A Two-State Random Walk Approach for Modeling Chlorine Decay in Water Distribution Network

Y. M. Mahrous, Abdullah S. Al-Ghamdi, A. M. M. Elfeki

Abstract-- Chlorination is one of the frequently used water disinfection methods in water distribution system. It has been successfully used to inactivate harmful micro-organisms and prevent the regrowth or recontamination of pathogens that might be present. However, maintaining residual chlorine besides keeping it below a certain level is essential because of concerns about formation of carcinogenic disinfection by-products within the distribution system. The stochastic two-state random walk model is employed to solve the advection-reaction transport equation and predicts how the concentration of dissolved chlorine varies in time and space in a water distribution network. Linear non-equilibrium particle transfer from water bulk phase (State 1) to pipe wall phase (State 2) is handled using a two-state Markov-chain process with absorbing state. The model was successful when applied to a single pipe. In the current study, New Haven’s network at Connecticut has been utilized for testing of the model for a complete network. The model shows a good agreement when compared with sampling results available in the literature and other models. The merit of using the two-state random walk technique in a Monte Carlo framework is the ability to estimate the uncertainty in the chlorine concentration along the pipe segments since the variability and fluctuation in the concentration is relatively high in water distribution network.

Index Term-- chlorine decay, Markov-chain, Random walk, pipes, stochastic method, Transport equation, and Water distribution system.

1. INTRODUCTION

As treated water discharges into water distribution system, it is most likely to get a regrowth or recontamination of pathogens. Factors such as flow velocity, temperature, type of treatment and the material of the pipe can highly affect the level of contamination. Even though an optimization between these factors can minimize the contamination to certain level, disinfection is the most crucial stage that should be applied to minimize the risk of contamination to an acceptable level. Despite the fact that free chlorine is decayed in the water bulk and on the inner wall of the pipe, chlorination is considered to be the most popular disinfection method used in water distribution systems. This is due to its comparatively low price, effectiveness in killing micro-organisms and chemical stability in water [1, 2].

As chlorine transported by the flow, it get consumed in both water bulk and on wall of the pipe. The bulk chlorine decay is defined as a chlorine reaction with dissolved and suspended matter which is mostly natural organic matter present in water, thus the reaction of chlorine with compound attached or derived from pipe material is insignificant. Inorganic compounds such as ammonia can also react with chlorine [3]. The biofilm covering the pipe wall, consists of microorganisms like bacteria, fungi, algae and their metabolites, is the second factor that contributes in the chlorine consumption. According to Lechevalier et al. [4], this biomass can easily grow in temperature as low as 6 C. but, the deposits from the bulk flow can impede the contact of chlorine with the growing biomass [5].

Maintaining residual chlorine is essential to inactivate harmful micro-organisms that might be present. But, chlorine should be kept below a certain level because of concerns about formation of carcinogenic disinfection by-products within the distribution systems. Therefore, monitoring data for chlorine concentration along the water distribution systems is considered to be the most important action that the water suppliers should satisfy. But, beside the high cost, it is impossible to have a widespread monitoring chlorine concentration data in a reasonable time for even a medium-sized city.

Mathematical modeling of water-quality behavior in distribution systems can be the best alternative option for mentoring. This option, in several ways, reduced the cost of predicting the spatial and temporal variation of a number of water quality constituents including chlorine [6]. Mathematical modeling has offered several advantages in the simulation of chlorine throughout the water distribution system. On the other hand, in most cases, it is difficult to predict chlorine decay in extensive and complex distribution systems. That is due to the reaction with the compounds present in bulk water, which remains unknown in most cases, and with the biofilm on the pipe wall or pipe material [7] beside the complexity of the system itself. Musz et al. [8] examined three of the most popular computer models in water quality modeling. They are input-output model I/O, developed by Zierolf M L et. al [9], inverse chlorine decay model, developed by Islam et al [10], and the forward simulation model [11]. Musz et al. [8] concluded that these models have disadvantages which may prevent a proper assessment of water quality in the whole water distribution system, limiting their usage only to small networks as well as simulating changes in fixed hydraulic conditions [8].

