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Chlorine decay in pipeline systems under sequential transients based on probability density function

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ABSTRACT

The dynamic hydraulic condition in water distribution systems significantly affects the decay of chlorine concentrations. There is strong correspondence between the turbulence intensity and chlorine decay and its regression analysis provides a feasible method to determine the chlorine decay coefficients. This study focused on the applicability of chlorine decay under dynamic conditions through transient events at designated intervals with predetermined intensities. To address field conditions for transient generation, the probability density function (PDF), based on the demand curve of the water consumption, was derived and implemented to the generation of transient events with irregular intervals and durations. The temporal variation of residual chlorine concentration in a pipeline system under irregular intervals and intensity of transient events based on predetermined PDF was obtained. The parameters of various chlorine decay models were calibrated using genetic algorithm and the regression equations. The parameters of *n*th and limited *n*th order chlorine decay models from regression equation were almost identical to those obtained by calibrations. The performance of the regression equation under various transient intensities and irregular introduction of transients demonstrated potential for the application of the developed method to field of water distribution systems.

Keywords: Chlorine decay; 2D Transient flow analysis; Hydraulic condition; Genetic algorithm

1. Introduction

Maintaining the designated concentration of residual chlorine is an important water quality criterion for water distribution systems (WDSs). However, residual chlorine concentration in WDS tends to decrease as it moves through the WDS. The factors affecting the rate of chlorine decay can be divided into two categories: water quality parameters and system parameters. Water quality parameters are related to the factors affecting rate of the general chemical reaction, such as initial chlorine concentration, organic compounds concentration, iron concentration, and water temperature [1–9]. Especially, biofilms are important factors for accurate chlorine decay modeling [10–14]. Unlike water quality parameters, system parameters of chlorine decay, namely pipe age, flow velocity, and pressure variations, are more related to the properties of the pipeline system [15–18]. The chemical reaction under dynamic hydraulic conditions is a distinguishing phenomenon that can only be found in a pipeline system [19].

Despite its importance, there have been limited studies exploring the relationship between hydraulic conditions of the system and chlorine decay. Several studies [15,20] noted a positive relationship between Reynolds number and chlorine decay coefficient; however, these experiments were conducted under steady-state flow conditions. Ramos et al. [17] performed experiments to explore the impact of transient flow regime. The study found that the transient event could attenuate the chlorine decay of the drinking water system. Kim and Kim [21] were the first to quantitatively explain the impact of transient event on chlorine decay. A succession of

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transient events was generated at regular intervals at the experimental pipeline system, and the turbulence intensity was calculated by a numerical simulation involving two-dimensional flow analysis. The study argued that the decrease in the total turbulence intensity during a transient event caused reduction in chlorine decay. The transient events generated on the pilot-scaled WDS had identical intensities and this acted as motivation for further generalization for the application of the proposed methodology [21]. In this study, the turbulence intensity was an important criterion, because it quantitatively represents the hydraulic condition of the system and the total reduction amount of turbulence intensity due to transient events was significantly influenced by chlorine decay.

The goal of this study is to validate the applicability of the generalized approach of Kim and Kim [21] for chlorine decay modeling in pipeline systems. This work is organized as follows. First, the probability density function (PDF), reflecting the transient occurrence pattern of the WDS, was specified to generate transient events with irregular intervals and intensities for the experimental pipeline system. The time-series variation data of residual chlorine concentration was obtained from the experimental pipeline system governed by the PDF. Second, the parameters of various chlorine decay models were calculated using the regression equations and compared with those obtained using the calibration scheme.

2. Materials and methods

2.1. Probability density function based on demand curve for water consumption

Starczewska et al. [19] found that various pressure transient events occurred in WDSs and the characteristics of each event depended on the location and source of the transient. In this study, the pattern of the transient event was assumed to be similar to the pattern of the water consumption of the system. In other words, the probability of occurrence of the transient event could be approximated as a PDF. The PDF used herein was constructed as a fifth degree polynomial, based on the proportion of water consumption in a certain period against the total water consumption in Seongnam-si, Korea [22]. Figs. 1(a) and (b) present the demand curve and its PDF, respectively.

