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DYNAQ: A Chlorine Decay Simulator in Water Supply Networks

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Abstract

Drinking water chlorination is an important issue for public health. Chlorine deficiency may lead to contamination of water whereas an excess amount of chlorine may cause trihalomethanes, which are suspected carcinogens. Therefore, it is very important to use the correct amount of chlorine in drinking water supply networks. Since chlorine is a highly reactive and decaying halogen, estimation of the concentration in drinking water supply networks has been the subject of many research projects. The objective of this paper is to describe a real-time chlorine decay and propagation simulation program developed for drinking water supply networks. The program can be used for other chemicals, biological changes and contaminant propagation in water supply networks. The proposed algorithm is based on a chronological activity list of events occurring in the network in order to enhance the efficient usage of computer storage, computational effectiveness and numerical accuracy. The program can handle dynamic hydraulic simulation and is less sensitive to the layout of the network and to the length of the simulation period than models available so far.

Key Words: Chlorine decay, Water supply networks, Computer modelling

DYNAQ: İçme Suyu Şebekelerinde Klor Kayıp Modeli

Özet

İçme suyu şebekelerinde klorlama halk sağlığı açısından önemlidir. Klorlamanın yeterli yapılmaması durumunda bakteriyolojik kirlenmeye, gereğinden fazlası ise kanserojen bileşiklere; trihalometanların oluşumuna neden olmaktadır. O halde klorun şebeke içinde gerektiği kadar ve yerde kullanılması zorunluluğu vardır. Klor suda reaksiyon gösteren bir halojen olduğu için şebeke içi hesabı oldukça detaylı araştırmalara konu olmuştur. Bu çalışmanın amacı içme suyu şebekelerinde reaktif klorun kayıp ve taşınım simulasyonlarını yapan programı tanıtmaktır. Program şebeke içinde diğer kimyasal, biyolojik değişiklikler ve ani kirlenmeler için de kullanılabilir. Sunulan algoritma bilgisayar kullanımı, hesap kolaylığı ve hassasiyetini sağlamak için şebeke içi değişimleri göz önüne almaktadır. Program zamana bağlı hidrolik çözümleri dikkate alırken daha önce geliştirilen programlara göre şebeke yapısına ve simulasyon süresinin uzunluğuna daha az bağımlıdır.

Anahtar Sözcükler: Klor Sönümü, İçme Suyu Şebekeleri, Bilgisayar Modellemesi.

Introduction

During the past decade, considerable attention has been focused on the development of algorithms for use in modelling water quality in pipe distribution systems. The various algorithms available to date have been based either on the use of steady-state models or on the dynamic approach. The steady-state models determine the spatial distribution of contaminants throughout the piping system under a given set of loading and operational conditions. A set of linear algebraic equations is used to describe concentrations at network nodes. An iterative solution can be used, as explained by Chun et al. (1985) and Wood et al. (1986), or the direct sparse matrix solution of Males et al. (1985) or the explicit graph-theoretical single-step substitution process of Liou and Kroon (1986) or the explicit marching out solution scheme of Clark et al. (1988). The dynamic models on the other hand, simulate the changes in the spatial distribution of contaminant throughout the piping system under a time-dependent customer demand and the other set of factors within the distribution system. The other factors include changes in storage tank levels, valve settings, storage tanks and pumps going on- or off-line, flow reversal in pipes and rapid demand changes (e.g., fire demands). Several numerical approaches have been adopted in the dynamic simulation of the contaminant advection process in a time-driven environment such as the Lagrangian transport model of Liou and Kroon (1986), the marching out solution method of Clark et al. (1988) and Grayman et al. (1988), and the discrete element method of Rossman et al. (1993). These algorithms are based on the assumptions of one-dimensional flow, quasi-steady network hydraulics, instantaneous and complete nodal mixing, ideal plug flow with negligible longitudinal dispersion and single contaminant with one or multiple sources. Contaminating substances are assumed to be either conservative or decaying subject to a simple first-order kinetic characteristic function. A comprehensive review and bibliography of the various approaches can be found in a study by Grayman and Clark (1990-1991).

Network Hydraulics

Distribution networks may be described as being composed of a number of pipe sections of constant diameter that are joined by fittings. The flow in pipes is maintained either by pumping or by the force of gravity. The end of each pipe is called a node. A node may be either a fixed grade or a junction. Junction nodes are points where pipes meet and where flow may be introduced or withdrawn. Fixed-grade nodes are points where a relatively constant pressure is maintained such as a storage tank or a reservoir. In order to obtain the hydraulic data such as velocities in pipes and pressures at nodes of a water distribution network, a solver requires simultaneous solution of the node continuity and pipe discharge equations. Several methods are available to solve these equations, among which Hardy-Cross, Newton Raphson and Linear (Rossman, 1993; Wood, 1986) are the most frequently used. The development of the equations and description of the solution methods are beyond the scope of the present study. KYPIPEF, a universally known, widely used and commercially available hydraulic program, is used to obtain the magnitudes of pipe velocities for each incremental hydraulic time step. These data are then used as an input information for DYNAQ, the dynamic water quality program developed for chlorine decay and transport calculations. In the following section the basics of the hydraulic program KYPIPEF developed at the University of Kentucky are explained.

