NUMERICAL SOLUTION OF THE ADVECTION-DISPERSION-REACTION EQUATION UNDER TRANSIENT HYDRAULIC CONDITIONS

Cristovao Fernandes and **Bryan Karney**

Department of Civil Engineering, University of Toronto

35 St. George Street, Toronto, Ontario

Canada, M5S 1A4. Phone/fax: (416) 978-7776

E-mail: fernand@ecf.utoronto.ca, karney@civ.utoronto.ca

Abstract: Solving or approximating the advection-diffusion/dispersion equation (ADE) is a challenging and important problem and has thus motivated a great deal of intense research. A specific complication arises from the nature of the governing partial differential equation: it is characterized by a hyperbolic non-dissipative advective transport term, a parabolic dissipative diffusive (dispersive) term and, possibly, an additional reaction/decay mechanism. In most pipeline applications, the numerical transport scheme is coupled to a steady or nearly steady hydraulic model. By contrast, this paper presents an implicit finite difference scheme for the solution of the advection–dispersion-reaction (ADR) superimposed on unsteady, method of characteristics (MOC) based, hydraulic solution. This contribution represents one of the first serious attempts to analyze the impact of water hammer conditions, and in particular fluid inertia and compressibility, on the evolution of water quality in pipe networks.

Keywords: water quality, transient, water hammer, chlorine, and distribution systems

1 INTRODUCTION

As water transits through a distribution system its quality undergoes important changes as a result of complex physical, chemical and biological processes. Thus, an appropriate water quality models represents a valuable tool for predicting the fate, transport and transformation of various water-born substances, especially for design and operational purposes. One potential water quality degradation process has been almost completely neglected in the modeling literature is the impact of transient flow conditions. The risk of pipe failure due to a significant pressure variation - or the possibility of making biofilms, corrosion and/or tuberculation on the pipe wall more susceptible to transport by high velocities - are two obvious and significant consequences. Another mechanism is associated with the role of velocity profile and shear stress that can affect mass transport in the system (Brunone et al., 2000).

This paper addresses one aspect of water quality modelling by presenting a numerical solution for the advection-dispersion-reaction equation considering water hammer effects,

with particular emphasis to low velocity or laminar flow conditions. The proposed approach is an implicit finite difference scheme superimposed on a method of characteristics (MOC) transient simulation program. The case study analyzed reflects the potential of the method, especially as a foundation for the integrated analysis and design of water distribution systems as suggested by Fernandes and Karney (1999).

2 WATER QUALITY MODELLING IN WATER DISTRIBUTION SYSTEMS

Quite generally, water quality models are products of two basic modules. The first predicts the hydraulic conditions in the system. Traditionally steady state models have been used and more recently rigid water models have gained importance for the analysis and design of water distribution systems. In this paper, full one-dimensional transient model is coupled to the transport mechanism. In fact, the hyperbolic partial differential equations of momentum and continuity (Wylie and Streeter, 1993) are first solved and then the same numerical grid is used as the basis of the water quality simulation.

More precisely, the second or water quality component, is dependent on the hydraulic model to evaluate flow paths in the pipeline system, the mixing from different sources, the dilution of contaminants and the travel/detention times. The primary water quality processes within a pipe are advection, diffusion and dispersion, chemical reactions, biological reactions, interactions at the inner pipe surface and external sources and sinks. These processes can include the simultaneous transport of multiple substances and their interactions. The mass transport of a single chemical, herein described for chlorine decay, is the 1-D advection-dispersion-reaction equation (ADR), and without source and sink terms, represented by

$$\frac{\partial C_i(x,t)}{\partial t} + u_i \frac{\partial C_i(x,t)}{\partial x} = D\frac{\partial^2 C}{\partial x^2} - KC_i(x,t) \quad (1)$$

in which $C(x,t)$ is the substance concentration at a point x is the spatial dimension, u_i the transient velocity, D is the dispersion coefficient, and t is the temporal variable. The water quality models in water distribution systems presented in the literature are, quite generally, based on the solution of the unsteady advection equation with reaction (D=0) to represent the overall mechanisms of mass transport within the system. This assumption is usually justified by the general hydraulic nature of systems under turbulent flow conditions. In other respects, the flow characteristics are generally considered steady and uniform and the advection is assumed to be the main mass transport mechanism.

Under laminar flow conditions, these assumptions must be reconsidered, mainly because of the characteristics of the related transport mechanisms and the significance influence of longitudinal dispersion in the concentration evolution through the system. Axworthy and Karney (1996) and Buchberger et al. (1999) focus on these characteristics, not only describing the physical aspects of this problem but also emphasizing the importance of a new systematic approach to take these matters into account.

