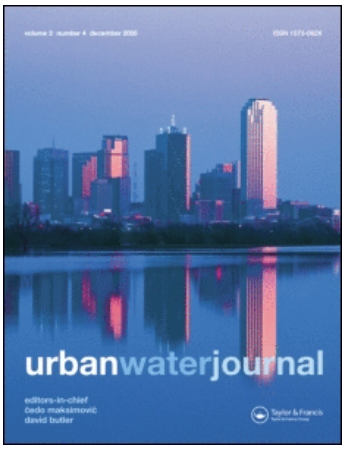

Urban Water Journal
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713734575

Modelling the advection equation under water hammer conditions

Cristovao Fernandes [a]; Bryan Karney [b]
[a] University of Parana Curitiba Brazil. [b] Department of Civil Engineering University of Toronto Toronto M5S 1A4 Canada.

Online Publication Date: 01 June 2004

To cite this Article Fernandes, Cristovao and Karney, Bryan(2004)'Modelling the advection equation under water hammer conditions',Urban Water Journal,1:2,97 — 112
To link to this Article: DOI: 10.1080/15730620412331290038
URL: http://dx.doi.org/10.1080/15730620412331290038

Urban Water Journal, Vol. 1, No. 2, June 2004, 97–112

Taylor & Francis
Taylor & Francis Group

Modelling the advection equation under water hammer conditions

CRISTOVAO FERNANDES*† and

BRYAN W. KARNEY‡

†University of Parana, Curitiba, Brazil ‡Department of Civil Engineering, University of Toronto, Toronto, M5S 1A4, Canada

(*Revised version received June 2004*)

The quality of water delivered by a distribution network may degrade for many reasons. This research considers one of these, focusing attention on the connection between water quality and the hydraulic events in a pipe system. More specifically, pressure and velocity variations associated with hydraulic transients or water hammer conditions, particularly through leaks and rapid device adjustments, have the potential to degrade water quality. In most previous applications, numerical transport schemes have been coupled to quasi-steady hydraulic models. By contrast, the current contribution couples a finite difference solution of the advection-reaction equation to a fully unsteady, method of characteristics (MOC) based, hydraulic solution. Depending on system properties, the effects of advection, compressibility and reaction may be evident in the modelled response. The numerical properties of consistency, stability and convergence of the proposed model are investigated both analytically and numerically. Although some case studies have revealed important water quality implications associated with dynamic conditions, particularly in cases of contaminated water intrusion, it should be admitted that many transient simulations exhibit few differences compared with quasi-steady results.

Keywords: Chlorine decay; Distribution systems; Intrusion; Transient; Water hammer; Water quality modelling

1. Introduction

As water transits through a distribution system, its quality undergoes important changes as a result of complex physical, chemical and biological processes. These transformations might be associated with changes in the quality of the source water, with the material and condition of the hydraulic elements such as pipes, valves, and tanks, or with the system's residence time (Grayman *et al*. 2000). Water quality can also be influenced by other factors, including the decay of chlorine-based residuals, bacterial regrowth, temperature, disinfectant residual and the presence of assimilable organic carbon (AOC) (LeChevallier *et al*. 1990). Further influences include biofilm-induced depletion of chlorine residuals, chemically and microbiologically engendered internal corrosion of the pipe wall, long detention times in pipes or storage tanks, and the growth and decay of disinfection by-products (DBP).

All these effects are superimposed on the hydraulic transport mechanisms that are usually assumed to be either steady or nearly steady, but may in fact be otherwise. It is possible that water quality could also be degraded by water hammer or hydraulic transient effects, not only by increasing the risk of pipe failure due to significant pressure variation, but also by making biofilms, corrosion and/or

*Corresponding author. Email: cris.dhs@ufpr.br

Urban Water Journal
ISSN 1573-062X print/ISSN 1744-9006 online
http://www.tandf.co.uk/journals
DOI: 10.1080/15730620412331290038

tuberculation on the pipe wall more susceptible to transport by high velocities and shear stresses (Brunone *et al*. 2000). Moreover, abnormally low transient pressures can draw contaminated water into an otherwise safe potable water delivery system (see also McInnis 2004 and Brunone and Ferrante 2004). However, apart from such intrusion events, the specific impact of inertia and compressibility effects has been largely neglected.

These considerations are clearly relevant to water quality models. The traditional techniques used to simulate the passage of a substance throughout the distribution system assume boundary conditions (e.g. source pressures and demands) that are, if not constant, at least highly regular or predictable. Can transients produce changes of greater significance than other transport mechanisms? While this far-reaching question is beyond the scope of this preliminary work, any comprehensive answer requires a tool that can account for transient flow. Accordingly, the specific issue addressed here is whether a more comprehensive representation of the hydraulic characteristics of the system can be easily achieved in a transport model, and whether such a comprehensive model can lead to a better understanding of the water quality degradation process.

The paper presents a numerical solution for the unsteady advection/reaction equation (ARE) considering hydraulic transient conditions. The proposed approach is a finite difference scheme superimposed on a method of characteristics (MOC) transient simulation. Issues of computational consistency, order and stability of the new procedure are considered. One application is given special attention. This is the impact of a transient episode in a simple system that draws contaminated/untreated water and creates a water quality event that would be quite unmarked by conventional steady state modelling.

1.1 *Overview of water quality modelling in distribution systems*

For all constituents of interest, computer-based water quality models combine two basic modules. The first determines hydraulic conditions, establishing flow velocity, flow direction and pressure values based upon continuity, energy and momentum relations. The second module relies on the hydraulic model to evaluate flow paths (advective transport), but also calculates the mixing of water from different sources, the dilution of contaminants, and the travel/detention times of the water (Elton *et al*. 1995). The water quality processes considered within a pipe generally include advection, chemical and biological reactions, interactions at the inner pipe surface and with external sources and sinks, and, possibly, diffusion and dispersion. Processes relating the simultaneous transport of multiple substances and their interactions have recently received attention (e.g. Bocelli and Uber 2001).

Mathematically, the mass transport of a single chemical is described by the advection-diffusion equation (ADE) derived from mass conservation and Fick's law. The resulting second order parabolic partial differential equation, including generic reaction and source/sink terms, can be written as (Celia *et al*. 1990):

$$\frac{\partial C_i(\vec{x},t)}{\partial t} + \vec{u}\,\nabla C_i(\vec{x},t) = \nabla\left(\boldsymbol{D}\nabla C_i(\vec{x},t)\right) + f\left(C_i(\vec{x},t)\right) + S\left(C_i(\vec{x},t)\right) \tag{1}$$

where $C_i(\vec{x},t)$ is the substance concentration, x is the spatial dimension, $\vec{u}$ is the velocity vector, $\boldsymbol{D}$ is the diffusion coefficient matrix, t is the temporal variable, $f(C)$ defines the chemical and biological reactions, and $S(C)$ defines any sources or sinks within the pipe. Equation (1) presents the general form for a single substance in the pipe. The underlying hydraulics, primarily characterized by the terms ($\vec{u}$) and $\boldsymbol{D}$, may be either steady or unsteady. (In the broader context, the reaction term f and the source/sink term S may also be influenced by system hydraulics, but these considerations are beyond the scope of this paper.)

Rather than solve the full transport equations, strategic simplifications are usually adopted. For turbulent flow, advection is the dominant mass transport mechanism. In fact, the diffusion/dispersion process is often an order of magnitude less than advection (Liou and Kroon 1987). Moreover, the flow is assumed to be one-dimensional (implying $\boldsymbol{D}$ and $\vec{u}$ are time-dependent scalars) and cross-sectional characteristics are treated as steady and uniform. Instantaneous and complete cross-sectional mixing of material is typically presumed. Finally, a first-order reaction term K is used to represent the effects of chemical and biological reactions. Under these assumptions, (1) reduces to:

$$\frac{\partial C(x,t)}{\partial t} + U(x,t)\frac{\partial C(x,t)}{\partial x} + KC(x,t) = 0 \tag{2}$$

This simplified equation is used as the basis for a transient pipe flow solution.

Water quality models universally simulate chlorine decay in distribution systems, but they differ in their numerical representation of hydraulic and mass transport components. Early models simulated individual constituents/disinfectants based on a steady state concentration distribution and a steady state hydraulic solution. More recently, extended period simulation (EPS, or so-called dynamic) water quality models were introduced to account for time-varying conditions through the advection equation. The water quality component is usually superimposed on an EPS hydraulic model (Liou and Kroon 1987, Grayman *et al*. 1988, Rossman *et al*. 1993, Boulos *et al*.

1994, 1995, Rossman and Boulos 1996). Such a modelling approach, despite assuming a plug-flow velocity profile and not directly accounting for shear stress, diffusion, inertia or compressibility effects, has proved useful in practice. This EPS approach to water quality modelling has been encoded in a variety of popular and commercial software applications, including the public domain program EPANET. Other water quality models (e.g. the rigid column approach of Islam and Chaudhry, 1998) have incorporated more sophisticated hydraulic or numerical schemes, but are not widely used.

1.2 *Hydraulic transients and water quality*

Before jumping into details, a key question should be directly answered: are transients so important that their impacts on water quality deserve special attention? Water distribution systems are complex in nature. Many distinct elements such as pipes of different sizes, material and diameters, and a range of boundary elements (e.g. reservoirs, tanks, valves, pumps, and booster chlorination devices) are needed to achieve the required quality and quantity objectives for the delivered water. Moreover, network elements sometimes carry large flows, with a potentially huge momentum under typical delivery conditions. It is the forces associated with adjustments to this momentum that is the physical foundation for the importance of transients in distribution systems.

In reality, system operation may sometimes be abruptly changed, inducing new hydraulic conditions. Pumps cycle on and off, valves are sometimes opened or closed, pipe breaks may suddenly occur, and water is withdrawn more or less continuously from the system, but at varying rates. This situation can create a dramatic physical response by virtue of the connection between fluid properties (water density and compressibility) and the governing constraint of mass conservation. In fact, the only mechanism for communicating operational changes throughout a pressurized system is through minute changes in fluid density. Since water is only slightly compressible, even a small change in density can produce a significant change in pressure. Elastic effects are manifested via pressure wave propagation, a mechanism that effectively communicates changes in the delivery conditions throughout the system. It is through pressure waves that the fluid momentum is adjusted. In fact, it is truly steady conditions that are ephemeral; pipe systems are dynamic and inertia and compressibility effects are important whenever a change occurs or is induced (i.e. almost always). As Karney and McInnis (1990) comment: ''water hammer (transient) conditions are nothing more than a call for the system to reassess its current status.'' This ''reassessment'' can significantly and dramatically alter the system's pressure and flow distribution.