KYPIPEF: The University of Kentucky Model

This model was developed to analyze the steady-state hydraulics of water distribution networks. The program is capable of handling a large number of storage tanks, pumps and pressure regulating valves. Furthermore, the extended period simulations (EPS) option of the program can handle situations in which water levels in tanks and water usage may vary over the simulation period. The input includes all the data necessary to define the network system characteristics for a steady-state simulation. The output of an EPS includes discharges in pipes, heads at nodes, and water levels in each tank throughout the simulation period. The basis of the program is a direct solution of the basic equations of the pipe system hydraulics using a linearization scheme and sparse matrix methods to handle the non-linear terms in the energy equations (Wood 1986).

DYNAQ: Chlorine Decay and Propagation Model

The chlorine decay and propagation models available to date treat the pipe segments as if they were a chemical reactor. For such a chemical reactor it is

assumed that chlorine enters from one end, decays in water (bulk decay) due to reaction with organisms and is consumed around the pipe wall due to a biofilm attached to the pipe wall and transported to the other end of the pipe by convection. Chlorine may also react with the pipe itself if the pipe consists of iron. The chlorine decay (reaction) and transport mechanism is schematically described in Figure 1.

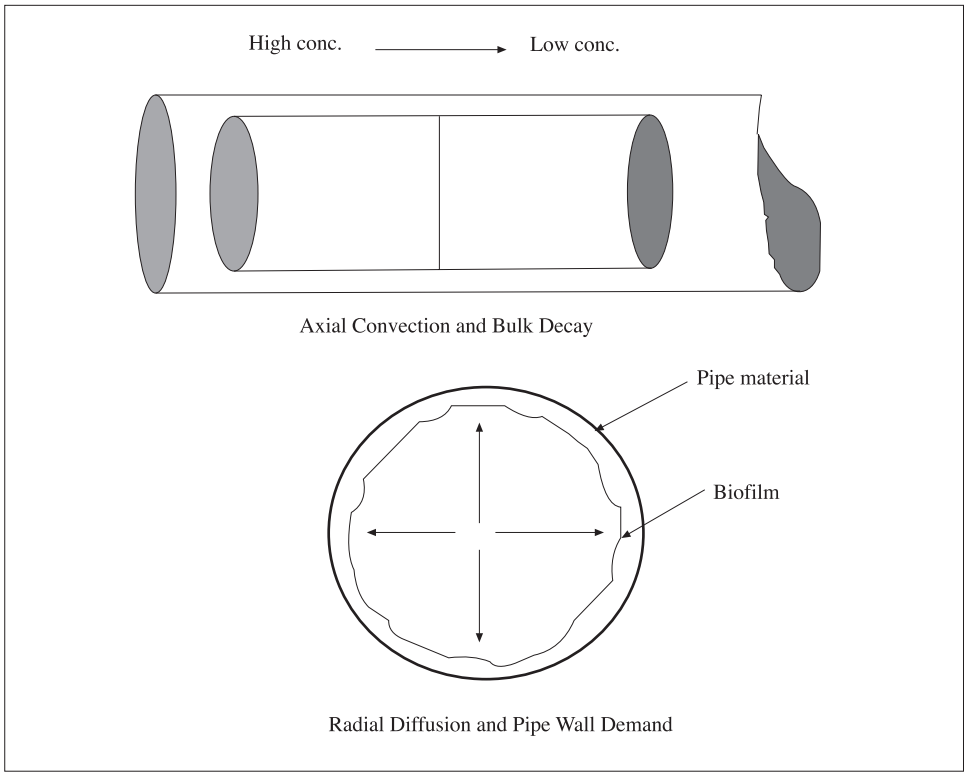

Figure 1. Schematic Description of 2-D Chlorine Transport

In most of the studies to date (Biswas et al., 1993; Rossman et al., 1994; Ozdemir and Ger, 1998), the chlorine decay mechanism has been treated as two-dimensional (2-D). The first dimension is the longitudinal axis of the pipe along which chlorine is transported and decayed (bulk decay). The second dimension is the radial direction along which chlorine is transported because of velocity gradients and diffuses due to the high pipe wall consumption. An analytical solution of 2-D chlorine decay and transport equation was given by Biswas et al. (1993). This study is valid for only fully turbulent flow conditions at which the velocity gradients are not prevalent; i.e., the Reynolds number in the pipe is greater than 30000. On the other hand, considerable chlorine decay occurs for flow in pipes with, Reynolds number of less than 30000 (Ozdemir and Ger, 1998), as shown in Figure 2. Therefore, it is necessary to investigate the chlorine decay and transport mechanism for a Reynolds number less than 30000 for which the flow cannot be said to be fully turbulent. The ordinate axis shows the non-dimensional form of chlorine concentration in a test pipe. The C value was obtained by normalization of the pipe outlet chlorine concentration with respect to the inlet chlorine concentration.

