A new approximate solution for chlorine concentration decay in pipes

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ABSTRACT

Biswas et al. (1993. A model for chlorine concentration decay in pipes. Water Res. 27(12), 1715–1724) presented an analytical solution of a two-dimensional (2-D) steady-state chlorine transport equation in a pipe under the turbulent condition and employed fractional error function and regression technique to develop an approximate solution. However, their approximate solution may not give a good result if the wall decay parameter is large. This paper provides a more accurate approximate solution of the 2-D steady-state chlorine transport equation under the turbulent condition. This new approximate solution has advantages of easy evaluation and good accuracy when compared with the approximate solution given by Biswas et al. (1993). In addition, this paper also develops a methodology that combines simulated annealing (SA) with this new approximate solution to determine the wall decay parameter. Two cases are chosen to demonstrate the application of the present approximate solution and methodology. The first case is to use this new approximate solution in simulating chlorine decay in pipes with the experiment-observed data given by Rossman (2006. The effect of advanced treatment on chlorine decay in metallic pipes. Water Res. 40(13), 2493–2502), while the second case presents the determination of the wall consumption at the end of the pipe network.

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1. Introduction

The Safe Drinking Water Act and its Amendments in the US commanded the establishment of maximum contaminant level goals for some harmful material that appears in the outlet of treatment plants to ensure secure quality of drinking water. This requirement led to more care for water quality aggravation in the distribution system. Before treated water enters the water distribution systems, disinfection is commonly performed to retain residual chlorine in a distribution system for avoiding microbiological growth in the pipe. In addition to cheapness, chlorine is a strong and sustained disinfection. The studies of chlorine residuals in the water distribution systems reported in the literature included the development of the model for chlorine disappearance in the transport process and described the mechanism for distribution of chlorine concentration in the network (e.g., Clark et al., 1991, 1993, 1995).

The model for chlorine transport in the pipes may include the first-order decay kinetics in bulk liquid and chlorine consumption at the pipe wall. The consumption process at the pipe wall is similar to the process of mass transfer from the bulk liquid phase to the pipe surface. LeChevallier et al. (1988) indicated that the transport of chlorine from the bulk liquid phase to the biofilm at the pipe wall is an important factor affecting the chlorine decay rate. In order to inactivate bacterial populations, higher chlorine concentrations are required in the biofilm as compared to those suspended in

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Nomenclature		J_0	Bessel function of the first kind of order zero
		J_1	Bessel function of the first kind of order one
A_0	dimensionless chlorine radial diffusivity ($LD_r/r_0^2 U$ $= \pi L D_r/Q$)	k	first-order chlorine decay rate constant in the bulk water (s^{-1})
A_1	dimensionless chlorine decay rate in the bulk water (kL/U)	L	pipe length (m)
		r	radial distance from the center of the pipe (m)
A_2	dimensionless wall decay rate ($V_d r_0/D_r$)	r_0	pipe radius (m)
c	point value of chlorine concentration in any location of the pipe ($mg L^{-1}$)	r_h	hydraulic radius of pipe
c_0	inlet chlorine concentration ($mg L^{-1}$)	R	dimensionless radial distance from the center of the pipe (r/r_0)
C	dimensionless chlorine concentration (c/c_0)		
C'	average chlorine concentration in the pipe under no wall consumption condition	U	average flow velocity throughout the distribution system ($m s^{-1}$)
C_{av}	dimensionless cup-mixing average concentration of the pipe at any cross-section	V_d	pipe wall surface reaction constant ($m s^{-1}$)
		x	axial distance from the inlet along the pipe (m)
D_r	radial effective diffusivity of chlorine in the water ($m^2 s^{-1}$)	X	dimensionless axial distance from the inlet along the pipe
$f(r)$	flow parameter term on the flow regime	λ_n	the nth root of eigenfunction
$F(R)$	dimensionless flow parameter term on the flow regime	ε	fractional error

the bulk liquid phase. In addition, the pipe material strongly affects the wall decay and could generally be grouped into two different types, that is, the reactive pipes such as unlined iron and unreactive pipes, e.g., PVC, MDPE, and cement-lined iron (Hallam et al., 2002). Therefore, the decay of chlorine at the pipe wall is usually considered as the first-order reaction parameter in relation to the degree of reactivity of the pipe material.

In order to simulate chlorine transport and decay behavior in a pipe, Biswas et al. (1993) considered a two-dimensional (2-D) steady-state chlorine transport equation. The equation includes the convective transport in axial direction, the diffusion in radial direction, and the consumptions by a first-order reaction in the bulk liquid phase and pipe wall. Commonly, the analytical or numerical approaches were used to solve the chlorine transport equation. Biswas et al. (1993) used the separation of variables technique to derive an analytical solution for the chlorine transport equation under turbulent flow. However, their solution is laborious to evaluate straightforwardly since it contains an infinite series with the roots of eigenfunction expressed in terms of Bessel functions. Thus, they introduced the concept of fractional error along with the regression technique to obtain an approximate solution for the chlorine transport equation. Their approximate solution was then used to determine the wall consumption parameter. However, the development of the approximate solution is not straightforward and the high accuracy occurs on narrow range of wall decay parameters due to a simplifying technique. For the numerical approach, Ozdemir and Ger (1998) applied a finite difference method to solve the steady-state chlorine transport equation. In addition, they also developed a numerical model and simulated chlorine decay under laminar and turbulent flow conditions. Rossman et al. (1994) developed a mass-transfer-based model that employed a lumped mass-transfer coefficient to account for the radial transport and estimated the wall consumption.