If the network is hydraulically dynamic, the next question is, ''What impact will this have on water quality conditions?'' Again, the answer is related to the complex interactions associated with the momentum transformations in the distribution system. The primary impact is likely upon mass transport characteristics due to the possibly intense flow changes that can be experienced. In fact, mass fluctuations within all pipe segments will occur as a result of flow acceleration or even reversal. The impacts of fast velocity fluctuations are felt throughout the system, possibly causing significant variations in spatial and temporal concentrations.

Another key issue pertains to fluid exchanges during transient episodes between the distribution system and storage devices or other system boundary conditions (e.g., reservoirs, tanks, relief valves, discharge control valves, orifices, etc.). Water may enter or leave the system (e.g., at relief valves or tanks) as a consequence of pressure fluctuations. This implies not only a physical exchange due to inertia properties, but also one that may exchange water with distinct chemical and biological characteristics between the system and the external environment. These interactions can promote a new set of water quality transformations that can only be evaluated if they can be tracked during the time that the phenomenon occurs. Moreover, these water quality implications may occur whenever dynamic hydraulic conditions are present within the network. Not surprisingly, these changes cannot always be captured by smoothed or average conditions in an EPS water quality model.

Of specific concern is the potential water quality degradation arising from negative pressures. If such pressures were to occur in a leaky pipe, the potential intrusion of ambient water into the system could compromise water quality. Since this water is probably untreated, it may bring pathogens, organic material, DBP precursors or other substances into the pipe network, without anyone's knowledge. As McInnis (2004) makes clear, such events could be responsible for considerable disease or disruption.

In summary, the nature of a distribution system with its elements (e.g. tanks, reservoirs, valves, pumps, etc.), plus the fact that water is a slightly compressible and dense compound, establish the dynamic characteristics of the whole system. These properties not only determine the magnitude of the hydraulic event, but also influence the associated chemical and biological transformations. In this context, the approach of current water quality models cannot assess these distinct impacts and must be extended. The current paper derives a transient advection/reaction model and investigates in a preliminary way the influence of hydraulic transients and compressibility effects on the mass transport of a single chemical constituent.

2. Proposed model

The identification of a suitable transient water quality numerical procedure should be closely related to the adopted hydraulic scheme. In the current case, hydraulic transient response can be appropriately modelled, including inertia and compressibility effects, through the method of characteristics (MOC). The water quality algorithm is built on this solution in conceptually the same way as simpler models described in the literature.

The hydraulic conditions are determined through the solution of the one-dimensional hyperbolic partial differential equations (PDE) of momentum and continuity given by:

$$\frac{\partial U}{\partial t} + g\frac{\partial H}{\partial x} + \frac{fU|U|}{2d} = 0 \tag{3}$$

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

in which: $U = U(x,t)$ is the instantaneous average fluid velocity; d = internal pipe diameter; $H = H(x,t)$ piezometric head; a = acoustic wavespeed; g = acceleration due to gravity; and f = Darcy–Weisbach friction factor, traditionally assumed equal to that determined under steady state conditions for each pipe. The MOC is used to transform these expressions into a system of four ordinary differential equations, representing a pair of compatibility equations valid along two characteristics lines (e.g. Wylie and Streeter 1993, Karney and McInnis 1992).

The proposed water quality module allows a direct algebraic solution for the advection-reaction equation by exploiting two important features of the hydraulic simulation. The first arises because the MOC solution numerically integrates the momentum and continuity equations over a fixed space–time grid (Karney and McInnis 1992). The resulting transport scheme has excellent computational speed and accuracy. The second feature is the fine level of temporal discretization (i.e. a small time step) associated with the hydraulic solution. These features are linked here to a suitable control volume definition, while accounting for the varying velocity. Thus, the space–time (x–t) grid arising from the MOC procedure is adapted to allow definition of a suitable finite difference scheme as depicted in figure 1. For simplicity, the characteristic lines are depicted only for point 1; similar characteristics exist at all points. Note in figure 1 that the hydraulic information is propagated exactly a distance Δx through the characteristic relation $\Delta x = a\Delta t$, where a is the wave propagation speed, and Δt is the water quality time step. Since a is normally large, Δt tends to be small.

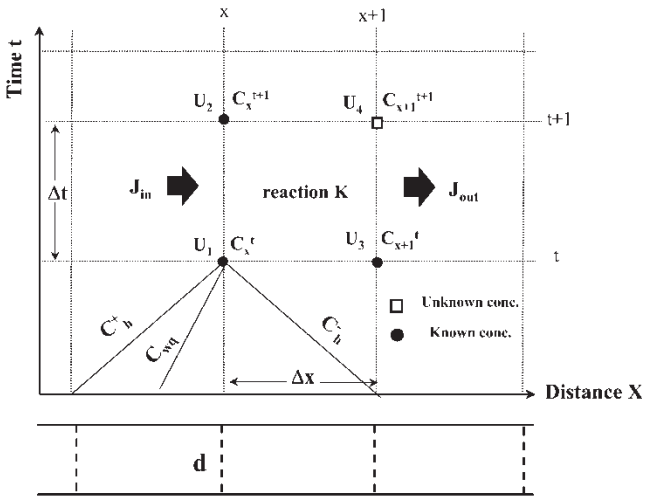

Figure 1. Space–time grid and control volume definition for the ARE solution.

In the derivation of the water quality model, the following definitions are useful: t = a time index for the ith time step; A = cross-sectional area of pipe; J_{in} = flux of constituent mass entering the control volume; J_{out} = - mass flux leaving the control volume; and ΔV = change of water volume. It is assumed that the disinfectant/constituent concentration at the upstream source is known for $C(0,t)$. The initial condition $C(x,0)$ is assumed to be known, either from measured results or from an extended period analysis.

In the transport equation given in (2), the finite signal propagation speed, associated with the velocity $U(x,t)$ and with the hyperbolic nature of the governing equations, now changes (possibly rapidly) with time and distance, creating a non-uniform advection speed. As a consequence, the typical time marching techniques usually suggested for solving PDEs of this nature are not necessarily appropriate. Previous algorithms for solving (2), including Lagrangian time-driven method, marching-out solutions, event-driven methods, and discrete volume element methods, have generally assumed a steady velocity field (Hoffman 2001). In the current formulation, the velocity flow field is unsteady and non-uniform in space, but still represented by an average cross-sectional value.

A direct application of (2) along the transport path creates an intrinsic mismatch in the time scales between the advection and water hammer velocities. In fact, the water hammer solution conveniently (and accurately) assumes that the advective velocity is much less than the wave propagation velocity a. Although this time step mismatch could be partially overcome by interpolating the velocity field during the advection calculation, an alternate procedure is proposed here. The adopted approach that is recommended is to "accumulate" the mass flux over a

number of hydraulic time steps, thus effectively "extending" the water quality time step; in this way, the advective transport time step and the hydraulic propagation time step are brought into closer agreement. More specifically, the water quality time step is obtained as a simple multiple of the hydraulic time step $\Delta t_h =$ from the MOC solution (Karney and McInnis 1992). Thus

$$\Delta t = N\Delta t_h \tag{5}$$

where $N =$ is an integer number representing the number of steps over which the accumulation occurs. If U_i denotes the velocities at these intermediate hydraulic steps, then $U = \frac{1}{N}\sum_{i=1}^{N} U_i$. Clearly, U now assumes the role of a time-averaged velocity over the water quality time step. In essence, the larger water quality time step effectively extends the C_{wq} characteristic line in figure 1 backward in time until it approximately spans a Δx step. The contrast to the usual extended period simulation (EPS) approach should be noted: in a typical EPS implementation, the water quality time step is usually a fraction of the hydraulic time step; in the current approximation, the opposite is true.

The mass balance equation for the defined control volume can be written as:

$$V\frac{\partial C}{\partial t} = (J_{\text{in}} - J_{\text{out}})A - KV\,\bar{C} \tag{6}$$

where $\bar{C}$ is the average concentration in the control volume, based upon the concentration at the grid points of the selected control volume. In this case the logical values to use are C_x^t, C_x^{t+1}, C_{x+1}^t and C_{x+1}^{t+1}. Clearly, the mass flux rate changes as the velocity changes. As a first solution, consider an approximation based on average concentrations at time t and $t + 1$ for both mass fluxes and decay rate. As usual, a finite difference procedure is derived by using Taylor series expansion of the dependent variable about the grid point (x,t).

The time derivative of concentration is approximated using an average of derivatives for positions x and $x + 1$. Neglecting the error term, the forward-time approximation can be written as:

$$\frac{\partial C}{\partial t} = \frac{1}{2}\left(\left.\frac{\partial C}{\partial t}\right|_x^t + \left.\frac{\partial C}{\partial t}\right|_{x+1}^t\right) = \frac{C_x^{t+1} - C_x^t + C_{x+1}^{t+1} - C_{x+1}^t}{2\Delta t} \tag{7}$$

The net mass flux rate from the control volume in figure 1 is based upon the average at time positions t and $t + 1$. Thus, the mass flux coming in the control volume is given by:

$$J_{\text{in}} = \frac{1}{2}\left(J_{\text{in}}|_x^t + J_{\text{in}}|_x^{t+1}\right) = \frac{1}{2}\left(C_x^t U_x^t + C_x^{t+1} U_x^{t+1}\right) \tag{8}$$

A similar expression holds for the flux leaving the control volume. Thus, the net mass flux rate from the control volume is given by:

$$J_{\text{in}} - J_{\text{out}} = \frac{C_x^t U_x^t + C_x^{t+1} U_x^{t+1} - C_{x+1}^t U_{x+1}^t - C_{x+1}^{t+1} U_{x+1}^{t+1}}{2} \tag{9}$$

Neglecting fluctuations in volume, the resulting expression is given by:

$$\text{Reaction} = KV\left(\frac{C_x^t + C_x^{t+1} + C_{x+1}^t + C_{x+1}^{t+1}}{4}\right) \tag{10}$$

in which the overall reaction term K is assumed to occur both within the bulk flow and at a certain rate between the bulk flow and the pipe wall material (Rossman *et al*. 1993).