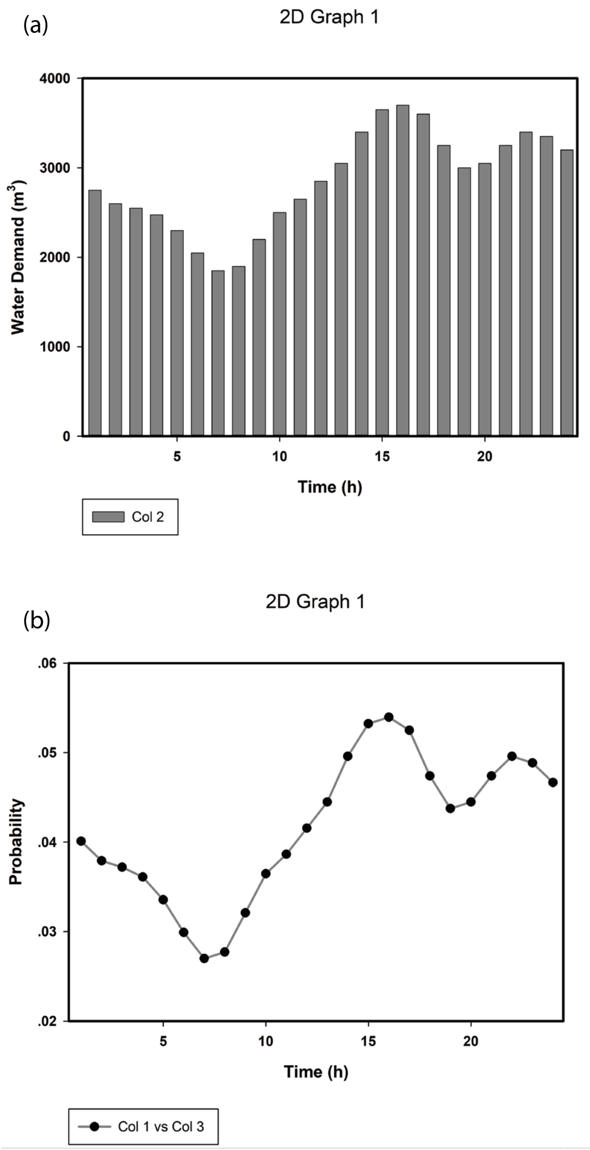

Fig. 1. Demand curve and PDF for water consumption. (a) Demand curve for water consumption. (b) PDF for demand curve.

2.2. Experimental setup

Fig. 2 shows the schematic and images of the experimental pipeline system. The specifications of the pipeline and chlorine monitoring system are as follows: the total length of pipeline is 125 m, elastic modulus of the pipe is 190 GPa, inner diameter and thickness of the pipe are 0.02 and 0.003 m, respectively, measurement range of the chlorine sensor (CLO 1-mA02pp., Prominent Inc., Baden-Württemberg, Germany) is 0.02–2 ppm, uncertainty of the sensor is ±0.02 ppm, and sampling rate is 1 Hz. There are two tanks in the experimental system, specifically, the pressurized and reservoir tank, used for different purposes. The pump was installed between the two tanks and it provided sufficient pressure head throughout the pipeline system before the reservoir tank. Prior to the experiment, the water in the pipeline and tanks were circulated for an hour throughout the pipeline system to remove all the bubbles and air that could exist in the pipeline system.

The transient generator, which was fabricated by Kim and Kim [21], was used and operated to generate irregular PDF-based transient events. Figs. 3 and 4, respectively, show the flowcharts of the transient generator operation and the developed software. The process shown in Fig. 3 is repeated until the end of the predetermined time (t_{finish}). In every time interval (t_{int}), the probability of transient event is calculated based on PDF ($f(t)$) and the value of determining factor (D_f) is also determined between 0 and 1 by the random number (uniform random) generation procedure. This process is complimentary to that of generating regular intervals of transient event in the previous study. The duration of valve closure should be noted when D_f satisfies the probability condition ($f(t) \geq D_f$). The valve closure duration represents the

