An application of the numerical Green’s function technique to advection-diffusion contaminant transport in water supply networks

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Abstract

The non-steady transport and decay of pollutants in drinking water distribution networks is traditionally modeled with pure advection models. This paper presents an eulerian-lagrangian numerical solution for the advection-diffusion equation in water supply networks. Because of the diffusion term, the numerical scheme produces a large linear system of equations. A technique that uses numerically computed Green’s functions and nodal mass balance considerations is proposed to decompose this large system in three tri-diagonal systems for each pipe and one (much smaller) system for the concentration at the pipe junctions. In this way, the system is efficiently solved and the model can be applied to large networks at reasonable computer cost. The model is applied to simulate the fluoride propagation in a real network for which published data of field measurements and simulation with the U.S.E.P.A. EPANET model are available. Comparisons are presented in the paper that clearly show that while in pipes with high and medium values of flow velocity the two models give very similar results, in the pipes with low values of flow velocity the new advection-diffusion model more closely predicts the concentration evolution, provided an appropriate value for the dispersion coefficient is used.

1 Introduction

Several authors have proposed models for the non-steady transport and decay of pollutants in drinking water supply networks that consider advection and reaction in the network pipes and assume complete mixing
at the nodes. A survey of those models can be found in [1] and [2]. In all of them diffusion is neglected, believing that it is unimportant in water supply networks, although no assessment of its relative importance under different flow and other conditions has been made.

In a previous paper (Aldama et al. [3]) the writers presented an efficient numerical solution for advection-diffusion transport in pipe networks. To achieve computational efficiency, a special technique was devised that employs numerically computed Green’s functions in each pipe. In this paper, a further development of the numerical solution is presented together with an application to a real water supply network and a comparison with the results of the USEPA-EPANET model and with field measurements carried out by the USEPA.

2 Problem statement

The non-steady advection-diffusion contaminant transport in a pipe flowing full is described by the following partial differential equation:

$$\frac{\partial C}{\partial t} = -V \frac{\partial C}{\partial x} + K \frac{\partial^2 C}{\partial x^2}$$  \hspace{1cm} (1)

where $C$ is the contaminant concentration, $V$ is the mean flow velocity and $D$ is the dispersion coefficient. Before applying the contaminant transport model, a hydraulic model is applied, so the flow velocity $V(x,t)$ in eqn (1) is considered a given function.

The following boundary conditions hold at the network nodes:

a) At some nodes, like sources and chlorination points, the concentration $C$ is given as a known function of time.

b) At all the nodes where water is consumed, the flow rate extracted is given and the mass of the contaminant extracted with the water equals the given flow rate multiplied by the unknown concentration.

c) At the storage tanks connected to the network the following mass balance condition is to be met:

$$\sum (QC)_{in} - \sum (QC)_{out} = \frac{d (WC)}{dt}$$  \hspace{1cm} (2)

where $W$ is the volume of water in the tank, the summations are taken on the inflow and outflow pipes connected to the tank respectively, and $C$ is
the concentration which in principle can be different for the ends of the inflow and outflow pipes connected to the tank and inside it.

3 Numerical solution

In order to numerically solve eqn (1) for each pipe with the given boundary conditions at the network nodes, a two-stage eulerian-lagrangian solution is employed (Aldama et al. [3]).

3.1 Lagrangian stage

In the first (lagrangian) stage the advective part of the eqn (1), i.e.,

\[
\frac{\partial C}{\partial t} + V \frac{\partial C}{\partial x} = 0
\]

is solved for each pipe. The solution obtained is denoted by \( C^a \). The pipe length is discretized in some number of interior points ranging for 1 to \( N \), and the pipe ends are called rear node \( R \) and front node \( F \) (fig. 1).

For each time step of the numerical solution, the values of \( C \) for the points of the time level \( t^n \) are known and the values of \( C \) for the points of the time level \( t^{n+1} \) are to be computed. The backward method of characteristics is used. The points of the level \( t^{n+1} \) are projected back on the characteristic line to the time level \( t^n \). For the point \( i \) shown in fig.1, for example, the projected point is \( A \). Because of the pure advection nature of eqn (3), the value of \( C^a \) for point \( i \) will be the same as that for point \( A \), and can be found by interpolating between the known values for the time level \( t^n \). Virtually any interpolation scheme can be used, the simplest being a linear interpolation between the points \( i-1 \) and \( i \).