In general, to simulate the decay of chlorine concentration throughout the water distribution system, mathematical models are mostly used with assumptions of first-order decay, second order decay, power-law decay (nth order) and exponential decay or reacting balance equation like Liou and Kroon [12], Clark et al. [13, 14, 15], Rossman et al. [16], Clark et al. [17], Rossman L A, and Boulos [18], Islam...
et al. [10], Clark and Sivaganesan [19], Ucak and Ozdemir [20], Leeuwen et al. [21].

Rossman, Clark and Grayman, developed a mass-transfer-based water quality model that became the most widely used model. While dissolved chlorine moves with flow, a portion of it can transported to the pipe wall and react with the corroded material or with the biofilm attached to the pipe wall [6, 16]. For first-order kinetics, the rate of a pipe wall reaction can be expressed as:

$$\frac{dC}{dt} = \frac{4k_w k_f C}{D(k_w + k_f)}$$  \hspace{1cm} (1)

Time-driven method, presented by Liou and Kroon [12] and installed in EPANET 2, is a Lagrangian based approach method which can tracks the chlorine concentration and size of a series of non-overlapping segments of water that fill each link in the water distribution network. As time go on, the size of the first upstream segment in a link increases as water enters the link. Meanwhile, an equal loss in size of the last downstream segment occurs as water leaves the link. The in between segments remain unchanged with equal size and move downstream. This repeated sequence of steps gets change to adapt the new condition whenever the hydraulic condition changes. The network is re-segmented to reflect changes in pipe travel times and mass is re-assign from the old segmentation to the new one. This updating process happens to the inter network at fixed time step [12]. The determination of chlorine decay along the pipe, using Time Driven method, in EPANET software as presented by Rossman [22]:

$$C_t = C_{i-1} - \left( k_b + \left[ \frac{4 \cdot k_w \cdot k_f}{D(k_w + k_f)} \right] C_{i-1} \cdot (t-t_{i-1}) \right)$$  \hspace{1cm} (2)

Time-driven method is used by Ozdemir and Ucak as an approach to develop a computer program DYNAQ to model chlorine in distribution networks. The program uses a simplified expression of a two-dimensional (2D) chloride transport and decay equation within a single pipe that includes the bulk-flow reaction, radial diffusion, and a subsequent pipe-wall reaction of chlorine [20].

An analytical solution of a two-dimensional (2-D) steady-state model for the chlorine transport equation under turbulent flow was driven by Biswas et al. [23]. Under a condition of relatively small wall decay coefficient, this radial diffusion model described chlorine decay in a turbulent flow regime with good accuracy [24]. By neglecting the high order terms in the analytical solution of Biswas et al. [23], Hund-Der Yeh et al. [24] provide more accurate approximate solution of the 2-D steady-state chlorine transport equation under the turbulent condition when dealing with higher values of wall decay coefficient. Moreover, to determine the wall decay parameter, they developed a methodology to combine optimization algorithm with this new approximate solution [24].

The field of water quality modeling is relatively young field and more developments are needed for better assessment and much accurate simulation results in the environmental engineering practice.

In this paper, the method of two-state random walk method (RWM) which has been developed by Mahrous et al. [25] is applied for New Haven’s network in Connecticut to simulate the decay of chlorine concentration within the flow regime throughout the network. The aim beyond this method is to solve the advection reaction transport equation based on a stochastic approach rather than the deterministic one, which is called as a discrete particle-tracking model. It treats the transport of chlorine mass as a large number of representative particles, and moves each particle through the flow of water using the velocity field obtained from the solution of the flow equation to simulate advection. This lagrangian approach is practically free of numerical dispersion and artificial oscillation because it solves the transport equation indirectly. The absence of numerical dispersion has turned the method into a valuable option for modeling complex, high-resolution transport problems, inverse modeling, and uncertainty assessment of contaminant transport [26]. Moreover, RWM can be implanted over any type of flow model because of the simplicity of its explicit equations [27]. While the previous models present chlorine concentration as an average deterministic value along the water network, RWM give more step ahead. The decay of chlorine in water distribution system can conceptually better be modelled in a stochastic manner rather than in a deterministic one since the experimental evidence shows that chlorine concentration is fluctuating and decaying randomly in the pipe system. Therefore, a stochastic technique is used in the modeling of the underlying processes. The stochastic technique has some merits over the deterministic one:

(1) It can account for the variability and uncertainty that is inherent in the chlorine transport process in the water distribution system, and

(2) The stochastic technique that is going to be used is working with particle model that makes studying the underlying process at particle level more conceptual.