The primary objective of this study is to develop a new approximate solution for the 2-D steady-state chlorine transport equation under turbulent flow. With the advantages of simple function form, easy numerical evaluation, and good accuracy, this approximate solution can simulate chlorine decay on both field and experiment. In addition, it can also be employed to estimate transport parameters if coupled with an optimization approach.

2. Methodology

2.1. Mathematical background

The following are given by Biswas et al. (1993). The 2-D steady-state equation for describing the concentration of total free chlorine in the water flowing through a pipe, in the absence of axial dispersion, is written as (Biswas et al., 1993)

$$Uf(r)\frac{\partial c}{\partial x} = D_r \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) - kc \tag{1}$$

where c is the concentration of free available chlorine, ($mg L^{-1}$); U is the average flow velocity in the pipe, ($m s^{-1}$); $f(r)$ is a flow parameter depending on the flow regime (e.g., $f(r) = 2[1-(r/r_0)^2]$ for laminar flow and an approximation to $f(r) = 1$ for turbulent flow); r is the radial coordinate; x is the axial coordinate; D_r is the effective diffusivity of chlorine solution in the r-direction, ($m s^{-1}$); and k is the chlorine first-order decay rate in the bulk water, (s^{-1}).

The left-hand side term of Eq. (1) accounts for the advective flux in the axial direction while the first term on the right-hand side (RHS) of Eq. (1) denotes the diffusive flux in the radial direction and the second term on the RHS represents the decay of chlorine in the bulk flow.

The boundary conditions for Eq. (1) are as follows (Biswas et al., 1993):

$$x = 0, \ c = c_0 \quad \text{at} \quad 0 \leqslant r \leqslant r_0 \tag{2}$$

$$r = 0, \ \partial c/\partial r = 0 \quad \text{at} \quad 0 \leqslant x \leqslant L \tag{3}$$

$$r = r_0, \ D_r \partial c/\partial r = -V_d c \quad \text{at} \quad 0 \leqslant x \leqslant L \tag{4}$$

where c_0 is the inlet chlorine concentration (mg L^{-1}); L is the pipe length (m); r_0 is the pipe radius (m); and V_d is the pipe wall surface reaction constant and also referred to "intrinsic wall decay constant" (m s^{-1}).

Under the turbulent condition, Eq. (1) can then be put in dimensionless form as (Biswas et al., 1993)

$$f(R)\frac{\partial C}{\partial X} = \frac{A_0}{R}\frac{\partial}{\partial R}\left(R\frac{\partial C}{\partial R}\right) - A_1 C \tag{5}$$

subject to the following dimensionless boundary conditions (Biswas et al., 1993):

$$X = 0, \ C = 1 \quad \text{at} \quad 0 \leqslant R \leqslant 1 \tag{6}$$

$$R = 0, \ \partial C/\partial R = 0 \quad \text{at} \quad 0 \leqslant X \leqslant 1 \tag{7}$$

$$R = 1, \ \partial C/\partial R = -A_2 C \quad \text{at} \quad 0 \leqslant X \leqslant 1 \tag{8}$$

where $C = c/c_0$, $X = x/L$, $R = r/r_0$, $A_0 = LD_r/r_0^2 U$, $A_1 = kL/U$, and $A_2 = V_d r_0/D_r$. The dimensionless parameters A_0, A_1, and A_2 represent the radial effective diffusivity, the chlorine decay rate constant in the bulk water, and pipe wall surface reaction constant, respectively. The function $F(R)$ represents the dimensionless velocity profile and is assumed to equal one under the turbulent flow or $2[1-R^2]$ under laminar flow.

The analytical solution under turbulent condition to Eq. (5) with respect to the boundary conditions, Eqs. (6)–(8), can be obtained based on the method of separation of variables. The result expressed as the cup-mixing average concentration at any cross-section of the pipe is (Biswas et al., 1993)

$$C_{av} = \sum_{n=1}^{\infty}\frac{4A_2^2}{\lambda_n^2(\lambda_n^2 + A_2^2)} \times \exp[-(A_1 + \lambda_n^2 A_0)X] \tag{9}$$

with the corresponding eigenfunction

$$\lambda_n J_1(\lambda_n) - A_2 J_0(\lambda_n) = 0 \tag{10}$$

where λ_n represents the root of Eq. (10). In Eq. (10), the Bessel functions, J_0 and J_1, can be evaluated to the seventh decimal place using the functions given by Press et al. (1986) and λ_n can be found by Newton's method when solving Eq. (10) as a nonlinear equation. Note that Newton's method has the advantage of quadratic convergence in searching the roots (Yeh, 1987). The concentration C_{av} at any location in the pipe can be evaluated by Eq. (9) if the values of λ_n, A_0, A_1, and A_2 are available. Biswas et al. (1993) indicated that the estimated error of C_{av} is less than 5% as C_{av} is computed using only the first term of the infinite series in Eq. (9). Therefore, it may be appropriate to use the first three terms of the series in Eq. (9) to compute C_{av}.