Figure 1. Discretization in a pipe at the lagrangian stage
In simulating the non-steady flow in distribution networks it is common to use quasi-dynamic or extended period models, in which the flow distribution is assumed constant during each of the consecutive time segments considered in the simulation. The time increments used in the numerical solution for contaminant transport are much smaller that those used in the hydraulic extended period model. Each “hydraulic” time increment $\Delta t_h$ is divided in a number of “contaminant transport” or “water quality” time increments $\Delta t_q$. This way, the simulation of contaminant transport considers a constant flow velocity in each pipe, and the values of $C_i^a$ for the points from 1 to $N$ are obtained by a linear interpolation for the time levels with constant flow velocity, up to the time level where the flow velocity and the discretization related to it changes (fig. 2). Each point in the first time level defined by the new discretization is projected back on its characteristic line to the previous time level and a linear interpolation is applied between the corresponding points to obtain the values of $C_i^a$. When the characteristic line crosses the left boundary, point 1 in fig. 2, $C_i^a$ is calculated with a linear interpolation on that boundary.

Figure 2. Characteristic lines in a pipe before and after a change in the flow velocity.
To compute $C^a$ for point $R$ (the rear end of the pipe), the inflow pipes connected to the same node need to be considered. Assuming complete mixing at the network nodes, the concentration at node $i$, $C_i$ is computed as:

$$C_i = \frac{\sum (Q C)_m}{\sum Q_m - q_i}$$  \hspace{1cm} (4)

where $q_i$ is the flow rate extracted at the node, and the summations are taken only for the pipes inflowing to the node $i$.

To simulate the effect of the storage tanks connected to the network, the following procedure based on eqn (2) is used:

1. At each time step, after computing $C^a F$ for the front ends $F$ of all the inflow pipes connected to the tank, the sum of $C^a F$ multiplied by the corresponding flow rate $Q$ of the same pipes is computed.

2. Assuming a complete and instantaneous mixing inside the tank, the concentration at the ends of the pipes that outflow from the tank is computed as:

$$C_{out} = \frac{(W C)^n + \Delta t \sum (Q C)_m}{W^{n+1} + \Delta t \sum Q_{out}}$$  \hspace{1cm} (5)

where $W$ is the water volume in the tank. The value of $C_{out}$ computed with eqn (5) is then assigned to the rear end $R$ of each outflow pipe connected to the tank.

### 3.2 Eulerian stage

The diffusion term is considered at this stage by numerically solving the differential equation:

$$\frac{\partial C}{\partial t} = K \frac{\partial^2 C}{\partial x^2}$$  \hspace{1cm} (6)

in the time interval between $t^n$ and $t^{n+1}$ using for initial conditions the values of $C^a$ calculated in the lagrangian stage. The direct application of a finite difference approximation to eqn (6) in a network of pipes would produce a system of linear equations, not amenable for an efficient
numerical solution, especially when the pipe network is large. In order to obtain a more efficient numerical solution the Numerical Green’s Function Technique is applied. The basis of the technique is explained in a companion paper (Aldama, Tzatchkov and Arreguin [4], see also Aldama et al. [3]), so only the computational procedure applied to the case of the advection-diffusion equation will be explained here.

For each pipe three auxiliary numerical solutions of the difference equation (6) (called homogeneous solution CH, Green’s function GR and Green’s function GF) are computed, each of them with different initial and boundary conditions. The final solution for $C_i$ is expressed as a superposition of the homogeneous solution and the two Green’s functions multiplied by the (still unknown) values of $C_R$ and $C_F$ at the pipe ends, i.e.,

$$C_i = CH_i + GR_i C_R + GF_i C_F, \quad \text{for } i = 1 \text{ to } N \quad (7)$$

In order to obtain $C_R$ and $C_F$ at the pipe ends (which are the network nodes), a “network node equivalent” of the differential equation (6) is written first:

$$W \frac{\partial C}{\partial t} = \sum_{j=1}^{m} \left( \frac{\partial C}{\partial x} \right)_j K_j A_j \quad (8)$$

where $W$ is the volume of water contained in the node, $m$ is the number of pipes connected to the node, and $A_j$ and $K_j$ are the dispersion coefficient and the cross section area of each pipe $j$. In finite difference form, assuming that the volume $W$ is formed by the sum of the volumes of the pipe segments $\Delta x$ adjacent to the node, for a node $i$ the eqn (8) can be written as follows:

$$\left( \sum_{j=1}^{m} \Delta x_j A_j \right) \frac{C_{i}^{n+1} - C_{i}^{n}}{\Delta t} = \sum_{j=1}^{m} K_j A_j \left(C_{1,j}^{n+1} - C_{1,j}^{n} + C_{1,j}^{n} - C_{i}^{n} \right) \quad (9)$$

where in each pipe $C_{1,j}$ the concentration value for the first interior computation point adjacent to the node $i$. For each pipe $j$ the unknown $C_{1,j}^{n+1}$ is expressed by eqn (7) and substituted in eqn (9) thus providing a system of linear equations for the values of $C$ at the network nodes. The prescribed values for $C$ given by the boundary conditions are considered directly in the system of equations, modifying it prior to solving. For the
rear ends $R$ of the pipes that outflow from a tank, the same type of boundary condition is applied with the value of $C$ existing at the tank.