The model algorithm of this lagrangian based approach, for application of chlorine decay in a single pipe, is presented in Mahrous et al. [25]. For the sake of completeness, the algorithm is explained in the following paragraphs.

II. METHODOLOGY

In the random walk method, the transported quantity of chlorine mass is discretized by a set of moving particles say N. Each particle is carrying a part of the mass of the chlorine that is equal to the total chlorine mass at the source divided by the number of particles. The particles are moving in the pipe under the influence of advection by the flow. The mass reduction to each particle of the solute is estimated according to the mass decay process. The concentration is estimated by counting the number of particles within the cell. In our case, the method will allow us to track changes in chlorine concentration depending on time and space throughout the water distribution network. A two-state
random walk defined as a particular particle can be in one of two states for certain period of time. Each particle has the same transition probability to change from one state to another. These two states are the transient state, representing that the particle is in the water bulk phase (State 1), and the absorbing state (State 2), representing that the particle is absorbed on the pipe wall. The movement of the chlorine particles between the two states is a linear non-equilibrium process from water bulk to pipe wall states. The process of state-changes is handled using the concept of stochastic analogue of two-state Markov-chain process with absorbing state [28]. Unlike the regular Markov chain, for which the transition matrix \( \mathbf{p} \) is primitive (\( p_{ii} < 1 \)) and the chain never get stuck in a particular state, Markov-chain with absorbing state must have at least one absorbing state say \( i \) with \( p_{ii} = 1 \) and \( p_{ij} = 0 \) for all \( j \neq i \). The transition is always from non-absorbing states to absorbing states. Therefore, a two-state Markov-chain transition matrix may have the following canonical form:

\[
\mathbf{p} = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix}
\]

Where \( \mathbf{p} \) is the transition matrix, \( p_{11} \) is the probability of having a particle stay in transient state TR and it is determined by subtracting \( p_{12} \) from one.; \( p_{12} \) is the probability of having a particle transfer from TR to absorbing state ABS; \( p_{21} \) is the probability of having a particle transfer from ABS to TR; and \( p_{22} \) is the probability of having a particle stay in ABS. In our case, the sum of \( p_{11} \) and \( p_{12} \) is equal to 1, \( p_{21} = 0 \) and \( p_{22} = 1 \). Fig. 1 shows the conceptual model of particle transfer between State 1 and 2 [25].

Fig. 1. conceptual model of particle transfer between water bulk and pipe wall [25].

The random walk method is offering a good alternative to the classical solution method to the transport equation in the field of water quality modeling. It has been demonstrated by many authors to be more computationally efficient than the traditional numerical methods such as finite difference, finite element and characteristic methods when solving the traditional second-order advection-dispersion-reaction equation. Unlike many approaches, RWM does not modify the under solving partial differential equation or the nature of the physical problem, and convergence analysis are not needed within this approach. Most importantly, besides solving the PDE, the approach can also improve our understanding about the physical process by providing a description of the dynamics underlying the target PDE [27].

As presented in Mahrous et al. [25], the methodology and algorithm use the classical one dimension (1-D) advection-reaction equation. The equation is describing the decay of free chlorine concentration in the water flowing though pipe with neglecting the axial dispersion and diffusivity of chlorine solution and it is written as:

\[
\frac{\partial c_i}{\partial t} + u_i \frac{\partial c_i}{\partial X} \pm R(c_i) = 0 \quad (4)
\]

Where, \( c_i \) is the concentration of constituent in pipe \( i \) as a function of distance \( x \) and time \( t \); \( u_i \) is the mean flow velocity in pipe \( i \); and \( R(c_i) \) is the reaction rate expression, equals zero for conservative constituent [30].

A random walk method is, together with two-state Markov chain theory is used to solve Eq. (4). The following lines explain the methodology adopted and the formulation of the algorithm to be implemented in a spreadsheet.

A special case of random-walk scheme is given in Eq. (5) [25, 26].

\[
X(t+\Delta t) = X(t) + u(X(t)) \Delta t \quad (5)
\]

Where; \( X(t+\Delta t) \) is the tagged particle position at time \( t+\Delta t \); \( X(t) \) is the particle position at time \( t \); \( u(X(t)) \) is the velocity of the water at position \( X(t) \) at time \( t \).