2.2. Biswas et al.'s approximate solution (1993)

In the case of no chlorine consumption at the pipe wall (i.e., $A_2 = 0$), the cup-mixing average chlorine concentration can be expressed as (Biswas et al., 1993)

$$C'_{av} = \exp(-A_1 X) \tag{11}$$

A fractional error ε was defined to simplify the analytical solution as (Biswas et al., 1993)

$$\varepsilon = (C'_{av} - C_{av})/C_{av} \tag{12}$$

Substituting Eq. (11) into Eq. (12), C_{av} becomes

$$C_{av} = \frac{\exp(-A_1 X)}{(1 + \varepsilon)} \tag{13}$$

Once ε is assigned, the C_{av} can then be determined by Eq. (13). Biswas et al. (1993) used the regression technique to express ε in terms of A_0 and A_2 as

$$\varepsilon = 2.4416 A_0 A_2 - 0.1559 A_0 A_2^2 \quad \text{for} \quad 0.01 \leqslant A_2 \leqslant 10 \tag{14}$$

Eq. (13) along with Eq. (14) was then used to approximate Eq. (9) in computing the C_{av}.

2.3. New approximate solution

The C_{av} may be approximated by retention of the first term of the infinite series and neglection of higher-order terms in Eq. (9) as

$$C_{av} = \frac{4A_2^2}{\lambda_1^2(\lambda_1^2 + A_2^2)}\exp[-(A_1 + \lambda_1^2 A_0)X] \tag{15}$$

For $0 \leqslant \lambda_n \leqslant 12$, the Bessel functions J_0 and J_1 in Eq. (10) can be respectively written as (Yang and Yeh, 2002)

$$J_0(\lambda_n) = 1 - \frac{(1/4)\lambda_n^2}{(1!)^2} + \frac{((1/4)\lambda_n^2)^2}{(2!)^2} - \frac{((1/4)\lambda_n^2)^3}{(3!)^2} + \cdots \tag{16}$$

and

$$J_1(\lambda_n) = \left(\frac{\lambda_n}{2}\right)\left[1 - \frac{(1/4)\lambda_n^2}{(1!)(2!)} + \frac{((1/4)\lambda_n^2)^2}{(2!)(3!)} - \frac{(1/4\lambda_n^2)^3}{(3!)(4!)} + \cdots\right] \tag{17}$$

The value of λ_n increases with A_2, which equals $V_d r_0/D_r$. The parameter D_r is assumed equal to the eddy diffusivity suggested as $D_{eddy} = 1.233 \times 10^{-2} U r_0$ by Edwards et al. (1979). Rossman et al. (1994) used the EPANET program to simulate chlorine residual in the network in New Haven, Connecticut, in which the value of A_2 ranged from 7.3×10^{-4} to 7.0×10^{-2} under turbulent flow. Biswas et al. (1993) also studied this network and had the value of A_2 ranging from 1.49×10^{-5} to 1.3×10^{-2}. Additionally, experimental studies for chlorine decay (Ozdemir and Ger, 1998; Rossman et al., 2001; Rossman, 2006) indicate that the value of A_2 is from about 2.49×10^{-4} to 3.48×10^{-3} under turbulent flow. Accordingly, the value of A_2 is considered smaller than 0.1. The first root λ_1 is less than 0.5 when $A_2 < 0.1$. Therefore, the third and higher-order terms in Eq. (16) and the second and higher-order terms in Eq. (17) are relatively small and negligible. Accordingly, based on Eq. (10), λ_1 becomes

$$\lambda_1 = \sqrt{\frac{4A_2}{2 + A_2}} \tag{18}$$

Eq. (15) can then be expressed as

$$C_{av} = \left(1 + \frac{2A_2}{4 + 2A_2 + A_2^2}\right)\exp\left[-\left(A_1 + \frac{4A_0 A_2}{2 + A_2}\right)X\right] \tag{19}$$

As an approximate solution to Eq. (1), Eq. (19) is very simple and easy to use to compute the C_{av}. When A_2 is smaller than 0.1, the second term on the RHS of Eq. (19) is much less than 1.

Thus, the approximate solution is further simplified to

$$C_{av} = \exp\left[-\left(A_1 + \frac{4A_0A_2}{2+A_2}\right)X\right] \qquad (20)$$

3.   Results and discussion

3.1.   Accuracy comparisons

The present approximate solution is compared with both the analytical and approximate solutions given in Biswas et al. (1993). Three figures are plotted to investigate the effect of the parameters A_0, A_1, and A_2 on the corresponding predicted chlorine concentration. Figs. 1(a)–(c) show the curves for the chlorine concentration distribution, C_{av}, at the outlet ($X = 1$) versus the dimensionless wall decay rate (A_2) with different values of dimensionless radial diffusivity (A_0) for the dimensionless water decay rate (A_1) equal to 0.001, 0.1, and 1. The solid line, dotted line, and dashed line represent the analytical solution, present approximate solution, and Biswas et al.'s approximate solution (1993), respectively.