A particularly efficient numerical scheme can be used to solve this model. Recognizing that at the upstream boundary C_0^{t+1} is known, C_1^{t+1} is the only unknown in the first element, and can be obtained directly. Thus, solving from upstream to downstream, the previous equations yield only one unknown (i.e. C_{x+1}^{t+1}) for a given time step. Substituting equations (7), (9) and (10) into (6), and solving for C_{x+1}^{t+1}, results in the following direct solution to finite difference formulation:

$$C_{x+1}^{t+1} = \frac{E_1 C_x^t + E_2 C_x^{t+1} - E_3 C_{x+1}^t}{E_4} \tag{11}$$

where the known values of E are functions of known velocities at the four grid point base and the temporal and spatial discretization as follows:

$$E_1 = U_x^t\frac{\Delta t}{\Delta x} - \frac{K\Delta t}{2} + 1 \tag{12}$$

$$E_2 = U_x^{t+1}\frac{\Delta t}{\Delta x} - \frac{K\Delta t}{2} - 1 \tag{13}$$

$$E_3 = U_{x+1}^t\frac{\Delta t}{\Delta x} + \frac{K\Delta t}{2} - 1 \tag{14}$$

$$E_4 = U_{x+1}^{t+1}\frac{\Delta t}{\Delta x} + \frac{K\Delta t}{2} + 1 \tag{15}$$

Thus, equation (11) provides a direct solution of the finite difference approximation of the ARE based on transient hydraulic conditions of the MOC x-t grid.

3. Numerical analysis

A finite difference equation (FDE) is defined "as a consistent representation of a (PDE) if the truncation error, represented by the difference between the FDE and the PDE, disappears as the size of the grid spacing goes to

zero independently'' (Hoffman 2001). The analysis is performed based on the characteristics of the so-called first form of the modified differential equation (MDE). The resulting MDE, as indicated in appendix I, is obtained for Δt, Δx approaching zero in (20), and is given by:

$$\frac{\partial C}{\partial t} = \underbrace{\lim_{\Delta x \to 0} \frac{U_T C}{\Delta x}}_{I} - \underbrace{\left(\frac{U_3 + U_4}{2}\right)\frac{\partial C}{\partial x}}_{II} - KC \qquad (16)$$

where, for simplicity, $U_1 = U_x^t$, $U_2 = U_x^{t+1}$, $U_3 = U_{x+1}^t$, $U_4 = U_{x+1}^{t+1}$. The transient velocity parameter is given by: $U_T = \frac{1}{2}(U_1 + U_2 - U_3 - U_4)$.

Equation (16) indicates that the time derivative of the dependent variable C is a function of two components (I and II) and a reaction term. The first component (I) reflects the fact that the rate of mass accumulation depends on the difference between the transient velocities. Physically this represents a variation of the mass flux over Δt, reflecting the divergence of the velocity flow field; this term will only be non-zero as compressibility effects arise in the system. Furthermore, this term indicates the possibility of a short-term increase (or decrease) in concentration depending on U_T. If U_T is positive, there is an accumulation of mass that can cause a small transient increase in concentration above the source concentration. Another physical implication is that the associated pressure changes in the hydraulic solution arise (through the continuity equation) as a consequence of the numerical value of U_T.

The second component (II) indicates that the rate of accumulation of concentration is directly influenced by the transient velocities out of the control volume. Interestingly, this advective component highlights the potential impact of distinct hydraulic time scales on concentration calculations, particularly if $U_3 \neq U_4$. Significantly, the first MDE is reduced to the ARE in equation (2) if $U_1 = U_2 = U_3 = U_4 = U$ in equation (16). Under such a steady and uniform flow field, the FDE, given by equation (11), is a consistent representation of the advection/reaction equation.

The next step identifies the order of the FDE [equation (11)]. This analysis refers to the evaluation of the order of truncation error terms in the approximations of the partial derivatives in the PDE. It should be based upon the definition of the second form of the modified differential equation (MDE), as developed in appendix I (see equation (25)). From equation (25), the FDE approximation has a truncation error of $O(\Delta t) + O(\Delta x)$. The advective component is influenced by transient velocities that impact the wave front propagation. The dominant terms are odd spatial derivatives, implying a dispersive effect. Furthermore, the presence of a second order derivative term ($\frac{\partial^2 C}{\partial x^2}$) reflects an implicit numerical diffusion, proportional to the transient velocities in a given control volume.

Finally, stability is often analysed using the Von Neumann method (Hoffman 1992). As derived in appendix I, the stability criterion of a FDE is based upon the interpretation of the complex amplification factor G, obtained from analysis of the general Fourier component of the FDE being analysed, and given by:

$$G = \frac{E_1 - (E_3 e^{i\theta})}{E_4 e^{i\theta} - E_2} = \frac{E_1 - E_3(\cos\theta + i\sin\theta)}{E_4(\cos\theta + i\sin\theta) - E_2} \qquad (17)$$

where E_1 to E_4 are known constant values of the finite difference scheme and given by equations (12) to (15); and $i = \sqrt{-1}$.

Equation (17) clearly indicates that the numerical stability of the hydraulic module is the key characteristic for a stable water quality module. The transient velocities can be calculated based upon the flexible discretization algorithm on a fixed-grid MOC (Karney and Ghidaoui 1997). Karney and Ghidaoui (1997) show that the conditions to assure accurate and stable general solutions for the integration of hyperbolic equations of momentum and continuity are the Courant number $C_r = \frac{\alpha \Delta t}{\Delta x} \leq 1$ and a small time step discretization Δt. As a consequence, the physics of the system is appropriately reproduced through stable pressure and velocity predictions. This fact positively influences the water quality transport module as shown through equation (16), reflecting a stable behaviour of components (I) and (II).

As a consequence of the small $\frac{\Delta t}{\Delta x}$ ratio, the corresponding unsteady advection terms $\frac{U_1 \Delta t}{\Delta t}$, $\frac{U_2 \Delta t}{\Delta x}$, $\frac{U_3 \Delta t}{\Delta x}$ and $\frac{U_4 \Delta t}{\Delta x}$ are also small. Thus, even considering the reaction term, the values of E_1 and E_4 are larger than either E_2 or E_3. This is true because the additive terms for parameters E_1 and E_4 from equations (12) and (15) induce an amplification factor G less than 1, thus satisfying the Von Neumann stability criteria. However, these conclusions are not completely universal and depend somewhat on the nature and behaviour of transient velocities.

Even with this slight ambiguity, one way to assure numerical stability of the mass transport algorithm is to assume the stability criteria proposed by Karney and Ghidaoui (1997) for the hydraulic module. Thus, maintaining the hydraulic and the water quality time steps as small as may be reasonable, in order to avoid magnifying the values of transient velocities between time steps, will certainly produce values of E_1 and E_4 larger than either E_2 or E_3 in equation (17). If these conditions are assured, and even if reversal flows are considered, the denominator of equation (17) will have a higher value than the numerator, thus assuring stability.

Overall, convergence of a FDE is linked with concepts of consistency and stability as stated by the Lax equivalence theorem (Strikwerda 1989). Thus, in the current case, the question of convergence is assured since the FDE is consistent and stable.

4. Preliminary case studies: steady flow with advection

The first case study is performed on a single pipe under steady state velocity conditions where the analytical solution is known. Specifically, the purpose of this initial analysis is to compare the propagation of the concentration front through the pipe, based on the analytical solution of the ARE, with the results of the numerical formulation.

This section explores the case study proposed by Axworthy and Karney (1996), who investigated a simple series pipeline, consisting of 10 pipe segments and 11 junctions. Each pipe segment in the system is 100 m long with an inside diameter of 500 mm. The steady state flow rate is 0.7 L/s, which corresponds to a low velocity of 0.004 m/s, a Reynolds number of 1748 and a Darcy-Weisbach friction factor of 0.0366. Chlorine concentration is a constant 1.0 mg/L at the source ($C_i(0,t) = 1.0$ mg/L), but is not initially present in the pipe ($C(x,0) = 0.0$ mg/L). The overall decay coefficient of 6.417×10^{-6} s^{-1} corresponds to a bulk flow and wall decay constants of 0.5 d^{-1} and 0.3048 m/d, respectively.

In Axworthy and Karney (1996), concentrations were established at each node to track both the transport and decay of the constituent as it travels through the pipeline. The water quality time step and the duration of the simulation were chosen to be 900 s and 47 h, respectively. The numerical results for the solution of the advection-reaction equation based upon the finite difference scheme herein derived [equation (11)] are presented in figure 2. The heavier solid line indicates the analytical solution based on the closed form solution of advection equation with reaction for a uniform velocity profile (Axworthy and Karney 1996). Curve 1 is the solution based upon the numerical advective scheme derived here. As illustrated, the numerical scheme slightly over-predicts the nodal concentrations; although the difference is not significant in the beginning of the pipe, it gradually increases to a level of 12% at 600 m.

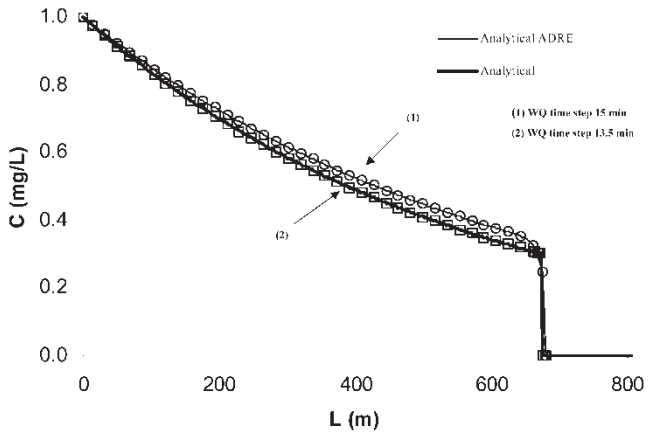

Figure 2. Comparison between analytical and numerical results.