The longitudinal dispersion is neglected due to its insignificant effects in transport mechanism under most operating condition. That means there is no intermixing of mass between adjacent parcels (segments) of water traveling down a pipe [3].

Linear non-equilibrium particle transfer from state 1 (water bulk) and State 2 (pipe wall) is to be handled. Consider a particle between two states: the aqueous State 1 and the absorbing State 2. At any instant of time, the particle can be transferred from State 1 to State 2. This can be handled by stochastic analogue of the two-state Markov-chain with absorbing state. This chain has state space \( \{1, 2\} \). The rates at which the particle leaves State 1 to State 2 are \( k_i \) (mass transfer coefficient).

Since chlorine is not conservative, the mass of its particles can be represented by the first order decay function of the form [25, 29]:

\[
M_p(t) = M_p(0)e^{-k_i t} \quad (6)
\]

Where \( M_p(t) \) is the mass of chlorine particle at time \( t \) (M); \( M_p(0) \) is the mass of chlorine particle at time zero (M); \( k_i \) is the bulk decay constant.

The probability of having a particle transferred from State 1(bulk phase) to State 2 (pipe wall phase) is represented by the modified equation [25]:

\[
p_{12} = \frac{4\lambda_i}{D} \Delta t \quad (7)
\]
Where \( p_{12} \) is the probability at which the chlorine particle will move from State 1, transition state, to State 2, the absorbed state and get decayed. Whenever \( p_{12} \) value is determined, it will be introduced along with \( p_{11}, p_{12} \) and \( p_{22} \) of the Markov chain transition matrix to set a linear non-equilibrium absorption or particle transfer from water bulk (State 1) to pipe wall (State 2) as in Eq. (3).

These four elements in the matrix in Eq. (3) will be introduced into the Markov chain cumulative transition matrix as,

\[
p_t = \begin{bmatrix} p_{11} & p_{11} \cdot p_{12} \\ 0 & 1 \end{bmatrix}
\]

for realization of states in the random walk process. Fig. 2 and 3 are graphically representing the Markov chain cumulative matrix for the two states in RWM process.

![Fig. 2. Graphical representation of Markov chain cumulative transition matrix for State 1 to State 1 or 2 in RWM process.](image)

![Fig. 3. Graphical representation of Markov chain cumulative transition matrix for State 2 to State 1 or 2 in RWM process.](image)

An excel spread sheet is developed to implement the algorithm. The idea is to generate random numbers between 0 and 1 by the built in function, RAND(). In order to realize a state of a particle each time step, a random number is drawn and if the number exists in the range between 0 and \( p_{11} \), it indicates that a particular particle will stay in the bulk flow, other than that it will be transferred to wall state. \( \lambda \) is global wall coefficient:

\[
\lambda = \frac{k_w k_f}{(k_w + k_f)}
\]

where \( k_w \) is the wall decay constant; \( k_f \) is the mass transfer coefficient.

\[
k_f = 0.0149 \frac{d}{D} \left( \frac{\nu}{3} \right)^{1/3} Re^{0.88}
\]

where \( d \) is the molecular diffusivity of the chlorine in water (1.21×10\(^{-9}\) m\(^2\)/s); \( D \) is the diameter of the pipe; \( \nu \) is the kinematic viscosity of the water (10\(^{-6}\) m\(^2\)/s); \( Re \) is the Reynolds number of the flow:

\[
Re = \frac{4Q}{\pi D \nu}
\]

Where \( Q \) is the flow of water in the pipe.

Most of the models in water quality practice are using the deterministic approach to determine the decay of chlorine throughout the network. In reality, taking lab test examination to measure the chlorine concentration for several sampling at the same moment will not give the same result when analyzing. A slight difference between the results would exist because of several affecting factors. One of them is the stochastic nature of the process. RWM is following the same principle. Each simulation result will be considered as one realization and it is slightly different from the next realization depending on the resolution of the chlorine dose applied. If the resolution is high, (large number of particles per chlorine dose) the differences between each realization is low indicating an inverse relationship. Therefore, in the current simulation, many realizations are generated and the average behavior over those realizations is estimated and the corresponding variability between the realizations is estimated using Monte Carlo method [31, 32, 33]. The ensemble mean concentration, \( <C(x)> \), is estimated by

\[
<C(x)> = \frac{1}{n} \sum_{i=1}^{n} C_i(x)
\]

Where, \( n \) is the number of realizations and \( C_i(x) \) is the concentration as a function of \( x \) along the pipe length at realization # \( i \).