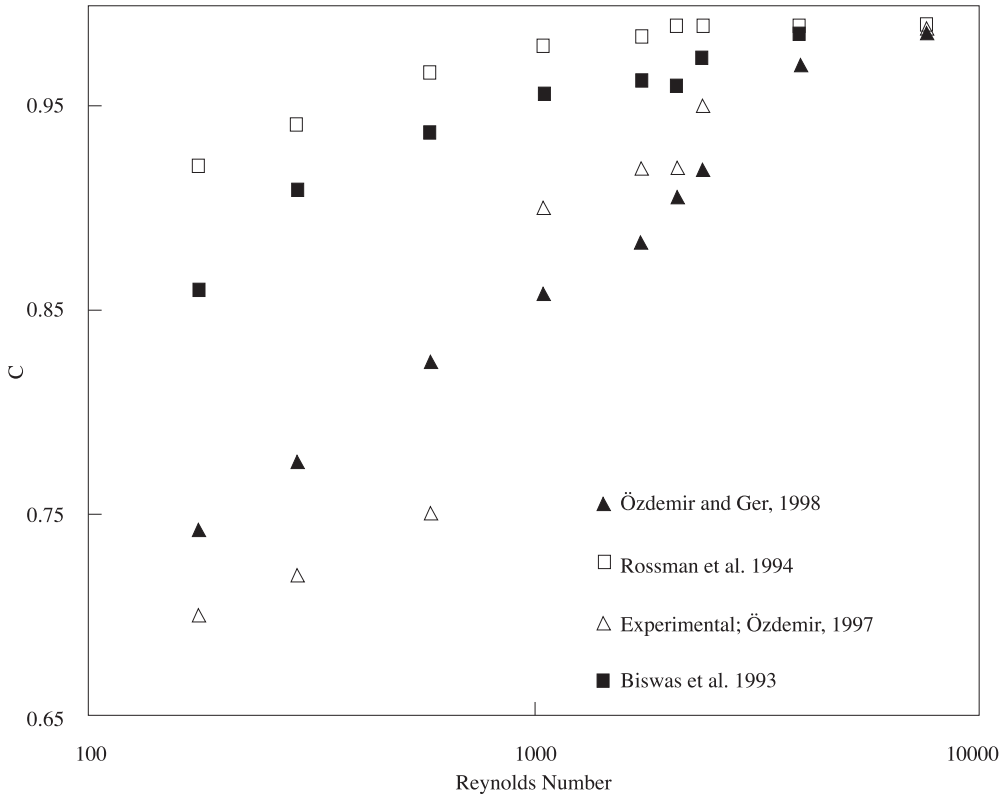

Figure 2. Comparison of Recent Studies for Chlorine Decay in a Single Pipe

Ozdemir and Ger (1998) studied the problem for flows with Reynolds numbers ranging from laminar to turbulent flow conditions. They solved the 2-D chlorine decay and transport equation by numerical methods. However, a 2-D numerical solution of the problem is a complex task to include in a drinking water supply network quality solver. Ozdemir and Ger (1998), therefore, proposed a very convenient single expression to calculate chlorine decay at any distance or time in a single pipe. DYNAQ, the program developed for drinking water supply network quality calculations, uses this expression to calculate chlorine decay at any time and location in the network.

The development of the chlorine decay and transport equations are summarized as follows:

The one-dimensional (1-D) equation of chlorine decay at any time or distance in a pipe is given as (Ozdemir and Ger, 1998)

$$C_{1D} = \frac{C_t}{C_{t-1}} = exp\{-(k + W_d/r_0)\}t \qquad (1)$$

where C_{1D} = non-dimensional 1-D chlorine decay; C_t = chlorine concentration at any time t; C_{t-1} = chlorine concentration at time t-1 (or initial chlorine concentration in the pipe); W_d = pipe wall chlorine demand; k = chlorine decay in water (bulk decay); r_0 pipe radius; and t = travel time of water (convection). The true decay C_T is approximated by the 2-D solution, C_{2D}:

$$C_T \approx C_{2D} \qquad (2)$$

A correction factor F_C is introduced such that it relates C_{1D} and C_{2D} as

$$F_C = \frac{C_{1D} - C_{2D}}{C_{2D}} \qquad (3)$$

In other words, if F_C and C_{1D} are known, without going through the cumbersome 2-D analysis, C_T can be estimated by

$$C_T \approx \frac{C_{1D}}{1 + F_C} \qquad (4)$$

By making the dimensional analysis, the correction factor F_C has been related to some non-dimensional parameters (Ozdemir and Ger, 1998) and given as the expression below:

$$Log(F_C x 100/Z) = -0.9538 Log(Re/1000) - 1 \quad (5)$$

where Z = non-dimensional parameter ($= 2W_d L/\nu$); Re = non-dimensional Reynolds number ($= Ud/\nu$); L = pipe length (L); d = pipe diameter (L); and ν = kinematic viscosity of water (L^2T^{-1}). The parameters k and W_d defined above should be estimated either from experimental studies or from the literature.

Furthermore, the complete mixing of incoming concentrations at a node is an additional assumption to be made in the numerical model for a network of pipes. Assuming instantaneous and perfect mixing at the network nodes, the nodal chlorine concentrations can be obtained from the mass balance principle as

$$C_k = \frac{\sum_{j=1}^{n} Q_j C_j}{\sum_{j=1}^{n} Q_j} \quad (6)$$

where C_k denotes the chlorine concentration at node k; Q_j and C_j are flows and concentrations of pipes leading to node k; and n is the number of pipes leading to node k.

For a variable-level tank, the change in concentration can be determined from the mass conservation relationship as

$$\frac{d(C_r V_r)}{dt} = Q_{in} C_{in} - Q_{out} C_r - k C_r V_r \quad (7)$$

where C_r and V_r are the fully mixed concentration and volume of the tank, respectively; C_{in} is the chlorine concentration of the incoming pipe; C_{out} is the concentration of outflow from the tank; and k is the decay rate for tank volume. Furthermore, full mixing is assumed within the tank; any outflow from the tank is assumed to have the fully mixed concentration of the tank.