This comparison demonstrates that the finite difference numerical scheme introduces some numerical dispersion, as well as indicating the influence of the advective and reaction components as one would expect. However, the tendency for dispersive transport is effectively eliminated by a more careful consideration of the match between physical and numerical velocities. In order to achieve this goal, a simple procedure was used to evaluate the wave front position of the concentration within the computational cell. In this case study, a new water quality time step of 13.5 min, better matching the hydraulic time step from the MOC solution, resulted in nodal concentrations represented by curve 2. As indicated in figure 2, the dispersion effects were largely eliminated.

For the steady state case, the magnitude of the numerical dispersion in the numerical result can be compared with the analytical result of the second modified differential equation (MDE). In a more compact representation, equation (25) (see appendix I) can be written as function of a_1, a_2, and a_3, as indicated through equation (27). These constant coefficients are values function of the steady state velocity, the reaction term, and the grid resolution. The parameters a_1, a_2, and a_3 are defined as indicated in equation (26, see appendix I). With the appropriate substitutions, the second MDE is reduced to equation (19) with the following constants: $a_1 = -0.004041$, $a_2 = 0.000125$, and $a_3 = 6.401 \times 10^{-6}$. The presence of a non-zero a_2 value indicates an implicit numerical diffusion associated with the proposed scheme. For the analytical solution presented by Axworthy and Karney (1996), the constants are: $a_1 = -0.004$, $a_2 = 0$, and $a_3 = 6.417\ 10^{-6}$. Thus, the "solid line" in figure 2 is the analytical solution of the second MDE that evaluates the order of the implicit numerical dispersion of the proposed model. Clearly, the agreement between the analytical solution and the numerical results indicates that the second MDE (17) gives an accurate estimation of the numerical errors of the explicit model for the solution of ARE.

5. Transient water quality response under turbulent flow

The next case studies help to better understand the significance of the solution technique in systems with turbulent flow. A key implication of turbulent flows is an efficient transfer of mass, momentum and energy within the fluid, where the velocity distribution is a primary contributor and advection dominates. Pipes experiencing turbulent flow are subject to higher corrosion rates, erosion, and more rapid scouring with its associated impacts on water quality (Brunone *et al.* 2000).

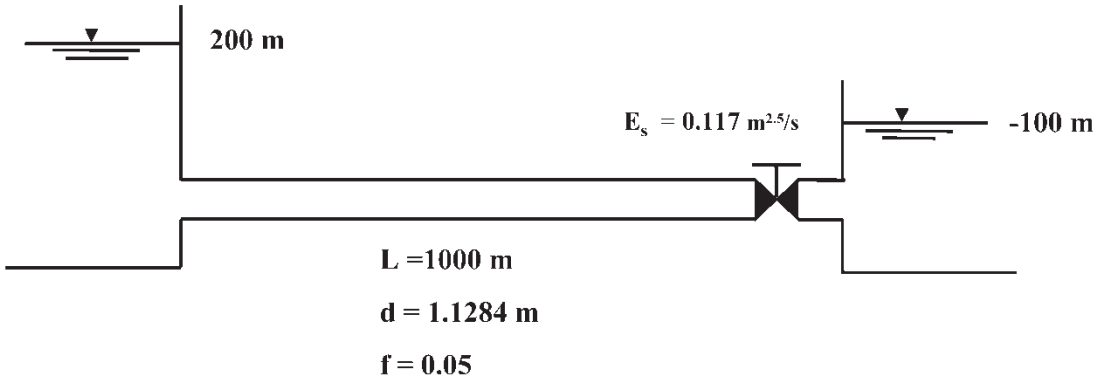

Figure 3. Simple pipe system.

5.1 *Response due to rapid valve opening*

In this case study, a full and rapid valve opening operation of a downstream valve in a single pipeline (figure 3) is simulated. This operation is a consequence of a linear change of valve flow in 2 s. The relevant parameters are: L (pipe length) = 1000 m, d (pipe diameter) = 1.1284 m, a = 1000 m/s, f = 0.05, E_S (valve size parameter, Karney and McInnis 1992) = 0.117 m$^{2.5}$/s, H_1 (upstream reservoir static head) = 200 m, and H_2 (downstream reservoir static head) = −100 m, Δx = 62.5 m. The hydraulic and water quality time step, are 0.01 s and 0.1 s, respectively. In addition, the overall chlorine decay coefficient (K) is 6.0 × 10^{-6} s^{-1} when the bulk flow and wall decay constants are 0.3 d^{-1} and 0.08 m/d, respectively. The boundary concentrations are defined as: $C(x = 0,t)$ = 0.5 mg/L, at the upstream reservoir, and $C(x,0)$ = 0.5 mg/L, through the pipeline. Given the size of the valve, the pipe characteristics and the reservoir heads, the expected steady state flow with a fully opened valve is 2.0 m^3/s.

The system response to the rapid valve opening is summarized in figures 4(a) and 4(b) for pressure and velocity evolution through time along the pipe. The opening of the valve initiates a flow increase and a pressure reduction at the downstream end. This disturbance creates a pressure and velocity wave that propagates to adjacent elements until the system finally adjusts to a new equilibrium condition. Restoration of equilibrium takes approximately 20 s in the current system. Note that compressibility and inertia effects cause an overshoot of the final head and discharge values. For example, at 5 s the pressure is temporarily greater than 200 m and the discharge greater than 2.0 m^3/s.

The impact of these events on the evolution of concentration is shown in figure 5. This figure shows that the concentration fluctuates over time as the flow develops. The model captures this influence, not only by the fluctuations observed but also by the short-term increase

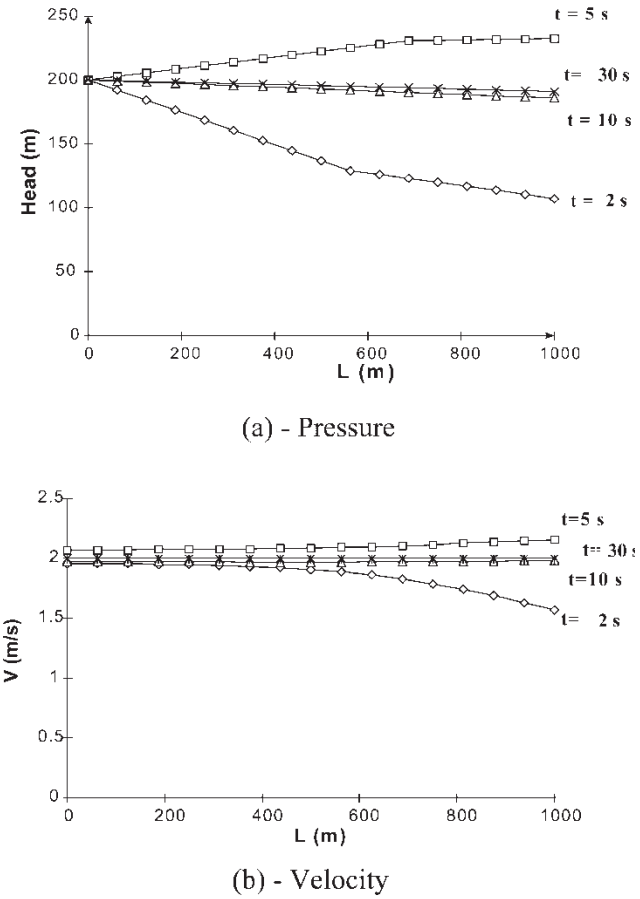

Figure 4. Pressure and velocity evolution during a transient event (K = 6 × 10^{-6} s^{-1}).

in concentration (e.g. t = 5 s) that reflects the imbalance of flows (i.e. compressibility) at this instant. As the transient flow comes into balance, the flow of water becomes uniform and, hence, concentration values stabilize. Interestingly, the direct impact of these transient events on

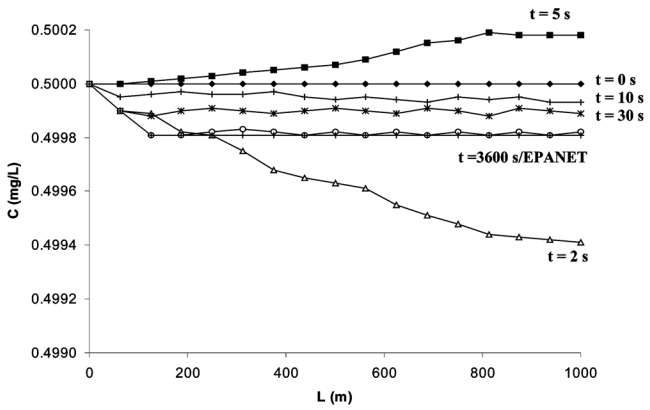

Figure 5. Concentration variation through pipe during a transient event ($K = 6 \times 10^{-6}$ s^{-1}).

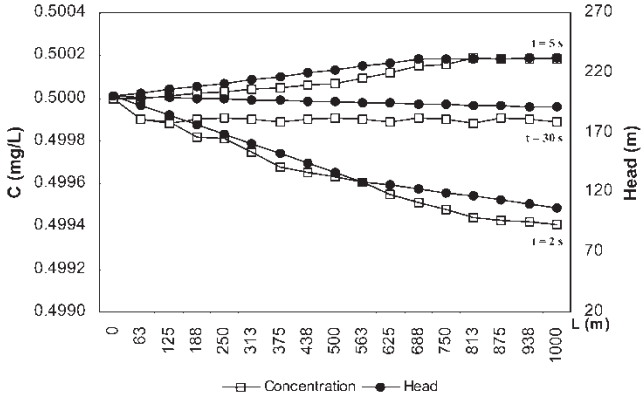

Figure 6. Physical response of the system through time.

concentrations in this system is small, even though their impact on system hydraulics is obviously significant.

For comparison, EPANET results are also included in figure 5 for a one hour water quality extended period simulation (Rossman 2000). The simulation includes a nodal demand, at the end of the pipe, with a flow variation over time corresponding to the hydraulic transient module, in order to fairly represent the transient episode. Although the EPANET results do not reproduce the short-term dynamics of the system, the overall response is quite similar. This similarity reflects the dominance of the advection and reaction components in this particular study.