As indicated in Figs. 1(a)–(c) for different A_1, the C_{av} value based on Biswas et al.'s approximate solution (1993) starts to
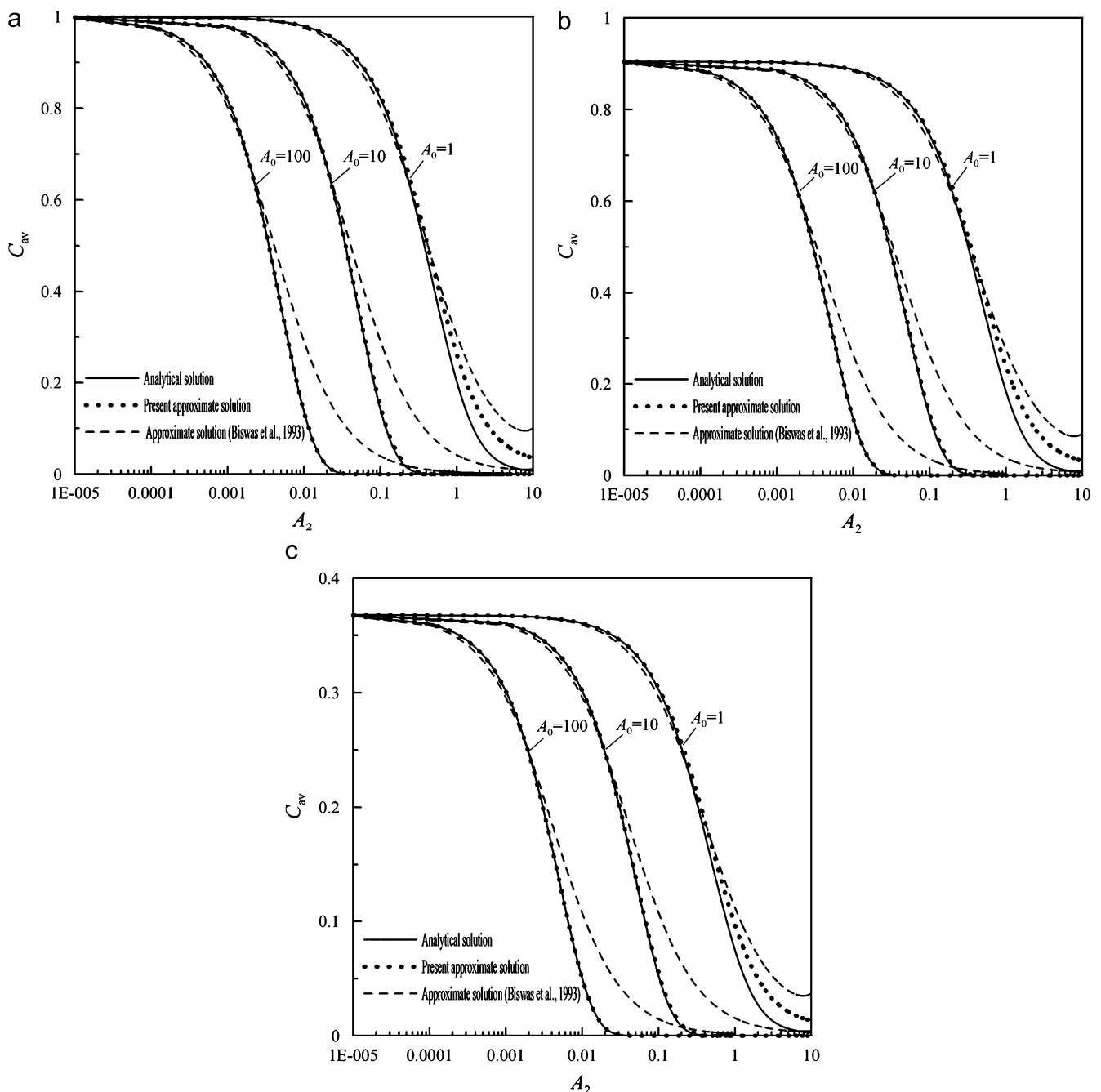
Fig. 1 – The curves of outlet chlorine concentration computed based on the analytical solution, present approximate solution, and Biswas et al.'s approximate solution (1993) against A_2 at (a) $A_1 = 0.001$; (b) $A_1 = 0.1$; and (c) $A_1 = 1$.

deviate from the analytical solution for A_2 at 0.003, 0.03, and 0.3 when $A_0 = 100$, 10, and 1, respectively. The present approximate solution is in good agreement with the analytical solution for A_1 ranging from 0.001 to 1 with A_0 equal to 100, 10, and 1 except in the region where $A_2 > 0.5$ and $A_0 = 1$. Those results indicate that the parameters of A_0 and A_2 have an apparent influence on the accuracy of those two approximate solutions. In addition, the present approximate solution generally gives better prediction for the chlorine concentration than that of Biswas et al.'s approximate solution (1993).

The poor accuracy of Biswas et al.'s approximate solution (1993) stems from the fact that the expressions of fractional factor, ε, in terms of A_0 and A_2 were developed using the regression techniques as shown in Eq. (14). On the other hand, the error of the present approximate solution is made mainly by neglecting the higher-order terms of the Bessel functions in Eqs. (16) and (17). If the first eigenvalue λ_1 is small, the errors of neglecting the higher-order terms in the Bessel functions of Eqs. (16) and (17) will be very small.