The Algorithm and Program Development

It is crucial to know the details of the network layout and hydraulics before taking any step into quality modeling. The velocities in each pipe constituting the network should be known. The program KYPIPEF gives a very efficient and detailed output of the network hydraulics that can directly be used as an input for DYNAQ, the program developed for the simulation of chlorine decay in a network. DYNAQ has three modules to perform the transfer of data, and run the algorithm. A brief explanation of the modules is given below:

READ1 and READ2 Program Modules

The modules are written in Fortran and compiled using the Microsoft Fortran Compiler. The module performs the following tasks in the following order: it reads the hydraulic output of KYPIPEF and stores the network layout. The order of nodes, pipe numbers and associated nodes, number of variable tanks and connecting pipe numbers, diameter and initial level of tanks and user-supplied initial node concentrations in the network are all recorded by these two modules.

MAIN Program

The algorithm of MAIN is a complex one and it works as a scheduler that creates, identifies and arranges activities in the network in chronological order. At this point, it is necessary to define some of the terminology used in the algorithm development.

Definition 1: A hydraulic event is an external phenomenon (external to the quality program DYNAQ) imposed by the hydraulic solution to the quality model that causes change in the magnitude of velocity and/or direction of flow in the pipes.

Definition 2: A sub-hydraulic event is an internal phenomenon occurring in the quality program module MAIN caused by a change of nodal concentration at any node in the network.

Definition 3: A hydraulic time step is the period between any two hydraulic events during which all flow and velocities remain constant. In a quasi-steady (extended period) simulation of a network hydraulics this period is usually one hour, but this can be decreased to any desired duration (e.g., half an hour, 15 minutes, 10 minutes etc.).

Definition 4: A quality time step is a period between any two concentration calculations. There is a preset maximum duration limit for actual quality time step in order not to lose the accuracy of the concentrations. This maximum is set to half an hour if the time used for hydraulic calculation is longer than half an hour. Otherwise this maximum takes the same value as that of the hydraulic time step. The quality time step is not a fixed value throughout the simulation and can vary according to chronological activities that are put in order.

Definition 5: A Chronological Activity List (CAL) is an ordered list of events occurring in the network during a quality time step. The list is updated after each quality time step. The activity list may include the following events: a) further sectioning of a pipe into new segments for displacement of the concentration front; b) attainment of concentration to at least one node in the network; and c) segmentation of new pipes entering the activity list due to concentration change of at least one node.

The algorithm developed to trace concentration fronts along the pipes and nodal mixing is illustrated in Figure 3. At the end of a quality time step, the distance of each front in pipe 1 and pipe 2 from node 1 $U_1\Delta t_1$ and $U_2\Delta t_2$, respectively (Figure 3a). According to the chronological activity list (CAL), the next sub-hydraulic event is a change in the concentration of node 1 in a quality time step smaller than Δt_1 and Δt_2. Given that Δt_1 is the smaller, after Δt_1 the concentration front from pipe 1 and the water ahead of the front in the second pipe is mixed at node 1 as formulated by equation (6). During Δt_1 the front in pipe 2 is moved to a new location with some additional decay. The next step is to make a new CAL such that while pipe 1 is dropped out of the list, pipe 3 is included. Before making any segmentation in pipe 3, Δt_3 (i.e., $\Delta t_2 - \Delta t_1$) and Δt_4 (i.e., L_3/U_3) are compared (Figure 3b). The smaller value becomes the new quality time step. Assuming Δt_3 is less than Δt_4, the next event is decided to be a second change in the concentration of node 1 as formulated by equation (6). In any case if Δt_4 is less than Δt_3, then the next event will have to be a change in the concentration of node 2 first followed by a second change at node 1. During Δt_3, the concentration at node 1 which was previously changed by pipe 1 is advected to a new location. In the next quality time step, there will be two concentration fronts in pipe 3 that move independently of each other. The first front has a lower concentration than the second one. Finally after Δt_5, the initial release from node 1 will reach node 2 and change its concentration (Figure 3d). This process will continue until all nodes in the network reach steady-state concentrations or until another hydraulic event occurs in the network. In a real network, there might be a number of fronts in a single pipe moving independenty of each other; the program DYNAQ is designed to handle such complexities. The macro flow chart of the program is shown in Figure 4.