Perhaps a more revealing way of presenting the results in figures 4 and 5 is provided in figure 6. This figure shows the combined plots of concentration and head variations with time for 2 s, 5 s and 30 s. As expected, the concentration profile in the system directly reflects the pressure evolution during the transient episode (i.e. 2 s and 5 s). At 30 s, when the system is almost under steady conditions, the concentration profile is stable, as is the head variation within the system. Clearly, though, this combination of system parameters does not promote a significant variation in concentration compared to the EPANET results. This similarity is due to the simulated combination of advection and reaction components. However, the minute changes in concentration nicely reflect the role of the compressibility in the hydraulic solution. Despite the initial fluctuation of concentration due to transient effects, there are only minor long-term differences between the two numerical solutions.

5.2 *Convergence to a steady concentration profile*

In order to better evaluate the proposed model, two additional computational experiments were performed and compared with EPANET results. One experiment involves a higher decay rate and the second demonstrates the propagation of a concentration front. The first experiment

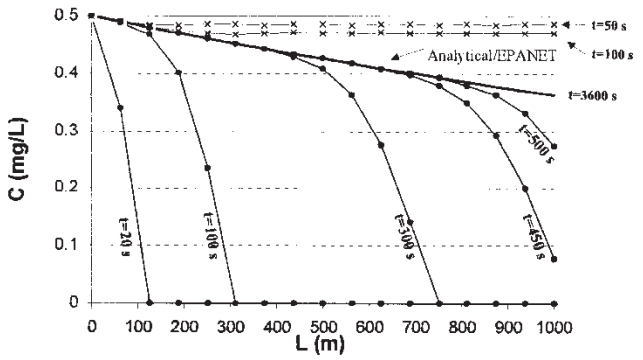

Figure 7. Concentration variation for two initial concentrations ($K = 6 \times 10^{-6}$ s^{-1}).

includes a 1 hour extended period simulation with an overall reaction decay of 6.0×10^{-5} s^{-1} (bulk flow, and wall decay constants are 5 d^{-1} and 0.90 m/d), initial concentration of $C(x = 0,t) = 0.5$ mg/L and $C(x,0) = 0.5$ mg/L, respectively. The hydraulic and water quality time steps are 0.05 and 0.5 s, respectively. The results in figure 7 emphasize the influence of a high decay rate. Transient effects are most significant during the first 20 s and appear as small (but stable) fluctuations in the trace. This plot also compares the steady state analytical solution of the ARE and EPANET results after a 1 hour extended period simulation. There is an excellent match between the two curves, with an overall relative error compared to the analytical solution of 0.01%.

The next set of computational experiments includes the analysis of the wave front evolution along a pipe, considering the same parameters as before, but with no initial concentration in the pipe (i.e. $C(x,t = 0) = 0$ mg/L). The results, also indicated in figure 7, show the concentration front evolution throughout the system. Approximately 450 s are required for the wave front to propagate through

the pipe (under steady state hydraulic conditions, this time is 500 s). The overall agreement between both the numerical results and the EPANET/analytical curve is again excellent.

An additional analysis was performed to compare modelling results for the wave front propagation at a specific time (300 s) and the analytical solution assuming a steady-state flow field for this transient case, as illustrated in figure 8. Curve 1, for a water quality time step of 0.5 s, highlights the challenges of reproducing the right position at the leading edge of the wave front. An analysis that considers a better match of the hydraulic and water quality time scales is presented through curve 2 (i.e. water quality time step equal to 1 s). The results clearly evince that the numerical differences are significantly removed; thus, better agreement is achieved when the two time scale grids are appropriately matched, as indicated by curve 2.

5.3 *Role of water exchange*

Linking transient and water quality considerations poses some challenging problems. In this case study, these issues are investigated using a specific boundary condition called an "external energy dissipater" (EED) (Karney and McInnis 1992). This element conveniently represents surge tanks, relief valves, leaky pipes, storage reservoirs, valves discharging to the atmosphere and many other common devices. The external flow is related to the head at the junction by the orifice equation and the hydraulic compatibility characteristic equations for any number of pipes are evaluated exactly as if it was at the downstream end of a single pipe. Accumulation of water in the element is accounted for through the continuity equation. In addition, this formulation updates the rate of mass transfer between the bulk fluid and the pipe wall, thus appropriately adjusting the overall reaction rate as the velocity changes.

In the current water quality formulation, the EED representing a tank is assumed completely mixed, with $C(t = 0) = Co$ as the pre-defined initial constituent concentration. The tank algorithm accounts for nonconservative constituents by including a first order decay rate within the tank. What makes this element interesting is that the tank concentration could be quite different from that found in the remainder of the pipe system.

A simple case study was designed to explore the properties of linking a hydraulic simulator that incorporates an external boundary condition at a junction, with a 1-D transport algorithm for full transient conditions in the remainder of the system. To this end, a full and rapid valve closing operation in the pipeline system is analysed in figure 9.

The specific linear valve closure operation considered here produces an ultimate steady flow reduction (via a valve operation) of 2.5 m^3/s to 0.5 m^3/s in 20 s. The flow is turbulent throughout and the system is characterized by the following parameters: a (wave propagation speed) = 1000 m/s, f (Darcy–Weisbach friction factor) = 0.031, E_S (valve size parameter) = 0.358 $m^{2.5}/s$, $H_1 = 120$ m, and $H_2 = 50$ m. In addition, the overall chlorine decay coefficient (K) is obtained using a first order bulk reaction rate of 1.0 day^{-1} and a wall reaction term of 0.45 m/day. Initial and boundary concentrations in the pipe are defined as: $C(x = 0,t) = 0.5$ mg/L and $C(x,t = 0)$ is the concentration distribution in the pipe after a 24 h residence time and decay mechanisms as previously defined. The tank is small and has a plan area of 2.5 m^2 and an initial length of water column of 4 m with an assumed initially depleted chlorine concentration of 0 mg/L. The hydraulic and water quality time steps are 0.01 and 0.1 s, respectively. The reaction rate in the tank was assumed to be 0.1 day^{-1}. The valve is relatively resistive even when fully open and the initial steady state level in the tank is thus 84 m.

The system response to the rapid valve opening requires approximately 800 s to establish the new steady state flow of 0.5 m^3/s. The head and flow variation through time, shown in figures 10 and 11, highlight the influence of transient effects in the tank. Positive flows are assumed

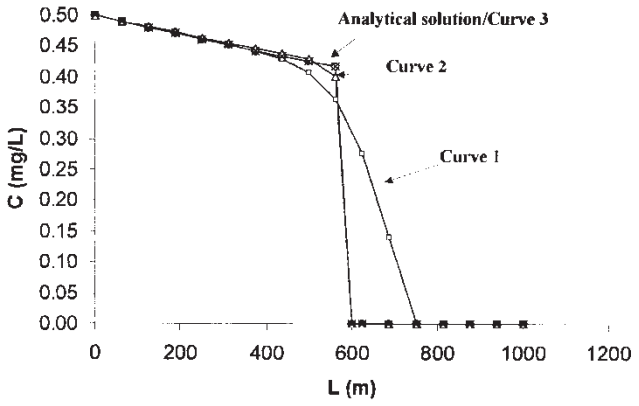

Figure 8. Wave front evolution at 500 s.

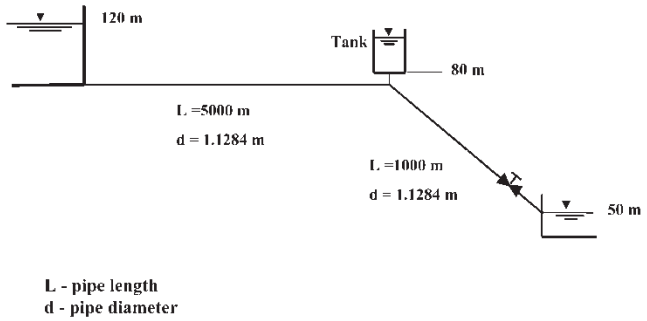

Figure 9. Pipeline system with storage.

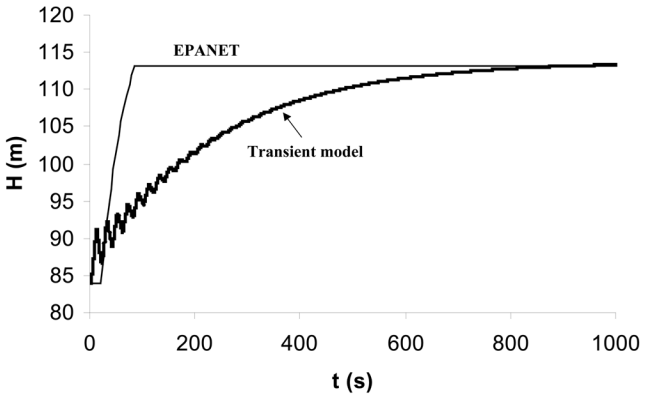

Figure 10. Water level variation within the tank.

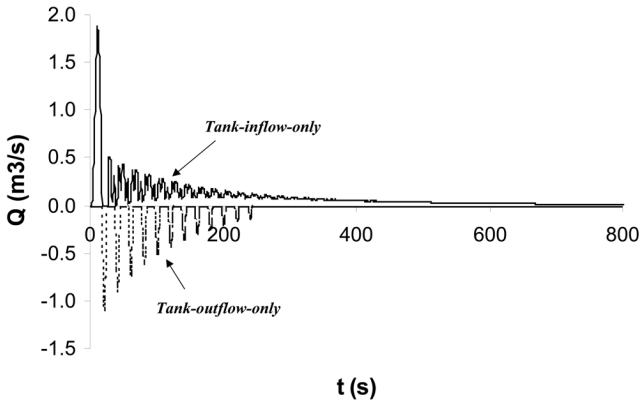

Figure 12. Alternative valve scenarios for the tank.