The concentration variance, \( \sigma^2_C(x) \), as a function of \( x \) along the pipe length is given by,

\[
\sigma^2_C(x) = \frac{1}{n} \sum_{i=1}^{n} [C_i(x) - <C(x)>]^2
\]

The coefficient of variation is given by,

\[
CV(x) = \frac{\sigma_C(x)}{<C(x)>}
\]
Where CV(x) is the coefficient of variation of the concentration as a function of x along the pipe length; $\sigma_C(x)$ is the standard deviation over the Monte Carlo realizations.

III. CASE STUDY AND DISCUSSION: EXPERIMENTAL RESEARCH

The presented two-state random walk method is employed to simulate the chlorine concentration in a network located in New Haven, Connecticut shown in Fig. 4. The network consists of eight main branch pipes. Seven sampling sites, in red circles, including the sites at the treatment plant and storage tank were established. Pipes 3, 16, 18 are dead-end pipes and the other pipes are main branch. The chlorine concentration were measured at the node denoted as a red circles. The approximate solution, given by Hund-Der Yeh et al. [24] is used to determine the $k_w$ in a field test conducted by the South Central Connecticut Regional Water Authority [11]. The diffusion coefficients (d) were determined by the eddy diffusivity given by Edwards et al. [34], and the chlorine bulk decay coefficient $k_b$ (6.4x10^{-6} s^{-1}) was obtained by bench kinetic tests performed with the water sample taken at the inlet to the network [23]. The characteristics of the network including pipe length, pipe radius, flow velocity along with the diffusion coefficient (d) and wall decay coefficient $k_w$ are presented in Table 1[23, 24].

![Fig. 4. Water network at New Haven, Connecticut [23, 13, 24]. Solid black circles represent pipe nodes, solid red circles represent chlorine measurement locations, and numbers represent pipe numbers.](Image 307x130 to 538x288)

The chlorine concentration decay is simulated throughout the network by employing the present method in seven segments. Each segment consists of more than one pipe. As shown in Figures 5a-10a, the outlet of some segments is the inlet of others. An average of ten Monte Carlo realizations is established in between an upper and lower limit with 95% confidence in which the realizations are fluctuating. As seen throughout the figures, the sampling results of Biswas et al. [23], the TDM (EPANET 2) simulated results, and the approximate solution of Hund-Der Yeh et al. [24], fit in between the upper and lower limits and prove a good agreement with the RW simulated results. Figures 5a, 7a, and 9a show relatively dramatic decrease in chlorine concentrations because of high value of wall decay coefficient (Table 1) and relatively low velocity due to the dead-end at the end of the segments. The large value of wall decay coefficient is virtually due to the significant biofilm growth that occurs in the dead-end pipes. Furthermore, the relatively low flow velocity causes higher retention time which consequently resulted in lower chlorine concentration due to the bulk decay reaction [23]. Table 2 presents the chlorine concentrations for the various segments quantitatively. The simulated outlet chlorine concentration with RWM indicate that the method give much better accuracy with higher values of $k_b$ and $k_w$ [25]. Note that as seen in Figures 5a-10a, the boundary limits (upper and lower limits) are increasing as go away from the source point. In another word, there is an increase in the limit of an uncertainty as the concentration of the chlorine goes far from the source. Figures 5b-10b shows the coefficient of variation CV(x) for Figures 5a-10a respectively. It show an increase in the coefficient of variation, CV(x), along the pipe segments as the flow goes far from the source. This is an indication of an increase in the uncertainty as the concentration moves far from the source.

![Fig. 5a. The sampling results of Biswas et al [23], simulated results of Hund-Der Yeh et al approximate solution [24], TDM (EPANET 2) and the average behavior of ten realizations of RWM between inlet and outlet for segment 1, 3.](Image 307x325 to 540x477)

![Fig. 6a. The sampling results Biswas et al [23], simulated results of Hund-Der Yeh et al approximate solution [24], TDM (EPANET 2) and the average behavior of ten realizations of RWM between inlet and outlet for segment 5, 6, 7.](Image 55x220 to 275x476)
Fig. 7a. The sampling results Biswas et al. [23], simulated results of Hund-Der Yeh et al. approximate solution [24], TDM (EPANET 2) and the average behavior of ten realizations of RWM between inlet and outlet for segment 5, 15, 16.