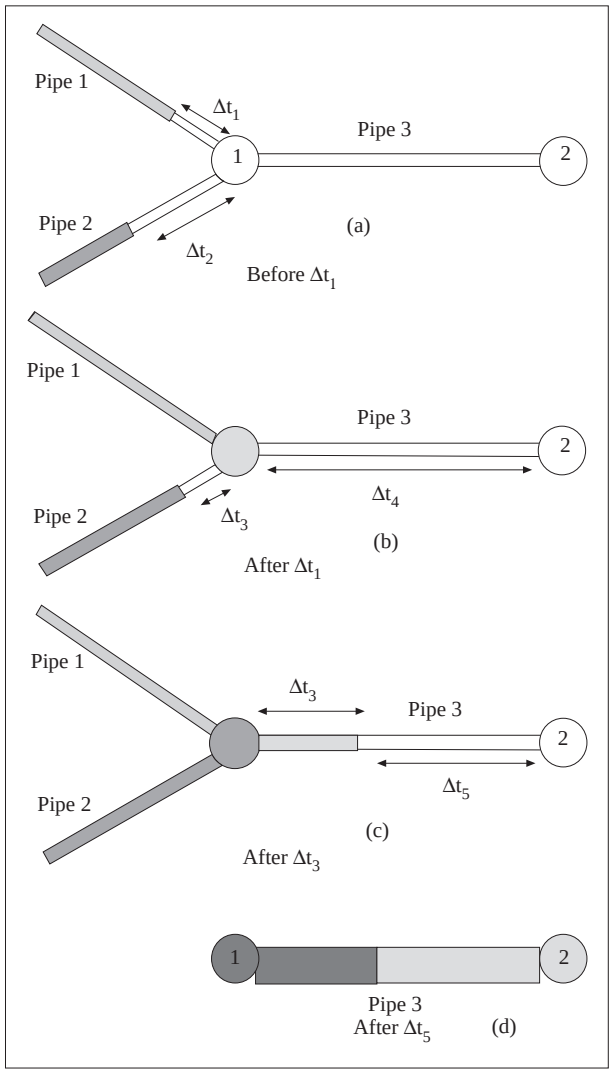

Figure 3. Concentration Front Movement and Decay

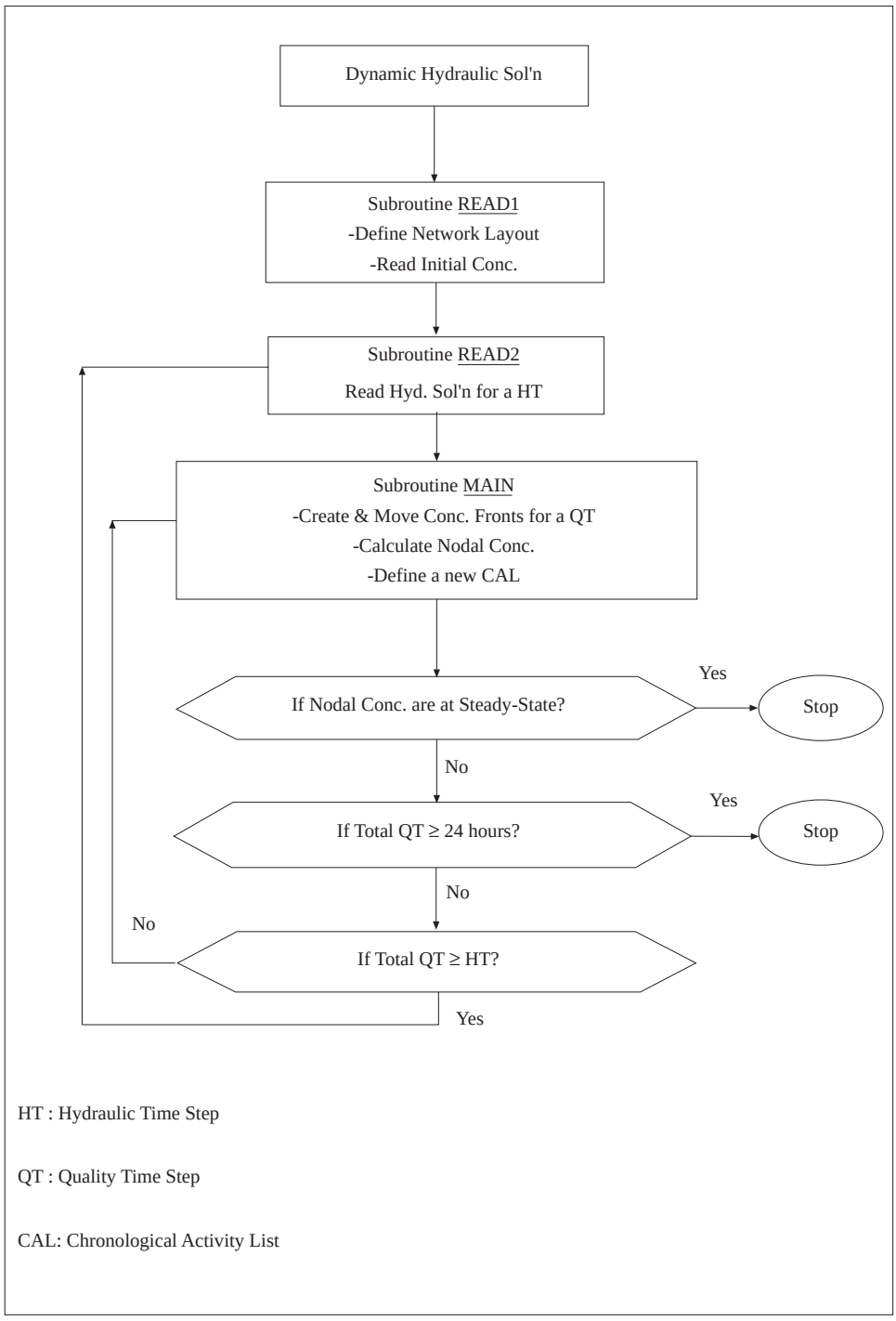

Figure 4. Flow Chart of the Program DYNAQ

Illustrative Example

An example network is considered to test the program DYNAQ for a dynamic simulation of chlorine decay in pipes. The network has one source at location 1, one storage reservoir (tank) at location 8, 13 pipes and 7 junction nodes. The characteristics of all pipes and nodes are given in Tables 1 and 2. Figure 5 is drawn to show the layout of the network. The steady-state hydraulic solution of the network is