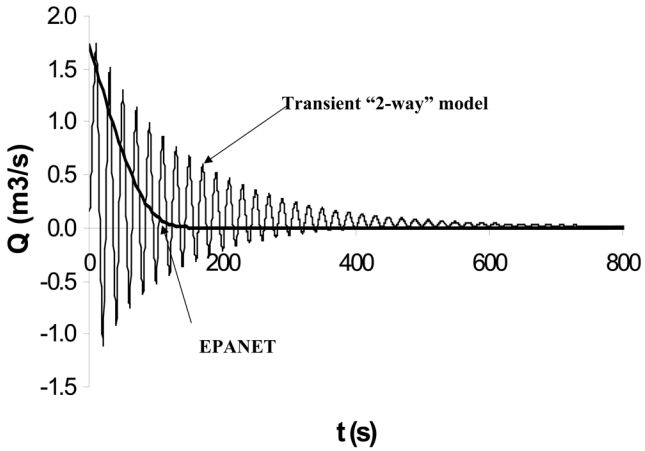

Figure 11. Flow into and out of the tank.

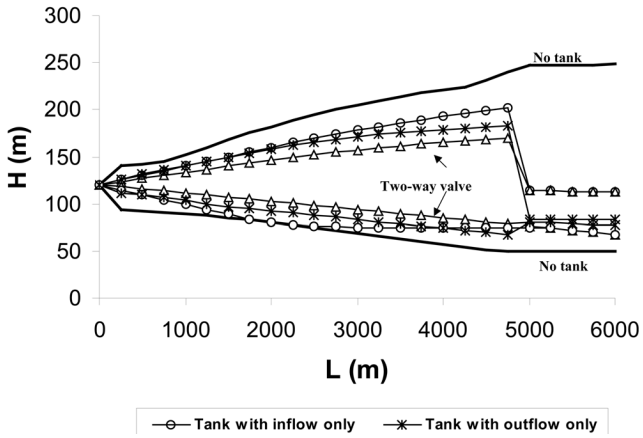

Figure 13. Maximum and minimum pressure distribution in the system.

from the pipe junction and into the tank. Transient variations are obvious in the tank for approximately 200 s, and the head changes are in the range of 84–114 m. The associated flows into the tank range from -1.0 m^3/s to $+1.6$ m^3/s. For comparison, figures 10 and 11 also show results for the same system using the quasi-steady state model EPANET. The control valve in EPANET is reproduced by a rule-based approach that establishes a new valve setting associated with a flow of 0.5 m^3/s after 20 s.

5.4 *Response with one-way tanks*

Two additional flow scenarios are created by using a ''one-way'' or check valve that allows flow either into or out of the tank. Scenario 1, defined as *tank-inflow-only*, allows flow going into the tank; Scenario 2, *tank-outflow-only*, permits flow to exit the tank, and the responses are summarized as indicated in figure 12. The *tank-inflow-only* scenario is expected to show the greatest impact of pipe water on the concentration in the tank, and the *tank-outflow-only* scenario conversely produces the greatest impact of tank water on the pipe concentrations.

The potential hydraulic implications of these scenarios are summarized through the overall maximum and minimum pressure distribution, as presented in figure 13. This plot indicates the importance of the storage device in attenuating the impact of the transient in comparison with the ''no reservoir system''. The ''two-way'' valve scenario, through its unrestricted exchange of flow, clearly limits the minimum and maximum heads.

The water quality implications of these hydraulic scenarios are represented in figure 14. The expected concentration in the tank reflects the transient flow behaviour as a consequence of the fast valve operation. The fluctuation of chlorine concentration persists for about 400 s and is more acute during the first 200 s during which the most significant pressure variation occurs in the tank. The concentration naturally reflects the imbalance of flows associated with the transient episode. In this case, chlorine

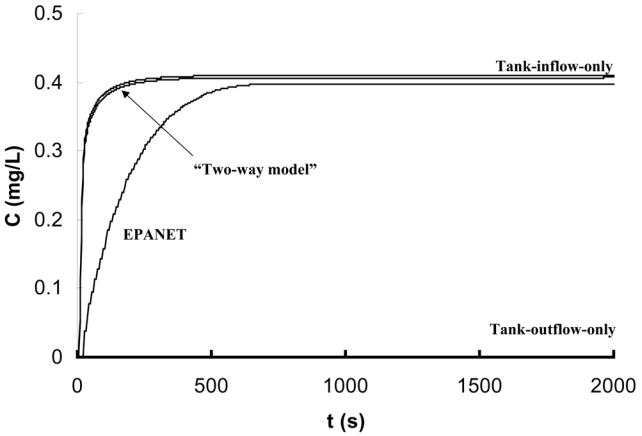

Figure 14. Concentration evolution in the tank.

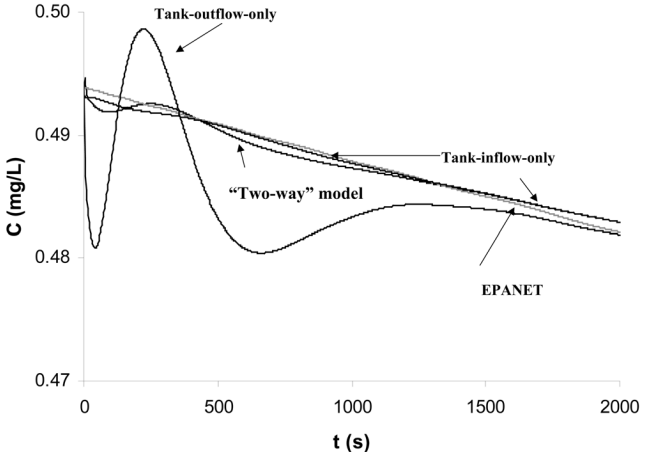

Figure 15. Chlorine concentration evolution at the downstream reservoir.

concentration in the tank builds up from 0 mg/L to 0.44 mg/L, stabilizing after 500 s when the system is essentially under steady state conditions. This concentration is practically the same obtained with EPANET model (0.39 mg/L). In this case, EPANET results are based on the same assumptions of the ''two-way'' tank, as previously described.

The *tank-inflow-only* scenario with the one-way valve into the tank clearly reveals the influence of fluid inertia on concentrations, indicating the mass rate being added to the system. The *tank-outflow-only* scenario, results in no chlorine being added to the tank, as expected, and is represented by the x-axis. EPANET simulates the system considering a ''two-way'' tank.

5.5 *Downstream concentration*

The curve labelled ''Two-way model'' shows the concentration evolution as a consequence of the flows oscillating in the tank (figure 15). The mass rate being added to or removed from the system and the inertia effects (e.g. velocity fluctuations) during the first 400 s of significant transient effects produce a concentration evolution curve that oscillates slightly between this interval of time when compared with the quasi-steady formulation. The concentration fluctuations are stabilized and are basically the same as the quasi-steady formulation at 2500 s. In this particular case, the tank not only attenuates the impact of pressure variations in the system but also attenuates the significant influence on concentrations caused by inertia effects observed in the system. The short-term decrease in concentration at 100 s is a consequence of the imbalance of flows that brings more water into the tank. The concentration variation tends to stabilize as the transient episode is attenuated.

5.6 *Additional case studies—contaminated tank*

Two additional case studies are introduced to explore potential water quality implications of a so-called transient intrusion event. These studies use the same system described in figure 9. The main difference is that the pipe system has an initial concentration equal to zero ($C(x,t = 0) = 0$ mg/L, pure water). The tank is assumed to have become contaminated by some unwanted conservative substance with an assumed initial concentration of 2 mg/L.

In the first experiment, the same valve closure operation (and hydraulic response) is again reproduced; that is, the flow is reduced from 2.5 m^3/s to 0.5 m^3/s in 20 s, as described in the previous section. The concentration profile at different locations within the system is presented in figure 16. Figure 16a shows the concentration fluctuation in the tank and the impact in the system is summarized by the concentration evolution at the downstream valve (figure 16b). The mass imported into the system as a consequence of the flow exchanged at the tank generates a maximum concentration of approximately 0.018 mg/L. Interestingly, the concentration evolution at the valve cannot be captured by the steady state simulator, since the tank in this case only captures the filling process.

By contrast, the concentration evolution at a location close to the tank is more dramatic (figure 16c). The concentration response can be significant when the transient episode is occurring in the system. Although faster in this case, concentrations can be up to 25 times higher than at the downstream end of the system, indicating that a user near a contaminated tank would be at considerable risk from exposure, but that dilution does improve the response elsewhere.

The final case study is based on the same system but the transient episode is now induced by a valve opening

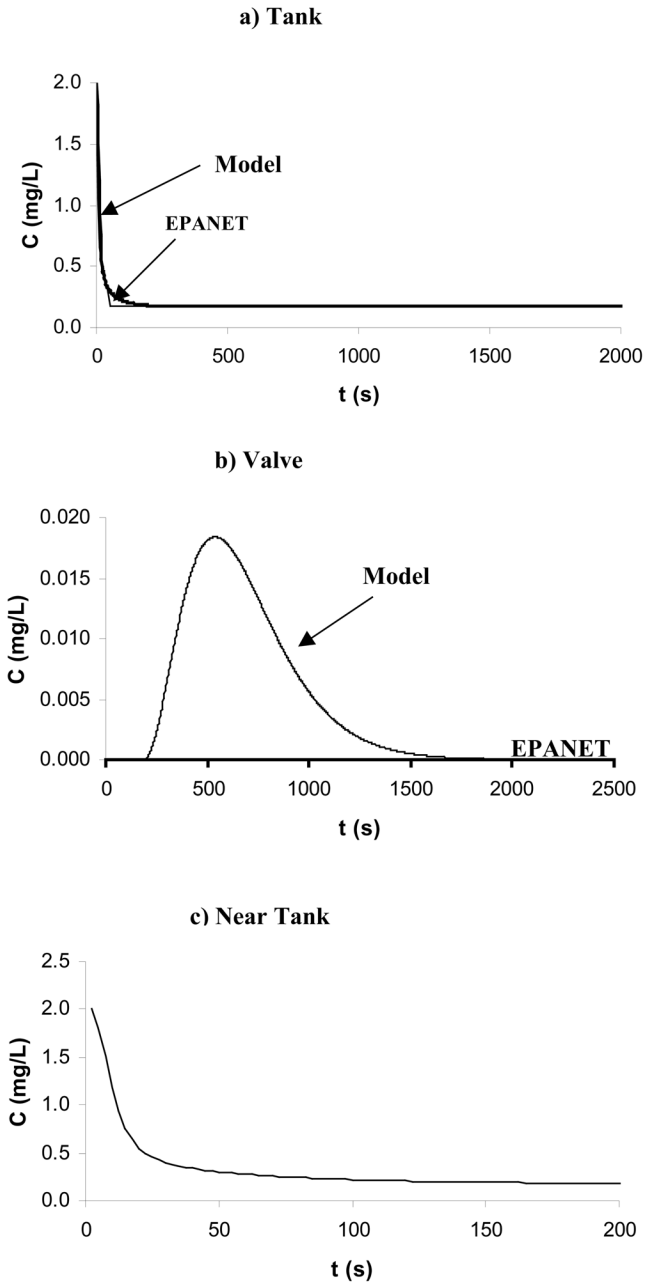

Figure 16. Concentration variation in different locations for valve closure.