3 NUMERICAL FORMULATION

Although formally parabolic, the ADE (eq. 1) propagates information by both advection and diffusion/dispersion. Because these processes occur at different time scales, the resultant numerical scheme should account for this interaction in order to achieve the required numerical criteria of stability, convergence and consistency. Moreover, transient (inertia and compressibility) effects dictate a not only a finite signal propagation speed, but also one that is now changing in time. As a consequence, time marching methods (Hoffman, 1992), usually suggested for solving PDE's of this nature, are not necessarily appropriate. For these and other reasons, the authors sought an alternative numerical procedure.

It has been reported that when diffusion dominates physical process, the standard finite difference method (FDM) or the finite element method (FEM) produces satisfactorily results. On the other hand, when advection is dominant many numerical non-physical oscillations and numerical diffusion have been described (Al-Lawatia et al., 1999).

Although these numerical issues commonly described in the literature, the definition of the numerical scheme to solve equation (1) was done mainly because two important features of the MOC solution for the hydraulic scheme. The first one arises because the MOC is a numerical procedure that is based upon the integration of momentum and continuity equations over a fixed-grid (Karney and McInnis, 1992). The result is a popular scheme with excellent computational speed and accuracy. Second, a small hydraulic step is required to guarantee the numerical accuracy and stability of the transient flow solution. The combination of both features can be linked to a suitable control volume definition, while accounting for the varying velocity. In this way, the finite difference method is used to present the solution for the advection equation with reaction taking into account the basic grid for the hydraulic simulation. The formulation presented here is an implicit finite difference scheme based upon the mass flux in a given control volume, considering transient velocities.

Previous algorithms for solving equation (1), including Eulerian methods and Eulerian-Lagrangian methods (Celia et al., 1990), have generally been based on the same assumptions, with the exception of the transient velocity field assumed here. One notable characteristic of these methods is the requirement of a small time step to properly account for the different time scales involved.

A direct solution of (1) along the transport path creates a mismatch in the time scales between the advection and water hammer velocities. Although this time-step problem can be partially overcome by interpolating the velocity field in the advection calculation, an alternate procedure is proposed here. Specially, the mass flux is accumulated over a number of hydraulic steps to appropriately extend the water quality time step. Thus, the space-time (x-t) grid arising from the MOC procedure (Fig. 1) is used to define a suitable finite difference grid.