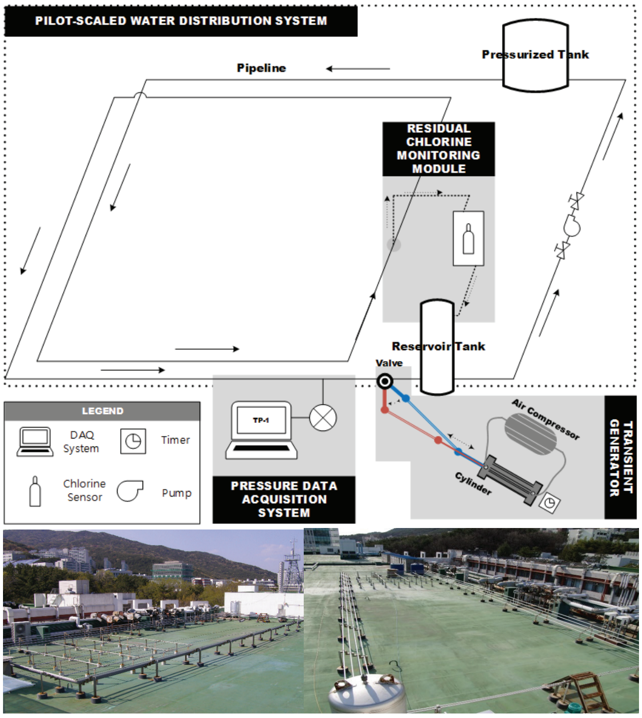

Fig. 2. Schematic and images of the experimental pipeline system.

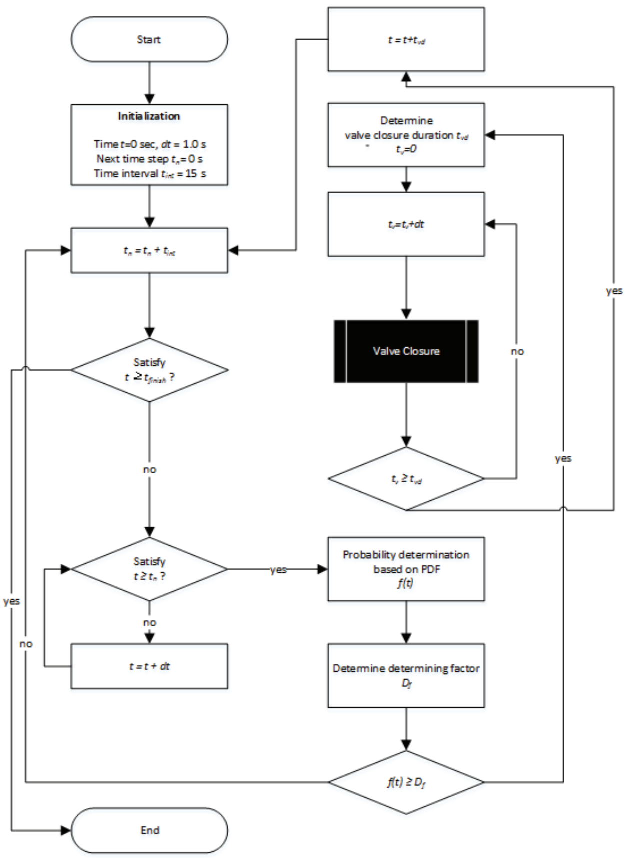

Fig. 3. Flowchart of PDF-based transient event generator.

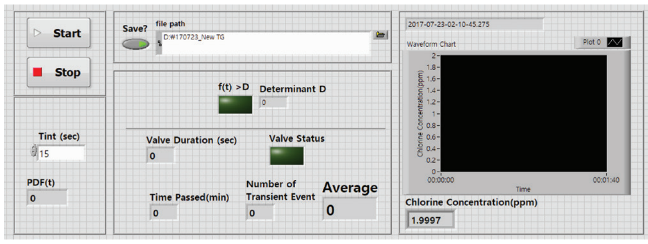

Fig. 4. Developed software for PDF-based transient event generator using LabVIEW.

turbulence intensity of each transient event. A longer valve closure duration implies a larger reduction in turbulence intensity. The duration was set randomly between 1 and 10 s. The control of transient generator was performed using National Instrument device (NI cDAQ-8178, NI-9203, and NI-9215) and LabVIEW 2015 software (Fig. 4).

The residual chlorine concentration of the experimental pipeline system was monitored while the transient generator introduced transient events on the system. Sodium hypochlorite (NaOCl) was used as the chlorine compound in experimental practices. Chlorine monitoring was initiated after the uniform residual chlorine concentration was checked throughout the pipeline system by measuring the chlorine concentration at five different sampling points of the system using a photometer.