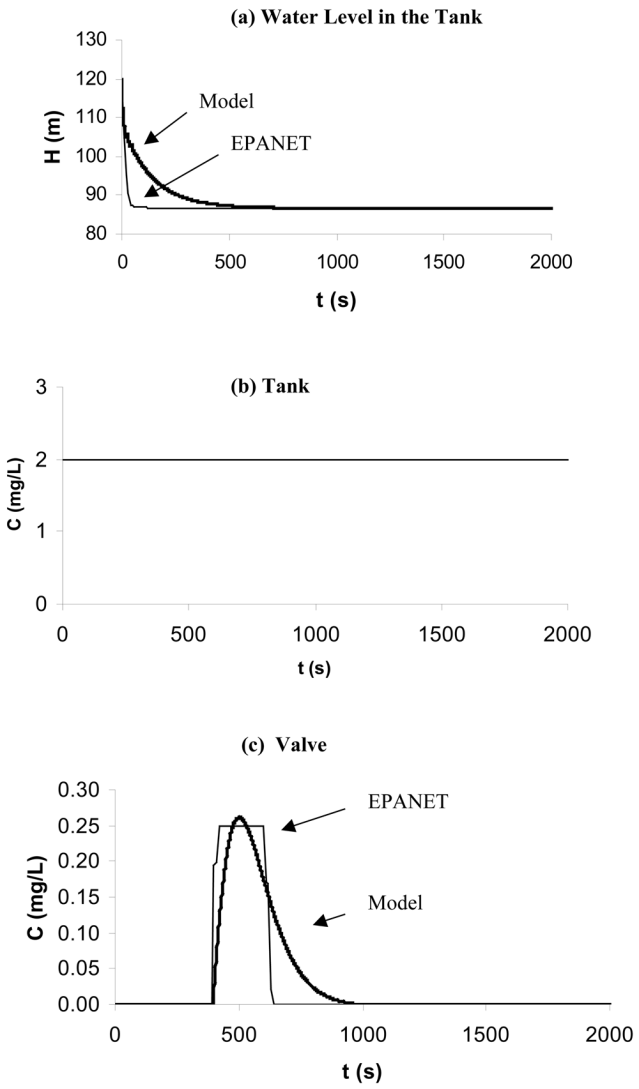

Figure 17. Concentration variation in different locations for valve opening.

operation that allows steady flows to change from zero to 2.5 m^3/s in 20 s. As before, the tank has an initial concentration of 2 mg/L of a conservative substance, and the system is initially uncontaminated ($C(x,t = 0) = 0$ mg/L). Figure 17a shows the water-level variation in the tank as a consequence of the valve operation that promotes a water level fluctuation decreasing from 120 m to 86.7 m in approximately 400 s as a consequence of the transient episode. EPANET results reproduce the physical response, but the steady balance occurs in approximately 100 s. Concentration in the tank is conserved at 2.0 mg/L as the reservoir is being emptied (figure 17b).

The significant impact is at downstream valve. Figure 17c summarizes the concentration evolution of the conservative substance as a result of delivery into the system during the transient. This response is approximated by EPANET, but in a way that under-predicts the duration of the intrusion event.

6. Discussion

It should be emphasized that the tank model formulated here is quite general. In essence, a storage or exchange of fluid is envisioned, and no actual tank need be present. In particular, the "tank" could even represent a leaky pipe

and its associated volume of soil surrounding the leak. Importantly, this last scenario implies that intrusion concerns, relating to drawing contaminated water into a pipe, such as at a leaky segment experiencing pressure fluctuation, may be partly mitigated by the usual ''in-and-then-out'' behaviour expected at a leak or external storage element. Nonetheless, the general concerns with intrusion events are not eliminated.

An interesting indication of how inertia effects can impact constituent concentration in the system is highlighted by the curve obtained from *Tank-outflow-only* scenario in figure 15. Here a check valve at the tank node is used to simulate the use of a reservoir as a ''one-way'' surge tank to compensate for low or negative pressures. In this case, flow is added to the system from the tank when the pressure difference is favourable. The impact is a decrease in concentration (to approximately 0.48 mg/L in the pipe), especially at the end of the transient episode (particularly after 100 s). As these transient effects are attenuated, the system compensates through a short-term relative increase in concentration until it arrives at the level of steady conditions after about 2000 s.

For the one-way valve that allows flow into the tank (*Tank in only Scenario*), the constituent concentration does not fluctuate significantly compared with the ''two-way'' model results. This relief-valve-like operation results in an overall water quality response quite similar to a protection system that simply floats on the hydraulic system.

7. Conclusions

This paper extends increases the range of applications available to water quality modelling. It presents a transient water quality modelling approach that faithfully represents a hydraulic model whether it is in a quasi-steady, an unsteady incompressible, or a rapidly unsteady state. A distinct numerical solution for the mass transport equation with reaction is developed and superimposed on the MOC hydraulic solution, one that is used whenever the advection process is dominant (i.e. turbulent flow conditions).

The strategy of superimposing the transport algorithm onto a MOC-based hydraulic solution of the pipeline system has revealed promising and encouraging results. The benefit of this contribution relies on an appropriate resolution of the dynamic balance between accuracy and simplicity. The transport algorithms are easily implemented in terms of coding strategy and do not require substantial memory; the numerical solution is stable, consistent and convergent, and the approach is intrinsically compatible with the transient hydraulic simulation.

Although water quality models can at times be quite simple, the protection of water quality itself is an extremely difficult and complex issue. There is no doubt that environmental degradation of source watersheds due to inappropriate soil and land use, inadequate environmental controls and other factors occurs. This is a stochastic condition with many variables that are not easily identified or controlled. One of these variables is the distribution system itself in which dynamic interactions can exacerbate these issues. For example, the addition of a new main can change the basic configuration of a system (and its hydraulic response), as can the switching of pumps, the operation of valves, and the water quality at the intake. In some cases, under rapidly changing conditions water quality predictions based on the current quasi-steady state modelling strategy need to be reconsidered.

These implications are particularly relevant to modelling the mass transport process in distribution systems. This paper provides a tool that permits representation of the system response under the influence of dynamic conditions. The resulting numerical procedure facilitates evaluation of system behaviour with complex boundary conditions, especially those requiring the coupled prediction of hydraulic and water quality conditions. In particular, it permits a better understanding of the role of compressibility and leaks on water quality and sets the stage for prediction of the interactions between the velocity profile and shear stress under different flow conditions. Moreover, these numerical schemes offer an alternative to traditional water quality models that compute transport components based solely on steady or quasi-steady state assumptions. In addition, the ARE model can serve as a benchmark technique for assessing the accuracy of other simplified methods for estimating contaminant and pathogen intrusion advection in distribution systems.

Acknowledgments

The authors acknowledge financial support from CAPES (Brazilian sponsoring agency), the Natural Science and Engineering Research Council (NSERC) of Canada and the Canadian Water Network.

References

Axworthy, D. and Karney, B.W., Modelling low velocity/high dispersion flow in water distribution systems. *J. Wat. Resources Plann. Mgmt*, 1996, **122**, 218–221.

Boccelli, D. and Uber, J., Evaluation of multicomponent model of chlorine residual dynamics in water distribution systems. In *Water Software Systems: Theory and Applications*, edited by B. Ulanicki, B. Coulbeck and J. Rance, Vol. 1, pp. 195–210, 2001 (Research Studies Press).

Boulos, P., Altman, T., Jarrige, A. and Collevati, F., An event-driven method for modelling contaminant propagation in water networks. *J. appl. Math. Modelling*, 1994, **18**, 84–92.

Boulos, P., Altman, T., Jarriage, P. and Collevati, F., Discrete simulation approach for network water quality models. *J. Wat. Resources Plann. Mgmt*, 1995, **121**, 49–60.

Brunone, B. and Ferrante, M., Pressure waves as a tool for leak detection in closed conduits. *Urban Wat. J.,* 2004, **1**, 145–155.

Brunone, B., Karney, B., Mecarelli, M. and Ferrante, M., Velocity profiles and unsteady friction in transient flow. *J. Wat. Resources Plann. Mgmt,* 2000, **126**, 236–244.

Celia, M., Russel, T., Herrera, I. and Ewing, R., An Eulerian-Lagrangian localized adjoint method for the advection diffusion equation. *Adv. Wat. Resources*, 1990, **13**, 187–206.

Elton, A., Brammer, L. and Tansley, N., Water quality modelling in distribution networks. *J. Am. Wat. Works Ass.*, 1995, **87**, 44–52.

Grayman, W., Clark, R. and Males, R., Modelling distribution water quality: dynamic approach. *J. Wat. Resources Plann. Mgmt*, 1988, **114**, 295–312.

Grayman, W., Rossman, L., and Geldreich, E., Water quality. In: *Water Distribution System Handbook*, edited by L. Mays, Chap. 9, 2000 (McGraw-Hill: New York).

Hoffman, J., *Numerical Methods for Engineers and Scientists*, 2001 (Marcel Dekker: New York).

Islam, M. and Chaudhry, M., Modelling the constituent transport in unsteady flows in pipe networks. *J. Hydraulic Engng*, 1998, **124**, 1115–1124.