shown in Figure 6. The source at node 1 is assumed to be a pumping station with a chlorination unit; the network is supplied with a continuous chlorine concentration of 1 mg/l Initial concentration in the network is assumed to be zero. The dynamic quality simulation starts at time zero. As shown in Figure 7a, the initial concentrations of all pipes and nodes are zero. As soon as the injection of chlorine starts at node 1 with an amount 1 mg/l, a front is created in three pipes connected to node 1, namely pipes 1, 2 and 3. A quality time step of 1200 s, which is also equal to the average travel time of water front from node 1 to node 4, is determined. In the chronological activity list CAL, the events are scheduled as concentration movements in pipes 1 and 2 and attainment of node 4 through pipe 3. Since node 4 is a source for two pipes with only one pipe discharging into it, the concentration of node 4 is the same as the concentration of pipe 3. Therefore, the colour of the pipe and node 4 are the same and are drawn in black. This case is shown in Figure 7b. In Figure 7c the concentration front is advected for one more quality time step that is equal to 1300 s. After the second quality time step, there are two nodal concentration changes in the CAL. The first change occurs at node 3 and the second change occurs at node 7. The dark grey colour shown in Figure 7c indicates that the concentrations are between 0.8 and 0.6 mg/l. The procedure detailed above continues in the same manner until the network reaches a steady-state condition. Figures 7d, e, f, and g are shown to indicate more steps until the first concentration front reaches the tank at node 8. There are many fronts traversing pipe 13 discharging into the tank until the system reaches the steady-state condition at time 19000 s (approx. 5 hours) as shown in Figure 7h. Even though concentrations at nodes and in pipes reach steady-state, the tank concentration will approach the concentration of pipe 13 asymptotically. This is because of the fact that while the inflow of water from pipe 13 tends to increase the concentration within the tank, there is a continuous decay taking place simultaneously within the tank.

Table 1. Pipe Characteristics

Pipe Number	Head Node	Tail Node	Length (m)	Diameter (mm)	Roughness Coeff.
1	1	2	300	150	120
2	1	3	400	150	120
3	1	4	200	150	120
4	2	3	600	100	120
5	3	4	600	100	120
6	2	5	500	100	120
7	3	5	400	100	120
8	3	6	300	100	120
9	3	7	350	100	120
10	4	7	200	100	120
11	5	6	50	100	120
12	6	7	300	100	120
13	6	8	200	100	120

Table 2. Junction Node Characteristics

Junction Number	Demand (l/sec)	Elevation (m)
1	-8.0	100
2	0.5	100
3	2.0	100
4	1.0	100
5	0.5	100
6	2.0	100
7	1.0	100
8	0	135

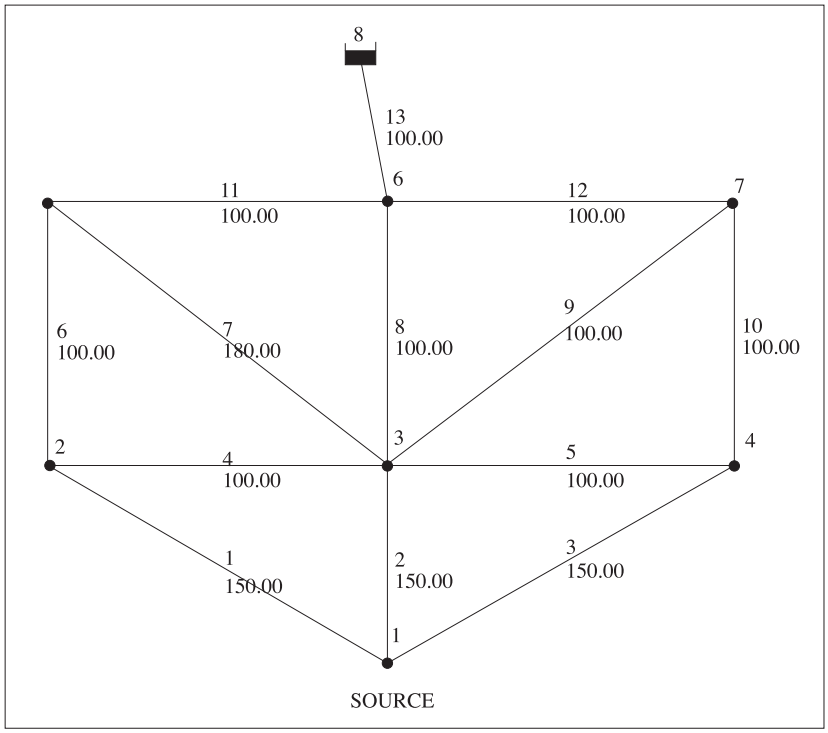

Figure 5. Example of a Water Distribution Network: Node Numbers, Pipe Number and Diameters