Fig. 2 shows the plots of the true and approximate values of λ_1 against A_2. The solid line represents the true λ_1 obtained from Eq. (10) by Newton's method and the dashed line denotes the approximate λ_1 calculated from Eq. (18). This figure indicates that both the value of λ_1 and the difference in λ_1 increase with A_2. In addition, Table 1 shows the relative errors of the approximate λ_1 to the true λ_1 for A_2 ranging from 0.001 to 0.5 and the relative error is about 1.2% at $A_2 = 0.1$. Accordingly, the present approximate solution gives accurate results when $A_2 < 0.1$ and is thus appropriate for most field cases.

3.2. Two case studies

The first-order reaction kinetics is usually used to represent the chlorine decay in the bulk liquid of the pipe and at the

Table 1 – Values of λ_1 at different A_2

A_2	Newton's method	Approximate method	Relative error (%)
0.001	0.04472	0.04471	−0.02
0.01	0.01412	0.01411	−0.07
0.1	0.44168	0.43644	−1.19
0.5	0.94077	0.89443	−4.93

pipe wall. The decay parameters can be determined based on an appropriate mathematical model and measured chlorine concentration data. Two cases are chosen to demonstrate the application of the present approximate solution. The wall surface reaction constant estimated based on the approximate solution is compared with those obtained from Biswas et al. (1993) and Rossman (2006) in Case 1 and from the South Central Connecticut Regional Water Authority (Clark et al., 1991) in Case 2.

3.2.1. Case 1

Rossman (2006) used a distribution system simulator, which consisted of a 27 m long loop with a 0.15 m diameter unlined ductile iron pipe, a recirculation pump, and a heat exchanger cooling system. An experiment was made to measure the reaction rate of chlorine in a simulated pipe for water treated by different forms of advanced treatment at US EPA's Test and Evaluation Facility in Cincinnati, Ohio. In Case 1, the present approximate solution is used to determine the pipe wall surface reaction constants V_d for water applied by three different treatments. The initial chlorine was about $6\,\mathrm{mg\,L^{-1}}$ and the values of k shown in the second column of Table 2 (Rossman, 2006) for lab-tested water under different treatments were determined based on the analysis of the kinetic test data. The wall surface reaction constants, V_d, for three sorts of lab-tested water can then be determined from the experiment-observed data based on the present approximate solution. In the experiment, the flow velocity was maintained constant, so a steady-state flow condition was considered. Note that the axial distance from the inlet along the pipe, x, is equal to the flow velocity multiplied by the flow time in the pipe. Under the turbulent condition, the eddy diffusion is greater than the molecular diffusion. Thus, the effective diffusivity in the radial direction, D_r, is only considered to the eddy diffusivity, which can be expressed as $D_{eddy} = 1.233 \times 10^{-2} U r_0$ (Edwards et al., 1979) because of turbulent flow. With the known values of pipe radius, pipe length, flow velocity, and chlorine bulk decay constant, V_d can be determined based on the present approximate solution, Eq. (20), when minimizing the objective function defined as the sum of square errors between the observed and predicted chlorine concentrations. In order to determine the optimal value of V_d for three sorts of lab-tested water, simulated annealing (SA) is applied. The SA is a generic probabilistic meta-algorithm for the global optimization problem based on the annealing concept, namely locating a good approximation to the global optimum of a objective function in a large search space. The initial temperature of the SA is chosen as 100 and
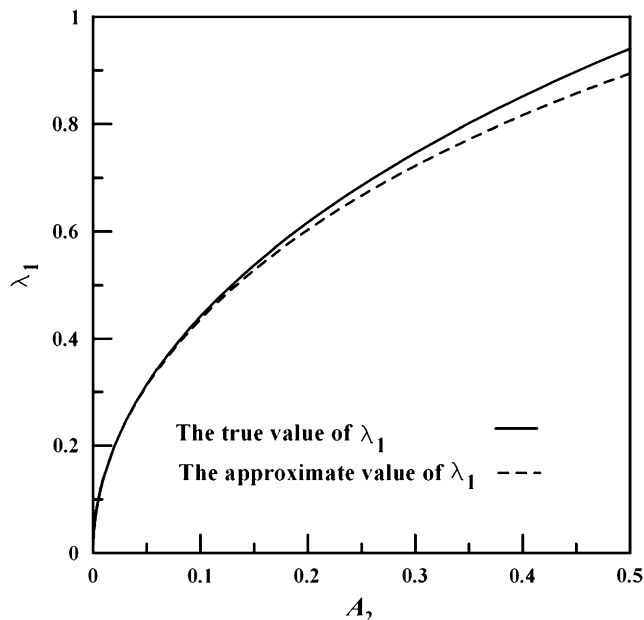
Fig. 2 – Plots of the true and approximate values of λ_1 against A_2.