Karney, B.W. and Guidaoui, M., Flexible discretization algorithm for fixed-grid MOC in pipelines. *J. Hydraulic Engng*, 1997, **123**, 1004–1011.

Karney, B.W. and McInnis, D., Transient analysis of water distribution systems. *J. Am. Wat. Works Ass.*, 1990, **82**, 62–70.

Karney, B.W. and McInnis, D., Efficient calculation of transient flow in simple pipe networks. *J. Hydraulic Engng*, 1992, **118**, 1014–1030.

LeChevallier, M., Coliform regrowth in drinking water: a review. *J. Am. Wat. Works Ass.*, 1990, **82**, 74–86.

Liou, C. and Kroon, J., Modelling the propagation of waterborne substance in distribution networks. *J. Am. Wat. Works Ass.*, 1987, **79**, 54–58.

McInnis, D., A relative-risk framework for evaluating transient pathogen intrusion in distribution systems. *Urban Wat. J.*, 2004, **1**, 157–166.

Rossman, L., *EPANET Users Manual*, 2000 (Water Supply and Water Resources Division. National Risk Management Research Laboratory, US Environmental Protection Agency: Cincinnati, Ohio).

Rossman, L. and Boulos, P., Numerical methods for modelling water quality in distribution systems: a comparison. *J. Wat. Resources Plann. Mgmt*, 1996, **122**, 137–146.

Rossman, L., Boulos, P. and Altman, T., Discrete volume-element method network water-quality models. *J. Wat. Resources Plann. Mgmt*, 1993, **119**, 505–517.

Strikwerda, J., *Finite Difference Schemes and Partial Differential Equations*, 1989 (Wadsworth and Brooks/Cole Advanced Books and Software: Pacific Grove, California).

Wylie, E. and Streeter, V., *Fluid Transients in Systems*, 1993 (Prentice-Hall: Englewood Cliffs, New Jersey).

Appendix I. Numerical analysis of the ARE formulation

This appendix summarizes the main properties of consistency, order, stability and convergence of the explicit finite difference scheme proposed [equation (11)].

Consistency

Writing the Taylor series expansion for the base point (x,t) in figure 1, and expanding all terms of the FDE represented by equation (11), the first form of the MDE can be expressed as:

$$\frac{\partial C}{\partial t}=\frac{2C}{\alpha_1}\left(\frac{U_T}{\Delta x}=K\right)-\left(\frac{\partial^2 C}{\partial t^2}\frac{\Delta t}{2}+\frac{\partial^3 t}{\partial t^3}\frac{\Delta t^2}{6}+K\right)-\frac{\alpha_2}{\alpha_1}\left(\frac{\partial C}{\partial x}+\frac{\partial^2 C}{\partial x^2}\frac{\Delta x}{2}+\frac{\partial^3 C}{\partial x^3}\frac{\Delta x^2}{6}+K\right)+-\left(\frac{\alpha_3}{\alpha_2}\frac{\partial^2 C}{\partial x\partial t}\Delta x+\frac{\partial^3 C}{\partial x^2\partial t}\frac{\Delta x^2}{2}+K\right) \tag{18}$$

where, $U_1=U_x^t$, $U_2=U_x^{t+1}$, $U_3=U_{x+1}^t$ and $U_4=U_{x+1}^{t+1}$. Additional definitions for clarity:

$$\alpha_1=2+K\Delta t+(U_4-U_2)\frac{\Delta t}{\Delta x} \tag{19}$$

$$\alpha_2=\frac{K\Delta x}{2}+U_3+U_4 \tag{20}$$

$$\alpha_3=1+\frac{K\Delta t}{2}+U_4\frac{\Delta t}{\Delta x} \tag{21}$$

Additionally, if the velocities are uniform, $U_1=U_2=U_3=U_4=U$, the MDE is reduced to the advection equation with reaction traditionally solved in water quality models and given by:

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}=-KC \tag{22}$$

Order

The order of a finite difference approximation of a partial difference equation is the rate at which the global error of the finite difference solution approaches zero as the sizes of the grid spacing approach zero (Hoffman 1992). This equation is obtained by eliminating the higher-order time and mixed time and space derivatives from the first form of MDE [equation (18)]. If a truncation over the second order derivative is considered the following equation can be obtained:

$$\left(1+\frac{U_T}{\alpha_1}\frac{\Delta t}{\Delta x}-\frac{K\Delta t}{\alpha_1}+\frac{KU_T}{2\alpha_1^2}\frac{\Delta t^2}{\Delta x}-\frac{2K^2}{3\alpha_1^2}\Delta t^2+K\right)\frac{\partial C}{\partial t}=\frac{2C}{\alpha_1}\left(\frac{U_T}{\Delta x}-K\right)+\left(\frac{\alpha_2}{\alpha_1}+\frac{2\alpha_3 U_T}{\alpha_1^2}+\frac{2K\alpha_3}{\alpha_1^2}\Delta x+\frac{\alpha_3 U_T^2}{\alpha_1^3}\frac{\Delta t}{\Delta x}-\frac{4K\alpha_3 U_T}{\alpha_1^3}\Delta t+\frac{2K^2\alpha_3^2}{\alpha_1^3}\Delta x\Delta t+K\right)\frac{\partial C}{\partial x}-\left(\frac{\alpha_2\Delta x}{2\alpha_1}-\frac{\alpha_2\alpha_3\Delta x}{\alpha_1^2}-\frac{K\alpha_3\Delta x^2}{\alpha_1^2}+\frac{\alpha_3 U_T\Delta x}{\alpha_1^2}-\frac{\alpha_2\alpha_3 U_T\Delta t}{\alpha_1^3}-\frac{K\alpha_2\alpha_3\Delta x\Delta t}{\alpha_1^3}\Delta x\Delta t+-\frac{\alpha_2\Delta t U_T}{2\alpha_1^2}+\frac{K\alpha_2\Delta x\Delta t}{2\alpha_1^2}-\frac{2\alpha_3^2 U_T\Delta x}{\alpha_1^3}+\frac{2K\alpha_3^2\Delta x^2}{\alpha_1^3}+K\right)\frac{\partial^2 C}{\partial x^2} \tag{23}$$

When the flow velocity is steady and uniform, the velocities $U_1 = U_2 = U_3 = U_4 = U$ and the constant U_T is zero. Thus, equation (23) is reduced to an expression as:

$$\frac{\partial C}{\partial t} = a_1 \frac{\partial C}{\partial x} + a_2 \frac{\partial^2 C}{\partial x^2} - a_3 \tag{24}$$

where a_1, a_2, and a_3 are constants values function of α_1, α_2, α_3, α_4, Δt , Δx and the reaction term K.

Stability

Stability is often analysed with the Von Neumann method. This method consists of establishing the exact solution of the FDE obtained for the general Fourier component of a complex series representation of the initial property distribution being analysed. Strikwerda (1989) demonstrates that the stability criterion of a FDE is based upon the interpretation of the amplification factor G. This factor is the single-step exact solution of the FDE for the general Fourier component, which must be less than unity for a bounded solution.

The amplification factor is determined by substituting the complex Fourier components for $C^t_{x\pm1}$ and $C^{t+1}_{x\pm1}$ into the FDE. In general, the behaviour of the amplification factor G is investigated over the range of $0 \leqslant (\theta = K\Delta x) \leqslant 1$, where θ refers to sine and cosine functions with a period of 2π and is given by:

$$C^{t+1}_{x\pm1} = GC^t_x \tag{25}$$

and the Fourier components given by the following equations: $C^{t+1}_{x+1} = GC^t_x e^{i\theta}$, $C^{t+1}_x = GC^t_x$, $C^t_{x+1} = C^t_x e^{i\theta}$, $e^{i\theta} = \cos\theta + i\sin\theta$ and $i = \sqrt{-1}$.

Thus, substituting the general Fourier components in the FDE [equation (11)], equation (17) can be obtained. To ensure a bounded solution, the amplification factor, that in general is a function of $\frac{U_i \Delta t}{\Delta x}$, is now dependent on values of E_1, E_2, E_3 and E_4. As a consequence, the values of transient velocities are remarkably determinant to the behaviour of the amplification factor.

For the particular case where velocities $U_1 = U_2 = U_3 = U_4 = U$ (the steady state case), and $\frac{U\Delta t}{\Delta x} = 1$, the absolute values of E_2 and E_3 are close to zero and, E_1 and E_4 close to 2. In this case, the amplification factor G [equation (17)] can be represented approximately by:

$$G = \frac{1}{(\cos\theta + i\sin\theta)} \tag{26}$$

Equation (26) represents an ellipse in the complex plane that lies within the unit circle, guaranteeing a stable amplification factor.

Appendix II. Notation

The following symbols are used in this paper:

Symbol	Meaning
A	= pipe cross-sectional area (m^2);
a	= wave propagation speed (m/s);
C	= constituent concentration at a given time and nodal location (mg/L);
$C_i(x,t)$	= constituent concentration at a time t and position x (mg/L);
C_r	= Courant number;
D	= diffusion coefficient matrix; coefficient of longitudinal dispersion (m^2/s);
d	= pipe diameter (m);
Δt	= water quality time step (s);
ΔV	= volume of the control volume (m^3);
Δx	= spatial discretization (m);
E_s	= valve size parameter ($m^{2.5}$/s);
E_1, E_2, E_3, E_4	= known values for concentration calculation in the explicit model;
$f(C_i(x,t))$	= function or set of functions defining the chemical and biological reactions;
F	= Darcy–Weisbach friction factor;
G	= amplification factor;
G	= acceleration due to gravity (9.8 m/s^2);
H_1, H_2	= upstream (downstream) reservoir static head (m);
J_{in}	= flux of mass that is coming in through the control volume (mg/m^2s);
J_{out}	= flux of mass that is coming out through the control volume (mg/m^2s);
K	= coefficient of chlorine concentration decay rate (s^{-1});
L	= pipe length (m);
$O(t)$	= valve opening operation time;
$S(C_i(x,t))$	= function defining any sources or sinks within the pipe;
t	= time nodal location;
$t+1$	= next time nodal location;
$\vec{u}$	= velocity vector (m);
$U(x,t)$	= velocity at position t and time x;