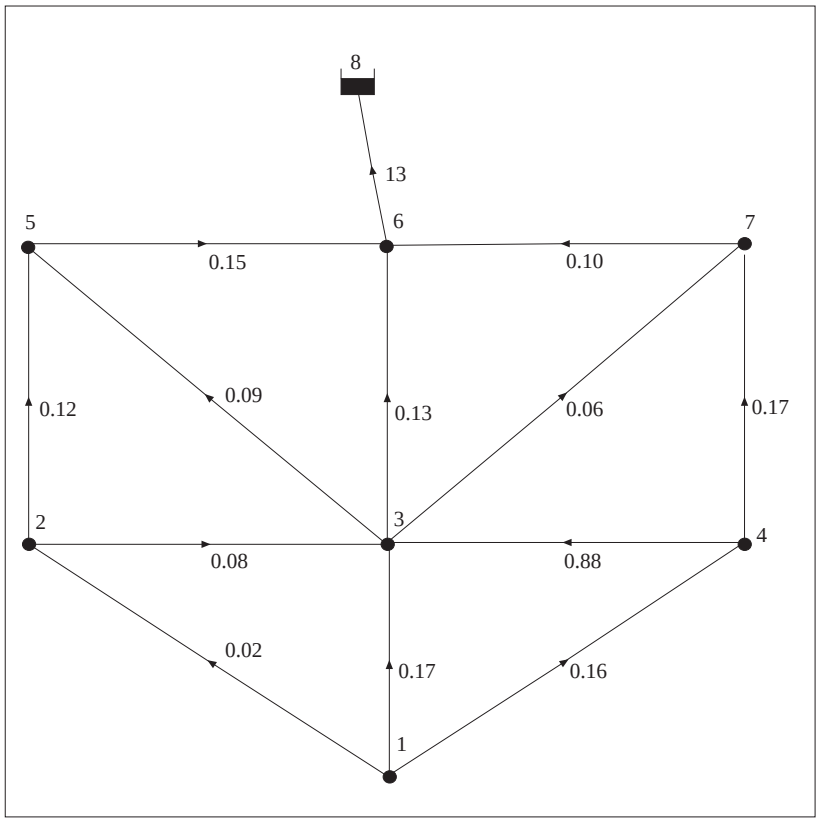

Figure 6. Hydraulic Solution (velocities are in m/s) of the Example Network

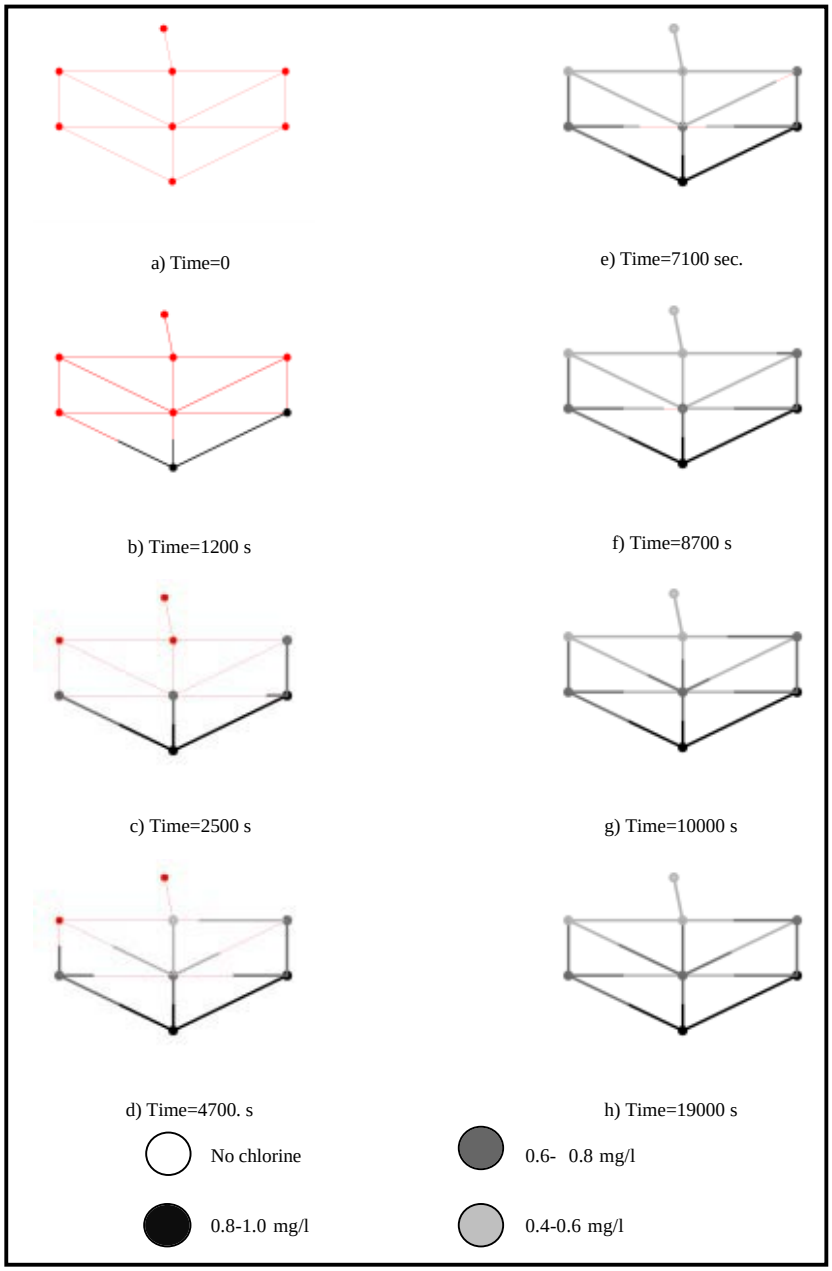

Figure 7. Real-Time Dynamic Simulation of the Example Network with DYNAQ

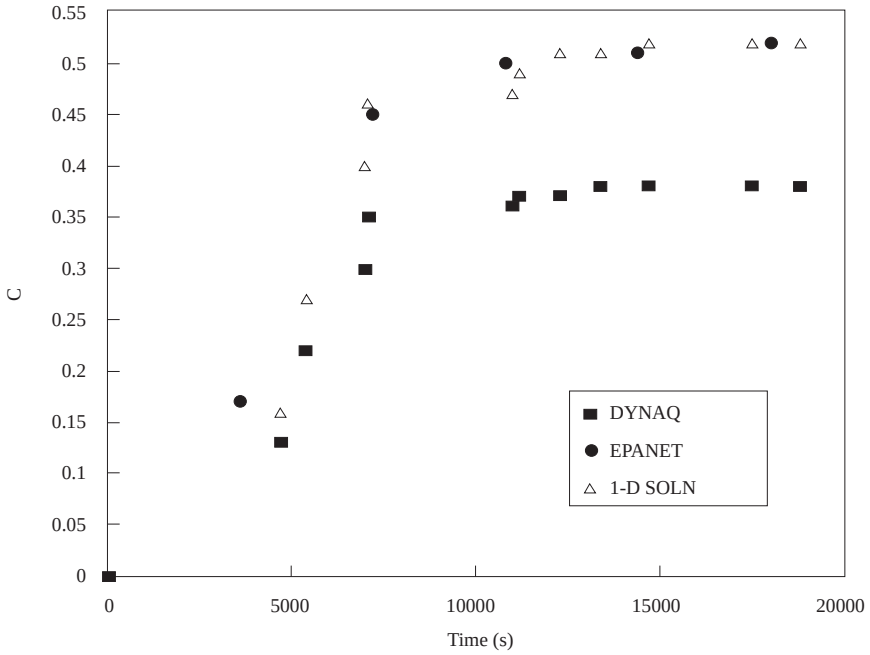

Figure 8. Concentration Change at Node 6

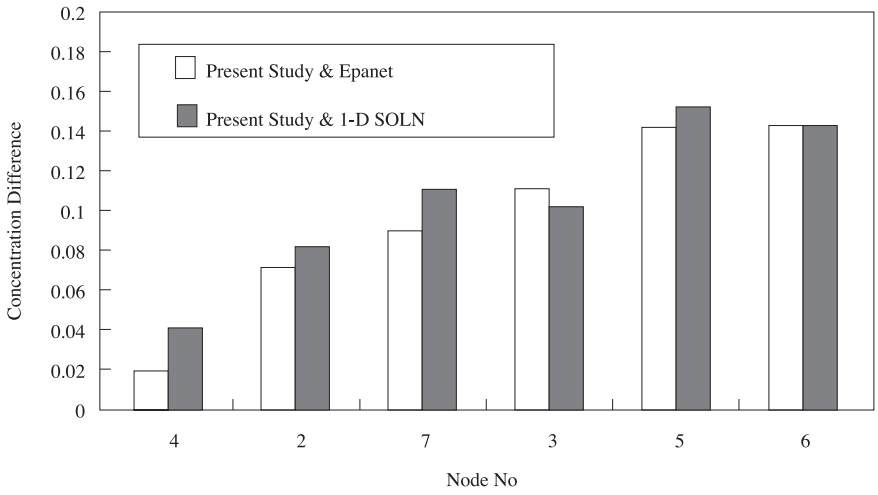

Figure 9. Concentration Difference (%) b/w Epanet and the Present Study with respect to Distance from the Source

Comparison of Results

The output of DYNAQ is compared with that of Epanet, a quality model frequently referred to in the US. To further enhance the comparison DYNAQ is coupled with both 1-D decay expression given as equation number (1). In Figure 8, the predictions of these three simulations for the concentration at node 6 are compared. The Epanet results and 1-D equation application overpredict the concentrations in the network. The discrepancy between the DYNAQ and 1-D equation and Epanet increases as the travel times increase, as shown in Figure 9. This difference in the ultimate (steady-state) concentrations of the nodes may become as large as 14 percent. This confirms the conclusions arrived at in studies by Ozdemir and Ger (1998) where the necessity of separate treatment of wall decay and bulk decay was emphasized.