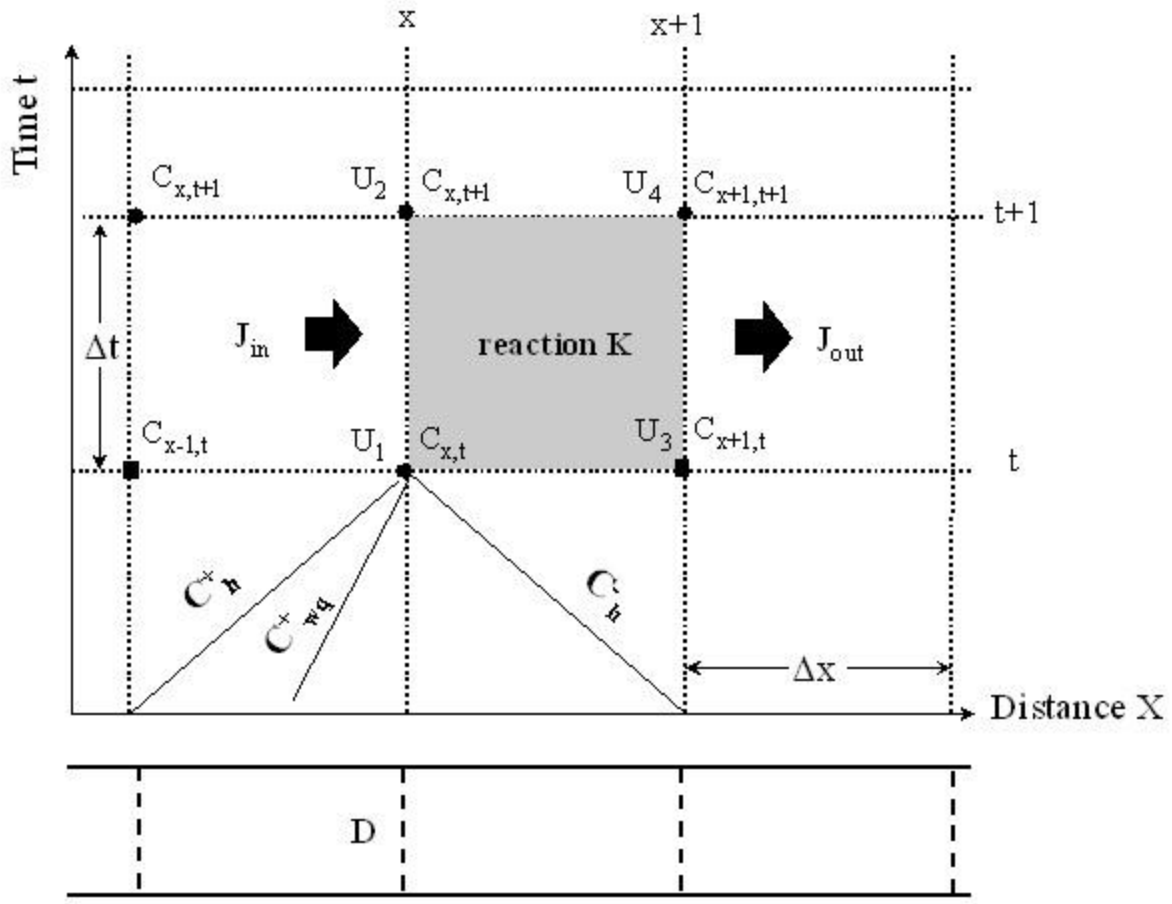

Fig.1 X-t grid and control volume definition

The following definitions are useful: t = as the index control for the i^{th} time step and x = spatial increment; A = cross sectional area; J_{in} = flux of mass entering the control volume; J_{out} = flux of mass that is leaving the control volume; ΔV = volume; and K= chemical reaction sink. It is assumed that disinfectant/constituent concentration source is constant and known for $C(0,t)$ (Dirichlet boundary condition). The initial condition $C(x,0)$ is assumed known, either measured from previous studies or from an extended period analysis. Thus, the mass balance equation for the defined control volume can be written as:

$$V\frac{\partial C}{\partial t} = (J_{in} - J_{out})A - KV\overline{C} \quad (2)$$

where $\overline{C}$ is the average concentration in the control volume, based upon the concentrations for the grid points of a given control volume (C_{x-1}^{t}, C_{x-1}^{t+1}, C_{x}^{t}, C_{x}^{t+1}). Clearly, the mass flux rate will change as the velocities change. As a first solution, consider an approximation based on average concentrations at time t and $t+1$ for both

mass fluxes and decay rate. This assumption is justified because of the small hydraulic time step in the MOC solution. As usual, a finite difference procedure is accomplished by using Taylor series expansion of the dependent variable about the grid point *(x,t).* Because velocities are changing, the time derivative is approximated using the average derivatives for time positions *i* and *i+1.* Thus, neglecting the error term, the forward-time approximation can be written as:

$$\frac{\partial C}{\partial t} = \frac{\left(C_x^{t+1} + C_{x-1}^{t+1}\right) - \left(C_x^t + C_{x-1}^t\right)}{2\Delta t} \quad (3)$$

The net mass flux rate from the control volume (see figure 1) is based upon the average at time positions *t* and *t+1* and is given, after expansions, by:

$$J_{in} - J_{out} = \frac{\left(C_{x-1}^t U_{x-1}^t + C_{x-1}^{t+1} U_{x-1}^{t+1}\right) - \left(C_x^t U_x^t + C_{x-1}^t U_{x-1}^{t+1}\right)}{2} + \frac{D}{2\Delta x}\left(C_{x+1}^t + C_{x+1}^{t+1} - 2\left(C_x^t + C_x^{t+1}\right) + C_{x-1}^t + C_{x-1}^{t+1}\right) \quad (4)$$