**Table 2 – Values of k and V_d for three sorts of lab-tested water**

Treatment	k (s^{-1})	V_d (m s^{-1})		
		First-order reaction model (Rossman, 2006)	Present approximate solution	Biswas et al.'s approximate solution (1993)
RO	8.10×10^{-8}	4.66×10^{-7}	4.50×10^{-7}	4.20×10^{-7}
CON	1.09×10^{-7}	6.73×10^{-7}	6.52×10^{-7}	6.43×10^{-7}
O$_3$	5.56×10^{-7}	1.30×10^{-6}	1.33×10^{-6}	1.53×10^{-6}

the temperature is decreased by the temperature reduction factor (0.85) after 8100 calculations. The annealing process will be terminated if the absolute differences between two successive objective function values are all less than 10^{-10} within 20 iterations or the number of evaluations is greater than 10^7. The SA has been successfully applied in forecasting THM Species (Lin and Yeh, 2005), parameter estimations (e.g., Yeh and Chen, 2007; Yeh et al., 2007a), and source identifications (e.g., Lin and Yeh, 2007; Yeh et al., 2007b).

As suggested by Rossman (2006), a first-order reaction model for describing the first-order decay of chlorine in bulk flow and at the pipe wall was expressed as

$$\frac{\partial c}{\partial t} = -\left(k + \frac{V_d}{r_h}\right)c \qquad (21)$$

where r_h is hydraulic radius of pipe. Table 2 lists the V_d's estimated by the present approximate solution, the first-order reaction model (Rossman, 2006), and Biswas et al.'s approximate solution (1993) for three sorts of lab-tested water. The table shows that the values of V_d estimated by these three models are close for the same lab-tested water. Note that the first-order reaction model neglects the radial diffusion and thus the estimated V_d slightly differs from those given by the other two solutions. Fig. 3 shows the experiment-observed data (Rossman, 2006) and the simulated results by the present approximate solution and Biswas et al.'s approximate solution (1993). The solid line represents the result of the present approximate solution and the dashed line represents the result of Biswas et al.'s approximate solution (1993). The symbols of circle, rhombus, and triangle displayed in Fig. 3 denote experiment-observed values for lab-tested water treated by reverse osmosis, conventional treatment, and ozonation, respectively. This figure indicates the simulated results of the present approximate solution are in good agreement with experiment-observed values from Rossman (2006). In contrast, the simulated results of Biswas et al.'s approximate solution (1993) are discordant in the case of the lab-tested water treated by ozonation with greater V_d value. This problem may be attributed to the fact that the chlorine concentration is inversely proportional to the quadratic of wall decay constant in Biswas et al.'s approximate solution as expressed in Eqs. (13) and (14). Chlorine concentration is considered to decay exponentially with increasing retention time as indicted in Eq. (21) and thus the chlorine concentration is inversely proportional to the exponent of k and V_d. The present approximate solution expressed as Eq. (20) conforms
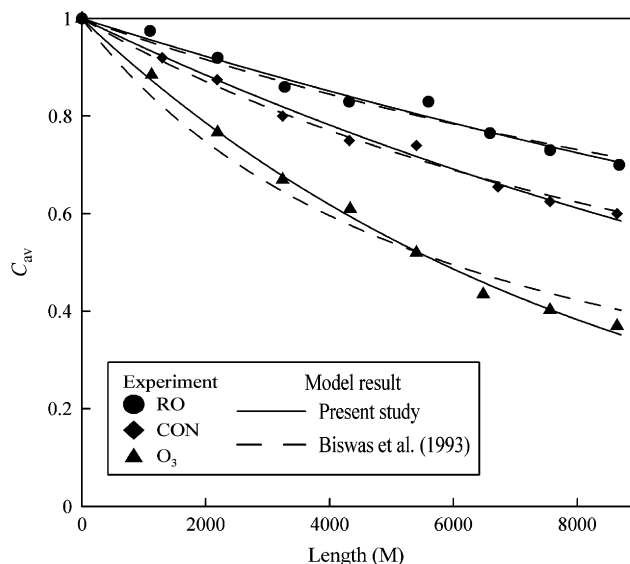

Fig. 3 – The experimental observation (Rossman, 2006) and simulated results of the present approximate solution and Biswas et al.'s approximate solution for three sorts of lab-tested water.

to the form of the first-order decay reaction. This may be the reason why the simulated results of the present approximate solution are better than those of Biswas et al.'s approximate solution (1993) when V_d is large.