Once the system of equations is solved, the values of $C$ inside the pipes are computed by eqn (7).

## 4 Dispersion coefficient considerations

When the water contained in a pipe is at rest ($V=0$ in eqn (1)), the contaminant can be transported in the water only by molecular diffusion, and coefficient $K$ equals the diffusivity $D$ of the given substance in the water, a very small value of the order of $1 \times 10^{-9}$ m$^2$/s. When the water in the pipe is flowing with some mean velocity $V$, the differences in the velocities at the different points inside the pipe cause a more intense mixing, which gives rise to dispersion coefficient $K$ in which the turbulent diffusion and the influence of the velocity distribution is accounted for.

In the classical work of G. Taylor theoretical formulae for the dispersion coefficient in laminar and turbulent flow in a pipe were obtained. Flow velocities in most pipes of a water distribution network are neither extremely low (for laminar flow to occur) nor very high (for fully developed turbulent flow to occur), so estimates of $K$ in the transition zone from laminar to turbulent flow are needed. While the use of such estimates in the proposed model is under research by the writers, in the example application that follows two possibilities are explored: a) Computing $K$ using the theoretical formula for turbulent flow for all network pipes regardless of the flow velocity. b) Assuming much greater values for $K$ in the pipes with very low flow velocities, and computing $K$ for the rest of the other pipes with the theoretical formula for turbulent flow.

## 5 Comparison with the EPANET model and field measurements

A public domain computer program for simulating the network hydraulics and contaminant transport in water distribution networks, called EPANET was developed by the US Environmental Protection Agency (EPA) (Rossman [5]). The program uses an extended period hydraulic model and a pure advection-reaction contaminant transport model. The EPANET program can be downloaded from an EPA Internet site, together with all the data needed to simulate three example networks. One of these example networks is the Cherry Hill Brushy Plains service area network, for which a series of field measurements
was carried out by the EPA in order to compare them with the predictions of the EPANET model (Rossman, Clark and Grayman [6]).

The proposed advection-diffusion model was applied to simulate the fluoride transport in Cherry Hill Brushy Plains service area network with the same data used in the EPANET simulation. Special care was taken to work with the same hydraulic data, boundary conditions, tank simulation algorithm, number of discretization points, time increments, etc., in order to assess the relative importance of the diffusion component considered in the proposed model. For the same reason, only the case of fluoride (which can be considered as a conservative substance in water) transport was simulated, in order to eliminate the influence of the reaction or decay which is important in the case of chlorine transport.

The predictions of the EPANET model compare fairly well with the field measurements of fluoride concentration for sampling points 3, 6, 11, 19 and 25; but for sampling points 10, 28 and 34 the model clearly fails to represent correctly the trend of concentration evolution, as can be seen in the corresponding graphics presented in the paper of Rossman, Clark and Grayman [6]).

The proposed model was applied first with dispersion coefficient $K$ computed using the Taylor’s formula for turbulent flow in all network pipes. The results obtained are very similar to the results of the EPANET model.

The flow velocity in some pipes of this network is very low (less than 0.03 m/s). When computing $K$ with the formula for turbulent flow with this low flow velocity, a very small value for $K$ is obtained. The relative importance of the diffusion term in eqn (1) is small and the computed solution behaves similar to that of a pure advection model. In the network pipes with medium or high values for the flow velocities, the computed value of $K$ is not small, but in those pipes advection is the dominant process exactly because of the relative importance of the flow velocities, so once again the two models give similar results.

As was noted, estimates of $K$ for flows that are not laminar nor turbulent, are under research by the writers. Nevertheless it is felt that for low velocities that approach laminar flow, much larger values of $K$ can be expected. With this idea in mind, the proposed model was applied with larger values of $K$ for the pipes with low flow velocity, to “calibrate” the contaminant transport model, as is done for network hydraulic models. Fig 3 shows the results for sampling point 10 with a $K=0.20$ m$^2$/s in pipes 8 and 10 (the average value calculated by the Taylor’s formula for turbulent flow would be approximately 0.0006 m$^2$/s). It may be seen that the proposed advection-diffusion model
Figure 3. Concentration evolution obtained by the proposed model (IMTARED), the EPANET model and field measurements.

represents more realistically the concentration evolution thanks to the consideration of dispersion.

6 Conclusions

An eulerian-lagrangian numerical solution of the non-steady advection-diffusion in water supply networks is proposed. The proposed solution employs the numerical Green's function technique in order to solve efficiently the system of linear equations produced by the numerical scheme. The numerical solution is applied to a real water distribution network for which results of simulations with the USEPA EPANET model and field measurements are available. In the network pipes with medium and high value of the flow velocities the two models give
similar results. In pipes with low flow velocities the measured concentration evolution is more closely represented by the proposed model than by the EPANET model, provided appropriate values for the dispersion coefficient $K$ are used.

References