2.3. Chlorine decay models and calibration of model parameters

Table 1 presents the existing and generic models for chlorine decay in WDSs. Existing models, namely first, second, third, fourth, limited first, limited second, limited third, limited fourth, and parallel first order models, are based on the fundamental chemical reaction laws. There are several limitations for existing chlorine decay models; (1) the reaction order (n) of the models are restricted to integer-type, (2) parallel first order model can consider only two reactants. Kim et al. [18] proposed comprehensive chlorine decay models, such as nth, limited nth, combined "1+1", combined "1+n", and combined "n+n". The integer reaction order (n) of existing models was extended to real number reaction order (n) and it was also possible to consider more than two reactants with the proposed comprehensive framework of the chlorine decay model.

The parameters of the candidate chlorine decay models in this study were calibrated using a genetic algorithm (GA) [23]. The objective function, root mean square error (RMSE), of the calibration can be defined as follows:

$$\mathrm{RMSE} = \sqrt{\sum_{i=1}^{n}\left[C_{\mathrm{obs}}\left(i\right) - C_{\mathrm{model}}\left(i, p_1, p_2, \ldots, p_k\right)\right]} \quad (1)$$

where i is the time step, C_{obs} is the observed chlorine concentration, $C_{\mathrm{model}}(i, p_1, p_2, \ldots, p_k)$ is the predicted chlorine decay concentration from a selected model, and p_k represents parameter of kth substance.

2.4. Transient flow analysis and turbulence intensity calculation

Turbulence intensity in transient flow is one of the primary controls for the rate of general chemical reaction [24].

Table 1
Existing and generic models for chlorine decay in water distribution system

Models	Governing equation	Parameters
First order	$C = C_0\exp(-kt)$	k
Second order	$C = \left(kt + \left(\frac{1}{C_0}\right)^{(1)}\right)^{-1}$	k
Third order	$C = \left(2kt + \left(\frac{1}{C_0}\right)^{2}\right)^{-\frac{1}{2}}$	k
Fourth order	$C = \left(3kt + \left(\frac{1}{C_0}\right)^{3}\right)^{-\frac{1}{3}}$	k
Limited first order	$C = C_* + (C_0 - C_*)\exp(-kt)$	k
Limited second order	$C = C_* + \left(kt + \left(\frac{1}{C_0 - C_*}\right)\right)^{-1}$	k, C_*
Limited third order	$C = C_* + \left(2kt + \left(\frac{1}{C_0 - C_*}\right)^{2}\right)^{-\frac{1}{2}}$	k, C_*
Limited fourth order	$C = C_* + \left(3kt + \left(\frac{1}{C_0 - C_*}\right)^{3}\right)^{-\frac{1}{3}}$	k, C_*
Parallel first order	$C = w_1C_0\exp(-k_1t) + (1 - w_1)C_0\exp(-k_2t)$	k_1, k_2, w_1
nth order	$C = \left(\left(n-1\right)kt + \left(\frac{1}{C_0}\right)^{(n-1)}\right)^{-\frac{1}{n-1}}$	k, n
Limited nth order	$C = C_* + \left(\left(n-1\right)kt + \left(\frac{1}{C_0 - C_*}\right)^{(n-1)}\right)^{-\frac{1}{n-1}}$	k, n
Combined "1+1"	$C = C_* + w_1(C_0 - C_*)\exp(-k_1t) + (1 - w_1)(C_0 - C_*)\exp(-k_2t)$	k_1, k_2, C_*, w_1
Combined "1+n"	$C = C_* + w_1(C_0 - C_*)\exp\left(-k_1t\right) + \left(k_2t\left(n_2-1\right) + \left(\frac{1}{(1-w_1)(C_0 - C_*)}\right)^{(n_2-1)}\right)^{-\frac{1}{n_2-1}}$	k_1, k_2, n_2, C_*, w_1
Combined "n+n"	$C = C_* + \left(k_1t\left(n_1-1\right) + \left(\frac{1}{w_1(C_0 - C_*)}\right)^{(n_1-1)}\right)^{-\frac{1}{n_1-1}} + \left(k_2t\left(n_2-1\right) + \left(\frac{1}{(1-w_1)(C_0 - C_*)}\right)^{(n_2-1)}\right)^{-\frac{1}{n_2-1}}$	k_1, k_2, n_1, n_2, C_*, w_1

Note: C is chlorine concentration (ppm), C_* is concentration of stable component (ppm), t is time (d), k, k_1, k_2 are decay coefficients (day^{-1}), n, n_1, n_2 are orders of decay model, and w_1 is weighting factor.