3.2.2. Case 2

In Case 2, the present approximate solution is employed to determine the V_d in a field test conducted by the South Central Connecticut Regional Water Authority (Clark et al., 1991). This network in New Haven, Connecticut, has been used many times in the past to test water quality models. The network shown in Fig. 4 is composed of eight main branch pipes. Seven sampling sites including the sites at the treatment plant and storage tank were established. The sampling results of chlorine concentration at the inlet and outlet points of these pipe segments are presented in the second and third columns of Table 3 (Biswas et al., 1993). The geometrical and flow parameter including pipe length, pipe radius, flow velocity (Biswas et al., 1993) and diffusion coefficients for all the pipes are listed in Table 4. The diffusion coefficients were determined by the eddy diffusivity given by Edwards et al., 1979. In addition, the chlorine bulk decay constant, k, was 6.4×10^{-6} (s^{-1}) (Biswas et al., 1993) obtained
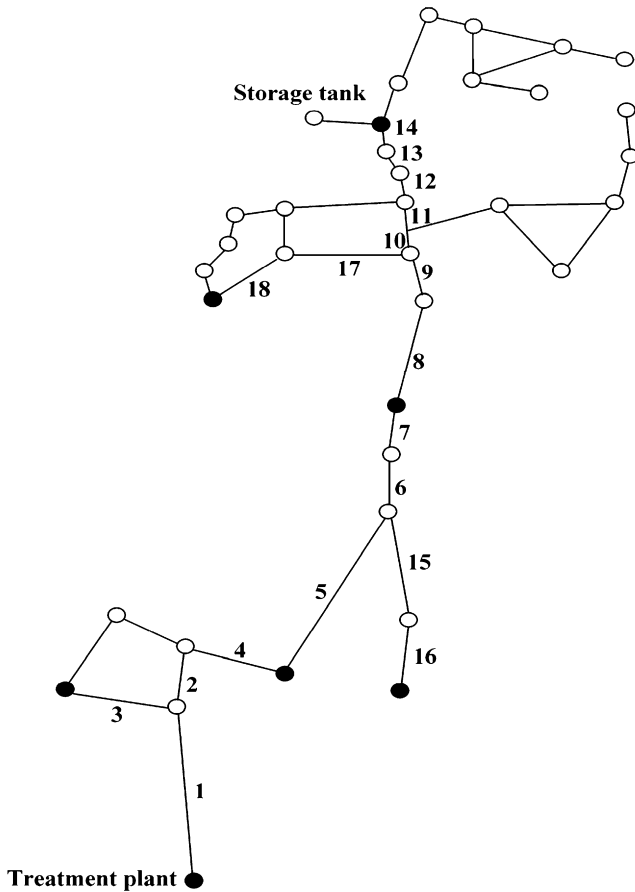
Fig. 4 – Water network at New Haven, Connecticut (Clark et al., 1991). Open circles represent pipe nodes, solid circles represent chlorine measurement locations, and numbers represent pipe numbers.

Table 3 – Chlorine concentrations at the inlet and outlet of various segments

Pipe in segment	Chlorine concentration at segment			
	C_{in} (Biswas et al., 1993)	C_{out} (Biswas et al., 1993)	$C_{out}/$ C_{in}	C_{av}
1,3	1.08	1.00	0.926	0.926
5, 6, 7	1.00	0.98	0.980	0.975
5, 15, 16	1.00	0.32	0.320	0.319
5–14	1.00	0.94	0.940	0.940
8, 9, 17, 18	0.98	0.16	0.163	0.161
8–14	0.98	0.94	0.959	0.964

by bench kinetic tests performed with the water sample taken at the inlet to the network.

In this network (Fig. 4), those pipes numbered 3, 16 and 18 are dead-end pipes while the other numbered pipes are main branch and chlorine concentrations were measured at the nodes denoted as solid circles. The present approximate solution expressed in Eq. (20) is used to determine the wall surface reaction constant, V_d, in this network. The average

value of V_d for the main pipes such as 5–14 in this network can be determined first. Assume that the wall surface reaction constant for the main pipes are all the same because those pipes were made by the same material. Based on Eq. (20), the dimensionless average concentrations at $X = 1$, the outlet of pipe 5, can be expressed as

$$C_{av}^5 = \exp\left[-\left(A_1^5 + \frac{4A_0^5 A_2^5}{2 + A_2^7}\right)\right] \qquad (22)$$

The superscript in each variable represents the pipe number. The dimensionless average concentrations at the outlet of other main pipes can be expressed in a similar manner. The chlorine concentrations are only measured at the inlet and outlet nodes of the segment and a segment usually contains several pipes. The C_{av} is the dimensionless concentration which is defined as the concentration at the pipe outlet divided by that at the pipe inlet. The outlet concentration of a pipe is in fact the inlet concentration of the next pipe. Thus, the dimensionless concentration C_{av} at the outlet of a segment is equal to the product of C_{av} of each pipe within the segment. The dimensionless concentration at the outlet of pipe 14 in the segment containing pipes 5–14 can be written as

$$\prod_{i=5}^{14} C_{av}^i = C_{out}^{14}/C_{in}^5 \qquad (23)$$

Furthermore, Eq. (23) can be simplified and expressed in term of A_2 as

$$\sum_{i=5}^{14} \frac{4A_0^i A_2^i}{2 + A_2^i} = -\left[\ln(C_{out}^{11}/C_{in}^7) + \sum_{i=5}^{14} A_1^i\right] \qquad (24)$$

where A_0 and A_1 are known dimensionless parameters and A_2 is a function of V_d. Note that V_d equals $A_2 D_r/r_0$ and is the only unknown in Eq. (24). Solving Eq. (24) by Newton's method, the average value of V_d for the main branches from pipe 5 to pipe 14 is obtained as 3.47×10^{-7} (m s^{-1}). This value presents the average wall surface reaction constant in the main branch. The same approach and the main branch V_d are then employed to further evaluate the V_d for the dead-end pipes 3, 16, and 18 as shown in Fig. 4. The estimated results for the V_d's for the numbered pipes in the network fall between 3.47×10^{-7} and 1.01×10^{-5} (m s^{-1}) and are listed in the last column of Table 4. Note that the value of V_d ranges from 0 to 7.06×10^{-5} (m s^{-1}) reported from field and experimental studies (Biswas et al., 1993; Rossman et al., 1994; Vasconcelos et al., 1997; Ozdemir and Ger, 1998; Munavalli and Kumar, 2006; Rossman, 2006). With the known geometrical and flow parameters and the estimated values of V_d, the dimensionless concentration C_{av} for all the segments in this network predicted by the analytical solution of Eq. (9) are listed in the fifth column of Table 3.