Fig. 8a. The sampling results Biswas et al. [23], simulated results of Hund-Der Yeh et al. approximate solution [24], TDM (EPANET 2) and the average behavior of ten realizations of RWM between inlet and outlet for segment 5-14.

Fig. 9a. The sampling results Biswas et al. [23], simulated results of Hund-Der Yeh et al. approximate solution [24], TDM (EPANET 2) and the average behavior of ten realizations of RWM between inlet and outlet for segment 8, 9, 17, 18.

Fig. 10a. The sampling results Biswas et al. [23], simulated results of Hund-Der Yeh et al. approximate solution [24], TDM (EPANET 2) and the average behavior of ten realizations of RWM between inlet and outlet for segment 8-14.
Fig. 8b. Coefficient of variation CV(x) for segment 5-14 (Fig. 8a).

Fig. 9b. Coefficient of variation CV(x) for segment 8, 9, 17, 18 (Fig. 9a).

Fig. 10b. Coefficient of variation CV(x) for segment 8-14 (Fig. 10a).

Table I

<table>
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<tr>
<th>pipe</th>
<th>Length (m)</th>
<th>Radius (m)</th>
<th>Flow velocity (ms⁻¹)</th>
<th>d (m²s⁻¹)</th>
<th>kₚ (ms⁻¹)</th>
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Table II
Chlorine concentrations at the inlet and outlet of various segments [24].

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<td>0.98</td>
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IV. CONCLUSION
This paper has employed a stochastic lagrangian approach known as a two-state random-walk method to solve the advection-reaction transport equation and numerically simulate the chlorine decay. This study is an extension for the study conducted by Mahrous et al. [25] for a single pipe. In this paper, the approach is implemented for a network to verify its ability to deal with much more complicated condition. More studies can be conducted for much more complicated network or whole system. New Haven’s network at Connecticut is utilized for this purpose. This network consists of eight main branch pipes and seven sampling sites including the sites at the treatment plant and storage tank. The scheme of the method, presented by Kitanidis [28] has been modified to deal with the chlorine decay in pipe flow network. Linear non-equilibrium particle transfer from water bulk to pipe wall state is handled using the stochastic analogue of two-state Markov-chain process with absorbing state [25]. The method showed high accuracy when dealing with large values of $k_0$ and $k_p$. The proposed model in the current study is verified with a good agreement by the sampling results of Biswas et al. [23], the TDM (EPANET 2) simulated results, and the approximate solution of Hund-Der yeh et al. [24]. The merit of using the two-state random walk technique in a Monte Carlo framework is the ability to estimate the uncertainty in the chlorine concentration along the pipe segments since the variability and fluctuation in the concentration is relatively high in water distribution network.

V. ACKNOWLEDGMENT
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VI. REFERENCES
APPENDIX I. NOTATION

The following symbols are used in this paper:

ABS: absorbing state;

\( C(x,t) \): point value of chlorine concentration in any location of the pipe (M/L^3);

D: diameter of the pipe (L);

d: molecular diffusivity of the chlorine in water (L^2/T);

\( k_a \): bulk decay constant (1/T);

\( k_c \): mass transfer coefficient (L/T);

\( k_w \): wall decay constant (L/T);

\( M_p(0) \): mass of chlorine particle at time zero (M) (M);

\( M_p(t) \): mass of chlorine particle at time t (M);

\( p \): Markov chain transition matrix;

\( p_c \): Markov chain cumulative transition Matrix;

Q: flow rate of water though pipe (L^3/T);

Re: Reynolds number;

RWM: random-walk-method;

TR: transition state;

t: time (T);

TDM: time-driven-method;

u: mean flow velocity of water (L/T);

\( \nu \): kinematic viscosity (L^2/T);

X(t): position of the particle at time t (L);

\( \lambda \): global wall coefficient (L/T);

\( CV(x) \): coefficient of variation;

\( \langle C(x) \rangle \): ensemble mean concentration (M/L^3);

\( \sigma_C^2 \): concentration variance;

\( \sigma_C \): standard deviation over Monte Carlo realizations;

x: distance along the pipe segment.

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