Nomenclature

C	=	non-dimensional concentration;
C_j	=	non-dimensional concentration of discharging water into the node;
C_k	=	non-dimensional concentration of node k;
C_{in}	=	non-dimensional concentration of discharging water into the tank;
C_r	=	non-dimensional concentration of the tank;
C_T	=	non-dimensional approximate concentration;
C_{1D}	=	non-dimensional 1-D solution;
C_{2D}	=	non-dimensional 2-D solution;
C_t	=	concentration at time t (ML^{-3});
d	=	pipe diameter (L);
F_C	=	correction factor applied to 1-D solution (non-dimensional);
k	=	bulk decay coefficient (T^{-1});
Q_j	=	discharge leading to node j (L^3T^{-1});
Q_{in}	=	discharge leading to the tank (L^3T^{-1});
Q_{out}	=	the amount of water discharging out from the tank (L^3T^{-1});
r_0	=	pipe radius (L);
Re	=	Reynolds number (U d / ν);
t	=	time (T);
U	=	average water velocity in the pipe (LT^{-1});
V_r	=	volume of tank (L^3);
W_d	=	pipe wall chlorine demand (wall decay) (LT^{-1});
Z	=	non-dimensional number (2 W_d L / ν);
ν	=	kinematic water viscosity (L^2T^{-1});
t	=	simulation time (T).

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