Especially, the reaction rate of chlorine compounds in the water bulk with biofilm at the pipe wall is also influenced by turbulence intensity [25]. Therefore, turbulence intensity represents the hydraulic condition of the system. Direct measurement of the turbulent intensity in a pipeline is extremely difficult simply because the installation and operation of fine resolution flow measurement devices such as laser Doppler velocimetry is difficult and cost demanding. In this regard, turbulence intensity of the system is calculated indirectly using the pressure head of the system, which is relatively easy to measure.

The total reduction in turbulence intensity caused by a transient event at time $T(\mathbb{I}_T)$ can be written as follows:

$$\mathbb{I}_T = \sum_{l=1}^{N} \Delta \bar{I}^{\,l}_{t(l)} \tag{2}$$

where $\Delta\bar{I}_t$ is the difference in accumulated turbulence intensity between the steady-state and a transient event during time t, l, and $t(l)$, respectively, represent a particular transient event and its duration for the lth event, and N is the number of transient events.

Because all transient events were performed under identical conditions in the experiment by Kim and Kim [21], Eq. (2) can be simplified as follows:

$$\mathbb{I}_T = N \times \Delta\bar{I}_{10\,\text{sec}} \tag{3}$$

Owing to this simplification, the quantified value of the hydraulic condition is not a number representing turbulence intensity, but a number of transient events.

To analyze transient flow in a pipeline, a two-dimensional model that could precisely analyze the pressure head and velocity profile of the system was used. The governing equations of two-dimensional transient flow analysis model are shown in Eqs. (4) and (5) [26]:

$$\frac{\partial \varphi}{\partial t} + \frac{a^2}{g}\frac{\partial V}{\partial x} = 0 \tag{4}$$

$$\frac{\partial u}{\partial t} + g\frac{\partial H}{\partial x} + \frac{1}{\rho r}\frac{\partial (r\tau)}{\partial r} = 0 \tag{5}$$

where $\varphi = p/\rho_l g + a^2[\ln(1-\alpha_v)]/g$ is an auxiliary variable that represents the piezometric head adjusted for vaporous cavitation, p is pressure, ρ_l is liquid density, α_v is volume of vapor/total volume, V is mean flow velocity, H is piezometric head, a is wave speed for homogeneous liquid in elastic pipe, g is gravitational acceleration, u is velocity, τ is wall shear stress, t is time, x is distance along the pipe, and r is the radial distance from the axis. The governing equations can be solved numerically using the predictor–corrector method [27].

Because the numerical analysis of turbulence is impossible [21], statistical mechanics of the ensemble averaging technique are integrated. To obtain temporal variation of the turbulence of the system, a minor modification was made to the initial velocity. The velocity difference between the ensemble average of velocity ($\bar{u}$) and ith velocity (u_i) is defined as the ith velocity fluctuation (u_i') and expressed as follows:

$$u_i' = u_i - \bar{u} \tag{6}$$

where $\bar{u} = \frac{1}{N_{\text{en}}}\sum_i^{N_{\text{en}}} u_i$, N_{en} is the number of ensemble sets of different initial flow velocities with minor modification, u_i is the velocity dependent on time and location.

The turbulence intensity (I) is defined as the quantity of the turbulence strength (T_{strength}) relative to the mean flow velocity, and defined as follows:

$$I = \frac{T_{\text{strength}}}{\bar{u}} \tag{7}$$

where $T_{\text{strength}} = \sqrt{1/N_{\text{en}}\sum_{i=1}^{N_{\text{en}}}(u_i')^2}$.

Turbulence intensity is accumulated over time $t(\bar{\mathbb{I}}_t)$ and the difference in accumulated turbulence intensity between steady-state and transient event ($\Delta\bar{\mathbb{I}}_t$), respectively, is expressed as follows:

$$\bar{\mathbb{I}}_t = \int_0^t I\,\mathrm{d}t \tag{8}$$

$$\Delta\bar{\mathbb{I}}_t = \bar{\mathbb{I}}_{t,\text{steady}} - \bar{\mathbb{I}}_{t,\text{transient}} \tag{9}$$

where $\bar{\mathbb{I}}_{t,\text{steady}}$, $\bar{\mathbb{I}}_{t,\text{transient}}$ are accumulated turbulence intensities for steady-state and transient conditions, respectively, over time t.