Substituting into equation (2), equations (3) and (4), implies the following implicit finite difference equation solved using the Thomas algorithm (Hoffman, 1992):

$$K_3 C_{x-1}^{t+1} + K_4 C_x^{t+1} - \frac{D\Delta t}{\Delta x^2} C_{x+1}^{t+1} = K_1 C_{x-1}^t + K_2 C_x^t - \frac{D\Delta t}{\Delta x^2} C_{x+1}^t \quad (5)$$

where the known values of *K* are function of known velocities at the four grid point base:

$$K_1 = 1 + U_{x-1}^t \frac{\Delta t}{\Delta x} - \frac{K\Delta t}{2} + \frac{D\Delta t}{\Delta x^2} \quad (6)$$

$$K_2 = 1 - U_x^t \frac{\Delta t}{\Delta x} - \frac{K\Delta t}{2} - \frac{2D\Delta t}{\Delta x^2} \quad (7)$$

$$K_3 = 1 - U_{x-1}^{t+1} \frac{\Delta t}{\Delta x} + \frac{K\Delta t}{2} - \frac{D\Delta t}{\Delta x^2} \quad (8)$$

$$K_4 = 1 + U_x^{t+1} \frac{\Delta t}{\Delta x} + \frac{K\Delta t}{2} + \frac{2D\Delta t}{\Delta x^2} \quad (9)$$

A numerical requirement for this procedure is to include of an artificial grid point with known initial concentration to allow the calculation of the dispersion term for the last grid point (boundary condition). In this formulation, the concentration of the artificial grid point is the value of the concentration of the last physical grid point, updated each time step.

4 CASE STUDY

In order to evaluate the potential of the proposed numerical scheme a full valve opening operation in a single pipeline is analyzed. The flow is laminar and characterized by the parameters included in Figure 2. The overall chlorine decay coefficient K=6.0 10^{-6} s^{-1}

when the bulk flow and wall decay constants are 0.3/d and 0.08 m/d. Initial concentration are defined as: $C(x=0,t)$ = 0.5 mg/L and $C(x,0)$ = 0 mg/L. This system requires about 20 s to establish the steady state flow velocity of 0.019 m/s.

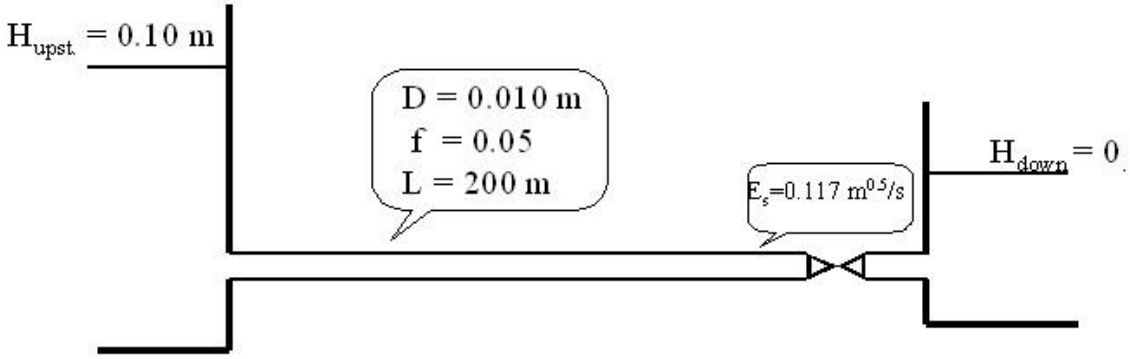

Fig.2 System description

Figure 3 summarizes the concentration evolution through the pipe at different time intervals for an extended period of 1hr. This plot summarizes the evolution of concentration by comparing two different curves, those with and without longitudinal dispersion. The ADR model refers to the solution of the proposed model, with longitudinal dispersion obtained based upon Taylor's theory. The AR model is the advection-reaction model solved by considering D=0 in (4). The influence of transient effects is significant for the first 20 s, and it takes approximately 1800 s for the front wave get through the pipe. It is evident that under laminar conditions dispersion is important and has a noticeable influence on constituent spreading. After 1800 s, the system is characterized by steady conditions and the model closely tracks the analytical solution of equation (1) (Axworthy and Karney, 1996). Additionally, due to space limitations, we have not included any formal numerical analysis to assure the specific range of cell Peclet number that are required to guarantee the numerical stability and consistency of the proposed model. However, numerical experiments show that for a range of Pe between 10^{-5} to 10^{-3}, results positively stable and consistent in the present example.