The sampled concentrations in the inlet and outlet of segments in the network are listed in the second and third columns of Table 3, respectively. In addition, the dimensionless sampled concentration at each segment is listed in the fourth column. The segments of pipes 5–7 and 8–14 consist of the main branch. Table 3 lists the C_{av} predicted based on the analytical solution and the measured concentration given in Biswas et al. (1993) at some inlets and outlets of the pipe

Table 4 – Parameters for different pipes in the network

Pipe	Length (m)	Radius (m)	Flow velocity (m s^{-1})	Diffusion coefficient (m^2 s^{-1})	V_d (m s^{-1})
1	731.5	0.152	0.546	1.02×10^{-3}	3.47×10^{-7}
3	396.2	0.102	0.195	2.45×10^{-4}	1.24×10^{-6}
5	822.9	0.152	0.512	9.60×10^{-4}	3.47×10^{-7}
6	121.9	0.152	0.494	9.26×10^{-4}	3.47×10^{-7}
7	213.4	0.152	0.485	9.09×10^{-4}	3.47×10^{-7}
8	579.1	0.152	0.457	8.56×10^{-4}	3.47×10^{-7}
9	182.9	0.152	0.445	8.34×10^{-4}	3.47×10^{-7}
10	121.9	0.152	0.372	6.97×10^{-4}	3.47×10^{-7}
11	91.4	0.152	0.329	6.17×10^{-4}	3.47×10^{-7}
12	76.2	0.152	0.338	6.33×10^{-4}	3.47×10^{-7}
13	182.9	0.152	0.329	6.17×10^{-4}	3.47×10^{-7}
14	91.4	0.152	0.323	6.05×10^{-4}	3.47×10^{-7}
15	365.8	0.152	0.014	2.62×10^{-5}	3.47×10^{-7}
16	304.8	0.102	0.014	1.76×10^{-5}	1.64×10^{-6}
17	457.2	0.102	0.168	2.11×10^{-4}	3.47×10^{-7}
18	426.7	0.102	0.049	6.16×10^{-5}	1.01×10^{-5}

segments. Table 3 indicates that the predicted C_{av} for the segments containing dead-end pipe agrees with the dimensionless measured concentration (C_{out}/C_{in}) for the same segment. This demonstrates that the present approximate solution can be applied to determine V_d for the field application problem. Table 4 indicates that the V_d's in the dead-end pipes 3, 16, and 18 are much greater than those in the main branch pipes. High value of V_d denotes that wall decay is significant. Biswas et al. (1993) also mentioned that significant biofilm growth occurs in the dead-end pipe where the flow velocity is relatively low if compared with that in main branch pipe. Low water flow velocity causes more retention time in the pipe, and consequently, yields lower chlorine concentration due to the bulk decay reaction. Once the chlorine concentration is lowered, the microorganisms formed as biofilm on the pipe wall are then increased. Consequently, the high values of pipe wall surface reaction result in large values of V_d for the dead-end pipes 3, 16, and 18 as demonstrated in the last column of Table 4.

4. Concluding remarks

An analytical solution for predicting the chlorine decay in the bulk water and at the pipe wall was presented in Biswas et al. (1993) and developed based on the 2-D steady-state chlorine transport with the first-order decay kinetics. This study develops a new approximate solution for describing the average chlorine concentration in the pipe by mainly neglecting the high order terms in the analytical solution (Biswas et al., 1993) and Bessel functions. The present approximate solution is expressed as an exponential form and in terms of three non-dimensional parameters, which physically represent the mechanisms of radial diffusion, first-order chlorine bulk decay, and chlorine wall decay. Generally, this approximate solution provides a better prediction for a wide range of the parameters except when the dimensionless wall decay rate is greater than 0.1. In short, this approximate

solution has been shown to have merits of easy evaluation and good accuracy if compared with Biswas et al.'s approximate solution (1993).

This approximate solution can be used either to predict the chlorine decay in pipes or to determine the wall decay parameter if coupled with an optimization algorithm such as SA. Two cases are chosen to demonstrate the application of the present approximate solution. In the first case, the approximate solution coupled with the algorithm of SA is used to determine the wall surface reaction constants for water treated by the methods of reverse osmosis, conventional treatment, and ozonation held at US EPA's Test and Evaluation Facility in Cincinnati, Ohio (Rossman, 2006). The simulated concentrations obtained by the present approximate solution are in good agreement with the experiment-observed solution for labtested water applied by those three treatments.

In the second case, the present approximate solution is also used to determine the wall surface reaction constant of the dead-end pipes in a field test conducted by the South Central Connecticut Regional Water Authority (Clark et al., 1991). The high values of wall surface reaction constant in the dead-end pipes determined by the present approximate solution may indicate the growth of biofilm on the wall pipe and thus lower the chlorine concentration.

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