3. Results and discussion

The initial flow velocity and chlorine concentration were 1.6 m/s and 1.6 ppm, respectively. The pressure head of the pipeline at steady-state was 4.1 m and maximum pressure during transient event was 183.5 m.

Fig. 5 shows the temporal variation in residual chlorine concentration and the pattern of transient events. As this study used the identical experimental pipeline and system conditions as those of Kim and Kim [21], the factors affecting rate of chlorine decay, such as pipe properties, flow velocity, concentration of humic acid, number of rechlorination events, and pressure head at steady-state were identical;

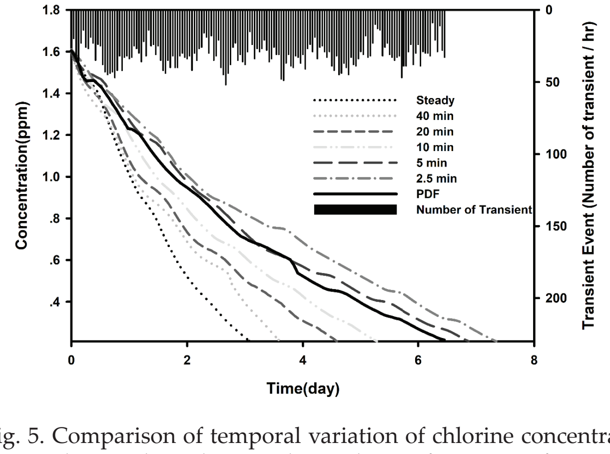

Fig. 5. Comparison of temporal variation of chlorine concentration under steady and unsteady conditions for various frequencies of transient event and PDF-based transient event generation.

Table 2
Number of transient events and total amount of turbulence intensity reduction for 4 d

Duration (t, s)	1	2	3	4	5	6	7	8	9	10	Total
Number of transient events (N)	384	402	384	409	378	382	380	395	385	388	3,887
Amount of turbulence intensity reduction during t s ($\Delta\bar{\mathbb{I}}_t$)	0.139	0.315	0.495	0.678	0.863	1.051	1.241	1.433	1.627	1.822	
Total turbulence intensity reduction ($N \times \Delta\bar{\mathbb{I}}_t$)	53.5	126.6	190.0	277.1	326.2	401.4	471.5	565.9	626.2	707.0	3,745.3

Table 3
Parameters for candidate chlorine models from calibration and regression equation in Kim and Kim [21] and corresponding determination coefficients (R^2) and root mean square error (RMSE)

Title	Parameters	Coefficient		R^2		RMSE	
		Calibration	Regression equation	Calibration	Regression equation	Calibration	Regression equation
First order	k (d^{-1})	0.275	0.207	0.87	0.76	0.144	0.193
Second order	k (d^{-1})	0.221	0.166	0.77	0.60	0.192	0.253
Third order	k (d^{-1})	0.181	0.131	0.62	0.43	0.244	0.301
Fourth order	k (d^{-1})	0.147	0.103	0.48	0.28	0.286	0.337
Limited first order	k (d^{-1})	0.281	0.211	0.87	0.76	0.144	0.195
Limited second order	k (d^{-1})	0.291	0.172	0.79	0.59	0.181	0.255
Limited third order	k (d^{-1})	0.297	0.137	0.79	0.36	0.181	0.318
Limited fourth order	k (d^{-1})	0.305	0.113	0.60	0.29	0.253	0.335
Parallel first order	w	0.745	0.667	0.87	0.76	0.144	0.193
	k_f (d^{-1})	0.275	0.207				
	k_s (d^{-1})	0.274	0.207				
nth order	n	0.551	0.553	0.87	0.87	0.142	0.142
	k (d^{-1})	0.241	0.230				
Limited nth order	n	0.542	0.530	0.87	0.87	0.142	0.142
	k (d^{-1})	0.235	0.232				
Combined "1+1"	w	0.879	0.823	0.87	0.75	0.145	0.201
	k_1 (d^{-1})	0.281	0.208				
	k_2 (d^{-1})	0.265	0.205				
	C^* (mg/L)	0.000	0.000				
Combined "1+n"	w	0.115	0.039	0.87	0.82	0.141	0.170
	k_1 (d^{-1})	0.813	0.071				
	n	0.570	0.625				
	k_2 (d^{-1})	0.236	0.241				
	C^* (mg/L)	0.052	0.069				
Combined "n+n"	w	0.204	0.186	0.84	0.82	0.159	0.169
	n_1	0.604	0.300				
	k_1 (d^{-1})	0.211	0.095				
	n_2	0.616	0.777				
	k_2 (d^{-1})	0.263	0.205				
	C^* (mg/L)	0.033	0.050				

however, the temporal variation in hydraulic conditions was different. Fig. 5 indicates that the chlorine decay rate for PDF-based transient event generation with irregular intensities and intervals corresponds to a value between 5 and 10 min of transient event intervals. The expectation for the total turbulence intensity reduction was also between that of 5 and 10 min intervals of transient events.