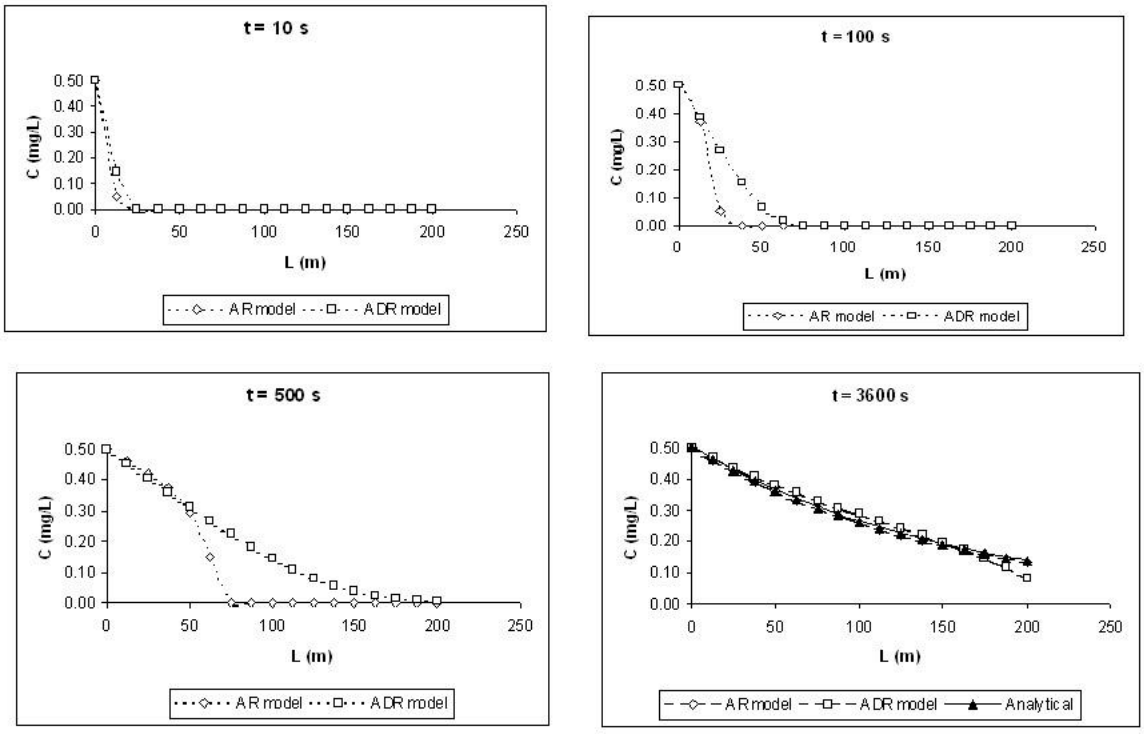

Fig.3 Wave front evolution through pipe under laminar transient conditions

5 FINAL COMMENTS

The numerical solution for the advection-dispersion-reaction equation proposed in this paper is an implicit finite difference method developed as consequence of the characteristics of the hydraulic solution given by the method of characteristics. The computational cell defined to represent the control volume is the chore justification of the proposed solution. The result is a quite simple formulation for the unknown concentration of a given constituent in a given time step. The model captured the impact of the transient flow propagation by increasing the concentration at a given point, but not affecting numerical stability and convergence. In this sense, the comparison with the analytical solution of the system analyzed by Axworthy and Karney (1996) is positively a good indication of the potential of this formulation. The results are potentially positive regarding that the purpose of identification the impact of transient conditions over main water quality issues in water distribution systems.

Acknowledgements

The authors acknowledge the financial support from CAPES (Brazilian Sponsoring Agency) and NSERC (Canada).

References

Al-Lawatia, M., Sharpley, R. C., and Wang, H.(1999). Second-order characteristic methods for advection-diffusion equations and comparison to other schemes. Advances in Water Resources, vol. 22, no.7, 741-768.

Axworthy, D., B. Karney. (1996). Modeling low velocity/high dispersion flow in water distribution systems. Journal of Water Resources Planning and Management, vol. 122, no.3, 218-221.

Brunone, B., B. Karney and M. Ferrante. (1999). Velocity profiles and unsteady pipe friction in transient flow. Journal of Water Resources Planning and Management, vol. 126, no.4, 236-244.

Celia, M., Russel, T., Herrera, I., and Ewing, R. (1990). An eulerian-lagrangian localized adjoint method for the advection diffusion equation. Advances in Water Resources, vol. 13, no.4, 187-206.

Fernandes, C. and Karney, B. (1999). Assessing water quality issues in water distribution systems from source to demand. In: Water Industry Systems: modelling and optimization applications. (Ed. D. Savic and G. Walters). Vol. 2, 231-239.

Hoffmann, J. (1992). Numerical methods for engineers and scientists. McGraw Hill.

Karney, B., McInnis, D. (1992). Efficient calculation of transient flow in simple pipe networks. Journal of Hydraulic Engineering, ASCE, 118(7), 1014-1030.

Wylie, E. B., and V. L. Streeter. (1993). Fluid transient in systems. Prentice-Hall.