.0714	0.72	0.45	0.1330	0.38
Second	0.36	0.0607	0.80	0.62	0.1100	0.58
Third	0.46	0.0508	0.86	0.86	0.0890	0.72
Fourth	0.59	0.0418	0.90	1.17	0.0703	0.83
Fifth	0.75	0.0340	0.94	1.61	0.0540	0.90

$$k = A \cdot \exp\left(-\frac{E_a}{RT}\right) \tag{2}$$

where A is the pre-exponential constant (d^{-1}), E_a is activation energy (J/mol), R is the ideal gas constant (J/mol·K), and T is absolute temperature (K).

Validation of the Arrhenius equation for modeling chlorine decay was conducted in several studies [4,6,9]. Kim et al. [8] proposed that the chlorine decay rate can be expressed by a linear relationship to Re, which can in turn be expressed as follows:

$$k = B(\mathrm{Re}) + C \tag{3}$$

where Re is Reynolds number, and B and C are constants determined using experimental data.

Using the relationship in Eqs. (2) and (3), it is possible to propose the combined equation for rate of chlorine decay as follows:

$$k = \left\{B\left(\mathrm{Re}\right) + C\right\} \cdot \exp\left(-\frac{E_a}{RT}\right) \tag{4}$$

Eq. (4) was applied to our experimental results. The optimized equation constants, B, C, and E_a/R, were obtained using four sets of experimental data (sets A23, A18, C23, and C18). The remaining data sets (B23 and B18) were used to validate the combined equation (Eq. (4)). The optimum coefficients for combined equation are summarized in Table 6.

Table 6
Optimum coefficients for the combined equation

Kinetic models	E_a/R (K)	B × 10^6	C (d^{-1}) × 10^6
First order	10,071	6.64	6.65
Second order	9,934	6.28	0.816
Third order	9,766	5.16	–6.22
Fourth order	9,485	2.87	–4.82
Fifth order	9,285	2.07	–9.95

Table 7
Validation result of combined equation

Condition	B18			B23		
	k	RMSE	R^2	k	RMSE	R^2
First	0.486	0.1090	0.81	0.954	0.2177	0.03
Second	0.736	0.0672	0.93	1.434	0.1542	0.51
Third	1.075	0.0501	0.96	2.076	0.1015	0.79
Fourth	1.567	0.0481	0.96	2.980	0.0621	0.92
Fifth	2.252	0.0586	0.94	4.236	0.0364	0.97

Table 6 shows the order of model reactions and calibrated parameters of Eq. (4). The pre-exponential terms of Eq. (4) tend to decrease as the order of reaction increases. As Re is dependent on the temperature of the water, with a positive correlation, it follows that the overall decay rate from Eq. (4) increased with temperature. Table 7 shows decay coefficients obtained from the combined equation using the optimum coefficients from Table 6.

The coefficients determined using optimum values from four of the calibration data sets, as per Table 7, showed a similar goodness of fit to those obtained from the calibration using GA. The decay coefficients obtained from validation ranged from 0.486 to 4.236 d^{-1}, and the corresponding values of RMSE and R^2 were 0.03–0.97. Although there was good overall agreement between the residual chlorine concentration obtained from the experimental data and that obtained using the combined equation, the results from the B23 data set showed significant differences when predicting the decay coefficient for first- and second-order kinetic models. Similar to the calibration data sets, the k tended to increase in higher order equations. Smaller RMSE and greater R^2 in high-order reactions were also seen in the validation results (Table 7). This implies that the performance of Eq. (4) is not superior to the performance of the GA.

4. Conclusion

The impact of temperature and hydraulic conditions on chlorine decay was explored for the prediction of chlorine concentrations in water distribution systems. A pilot-scale pipeline system was designed, and residual chlorine concentrations were obtained under various hydraulic and temperature conditions. The chlorine decay rates increased with temperature and Re. A combined equation for chlorine decay was proposed and applied to two experimental data sets. The predicted rate of chlorine decay showed good agreement with observed data. In this study, experiments were carried out in a highly controlled PE pipeline system to delineate the combined relationship between the chlorine reaction rate, temperature, and flow velocity, using tap water. Further generalization in experimental conditions such as pipeline material, different initial concentrations, wider ranges in discharge, flow velocity, and pressure need to be investigated to obtain a general equation for chlorine decay rate for real-life systems.

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Symbols

C_* — Concentration of stable component, ppm
C_{exp} — Residual chlorine concentration from experimental observation
C_{model} — Residual chlorine concentration from model prediction
E_a — Activation energy
f_{obj} — Objective function for genetic algorithm
A — Pre-exponential constant for Arrhenius equation
B — Constant for linear equation
C — Constant for linear equation
Re — Reynolds number
T — Absolute temperature
C — Chlorine concentration, ppm
R — Ideal gas constant
k, k_1, k_2 — Decay coefficients, d^{-1}
n — Order of decay model
w — Weighting factor

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