Table 2 summarizes the number of transient events and amount of turbulence intensity reduction for 4 d. The number of transients introduced into the experimental pipeline system was 3,887. The mean and standard deviation of transient events were 389 and 9.6, respectively, for various valve closure durations. The amount of turbulence intensity reduction during various valve closure duration was calculated using Eq. (9) and it was seen that $\Delta\overline{\mathbb{I}}_t$ increased with increasing valve closure duration. The net turbulence intensity during the experiment was 3,745.3 and this value was considered as the overall loss of the system chlorination activity [21]. The total turbulence intensity reduction of this study was greater than that for 10 min transient interval and lesser than that for 5 min transient interval.

The regression equations relating the total turbulence intensity reduction to the parameters of chlorine decay models can be obtained for parameters of candidate chlorine decay models. Table 3 shows the parameters of candidate chlorine models obtained from calibration method and regression equations. Among the 14 candidate models, first order, limited first order, parallel first order, *n*th order, limited *n*th order, combined "1+1", combined "1+*n*", and combined "*n*+*n*" models with parameters from calibration method showed good agreement between experimental data. This is similar to the result from Kim and Kim [21]; however, the overall "goodness of fit" of the models (R^2 and RMSE) was worse than the previous study because of the relatively unstable hydraulic conditions employed in this study. Even though there are differences between the coefficients from the calibration and regression equations, the performance of the generic models was better than that of existing models. This finding indicates that the relaxation of limitations on existing parameters or introduction of additional calibration parameters could help to predict chlorine concentration under complicated hydraulic conditions.

4. Conclusion

This research introduced the PDF of transients to determine the behavior of chlorine decay in real WDSs. The demand curve for water consumption was used to simulate the frequency of transient events in field conditions and the transient events had random durations ranging from 1 to 10 s. The parameters and fitness of chlorine decay models from GA and regression equations were compared with those of an existing study. The most significant conclusion is that the result verified the regression equation obtained from regular transient events. As per the good performance of the regression equation under various transient intensities, irregular introduction of transients, unsteady flow conditions, and delineated equations demonstrate potential for the application of the proposed method to field WDSs. Further work is required to verify the applicability in real-life WDSs. Calibration is important for hydraulic conditions under deteriorated systems, such as those affected by corrosion or partially blocked pipelines, which can lead to irregular wall conditions.

Acknowledgments

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Symbols

$\mathbb{I}_T$ — Total amount of the reduction of turbulence intensity
$\Delta\bar{I}_t$ — Difference in accumulated turbulence intensity between steady-state and transient state
I — Turbulence intensity
T_{strength} — Strength of turbulence
$\overline{\mathbb{I}}_{t,\text{steady}}$ — Accumulated turbulence intensity in steady-state over time t
$\overline{\mathbb{I}}_{t,\text{transient}}$ — Accumulated turbulence intensity in transient state over time t
N — Number of transient events
t_{finish} — Predetermined finish time
t_{int} — Time interval
C — Chlorine concentration, ppm
C_* — Concentration of stable component, ppm
k, k_1, k_2 — Decay coefficients, d^{-1}
n, n_1, n_2 — Order of decay model
w_1 — Weighting factor
φ — Auxiliary variable which represents the piezometric head adjusted for vaporous cavitation
p — Pressure
ρ_l — Liquid density
α_v — Volume of vapor/total volume
V — Mean flow velocity
H — Piezometric head
a — Wave speed for homogeneous liquid in elastic pipe
g — Gravitational acceleration
u — Velocity
τ — Wall shear stress
t — Time
x — Distance along the pipe
r — Distance from the axis in radial direction
$\bar{u}$ — Ensemble average of velocity
u_i — *i*th velocity
u'_i — *i*th velocity fluctuation
N_{en} — Number of ensemble sets

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