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52. A domain decomposition strategy for the numerical simulation of contaminant transport in pipe networks

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1. Introduction. In this paper, a very efficient domain decomposition strategy is proposed for the numerical simulation of advective-dispersive-reactive (ADR) processes in pipe networks. The problem is modeled by applying the ADR equation in each pipe, as well as boundary conditions at each of the network nodes. In order to numerically solve the ADR equation, each pipe is discretized by means of a finite difference scheme. The presence of the dispersion term, and the inclusion of the boundary conditions at each network node, often produces large, unsymmetric and unstructured systems of linear equations. These systems of equations must be solved at each time step considered in the simulation, leading to significant computational costs. The proposed domain decomposition technique is based on the use of numerically computed Green functions and nodal mass balance considerations. Thus, the large system of equations that represents the discretized network is decomposed exactly in three easy-to-solve tridiagonal systems that represent the ADR processes for each pipe, and one low order system for the concentration at the pipe junctions. In each pipe the sought solution is represented by the superposition of three numerically obtained auxiliary solutions: a homogeneous (zero boundary conditions) solution, and two Green function solutions (one for each reach end) multiplied by the unknown values of the constituent concentration at the two reach ends. To obtain the Green functions corresponding to each reach end, a unit value for the concentration is imposed at one boundary and a value of zero at the other, and the resulting tridiagonal system is numerically solved. The fluxes at each of the pipe ends are expressed in terms of the values of the concentration there. Henceforth, continuity balance relations are used to construct a system of linear equations for the values of the unknown quantities at the network nodes. The method is applicable to any type of network, branched or looped.

Computer-based mathematical models able to predict the time history and the spatial distribution of constituents in water distribution networks are useful in network design and operation. Such models can be used to analyze water quality degradation problems, to assess alternative operational and control strategies for improving and maintaining water quality, to design water-quality-sampling programs, to optimize disinfection processes and to evaluate water quality aspects of distribution network improvement projects. Several authors have proposed models of this type that consider advection and reaction and neglect dispersion [4], [3]; and several computer programs that implement such models are available [7], [3]. Field observations conducted in distribution networks [8], [3], have shown that the advection-reaction model predictions are in good agreement with the observed concentrations in pipes with medium and high flow velocities, but fail in dead-end pipes where low velocities prevail.

While relatively simple Lagrangian tracking explicit-type numerical algorithms are used in the network advection-reaction models, more complicated numerical solutions have to be applied when dispersion is to be considered. The numerical solution for advection-dispersion-reaction in networks poses three main problems:

a) Boundary conditions at the nodes common to several domains have to be formulated and considered in the numerical solution.

b) The direct application of the numerical schemes produces large non-banded, unsymmetric and unstructured systems of equations to be solved, especially when the network is

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large.

c) The computational difficulties increase when advection dominates over dispersion. Sharp concentration gradients are expected in this case, and a very fine discretization would be needed if Eulerian methods are to be applied, which makes them impractical. Because of the small values of the dispersion coefficient, contaminant transport in water distribution networks falls exactly in this category of advection-dominated problems.

In this paper a numerical solution for the advection-dispersion-reaction equation in pipe networks is presented with special emphasis on the domain decomposition strategy used to efficiently solve the resulting finite difference equations. More information about the rest of the solution procedure can be found in [2], [10], [10], [12] and [11]. An Eulerian-Lagrangian numerical scheme is applied. The solution is applicable to advection-dominated and dispersion-dominated transport and is stable for a broad range of flow velocities that can be met in real distribution networks. The model is applied to simulate the variation of fluoride and chlorine concentration in a real distribution network and its predictions are compared to field observations and to the EPANET computer program that considers advection-reaction only.

2. Problem statement. The non-steady advection-dispersion-reaction process in a pipe flowing full is described by the following partial differential equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} - KC \tag{2.1}$$

where C = constituent concentration; u = cross-sectional average flow velocity; D = dispersion coefficient; K = first order decay constant; x= distance along pipe; and t = time.

The following boundary conditions hold at the network nodes:

a) At some nodes, as constituent sources, the concentration C is given as a prescribed function of time.

b) Mixing at the network nodes. Two or more pipes, each of them with different flow and constituent concentration, may convey inflow to a node. Water is mixed at the node and a new concentration is obtained, then water leaves the node with that concentration to the outflowing pipes and to the consumption abstracted. A complete and instantaneous mixing is usually assumed in the network models.

c) Mass conservation at the network nodes. The well-known differential equation 2.1, is obtained by applying the mass conservation principle to an elementary pipe segment with a length dx in a time period dt, such that $dx = u.dt$. The same derivation can be generalized to the case of a junction where several pipes meet. Given that the flow velocity u_j in each pipe j is different, the segment length of each pipe considered in the elementary node volume will be different in order to handle the balance of the incoming and outcoming quantities in the same period of time dt, so that $dx_j = u_j.dt$. The following nodal equivalent of equation 2.1 is thus obtained:

$$\sum_{j=1}^{m}\left(\frac{dx_j}{2}A_j\right)\frac{\partial C}{\partial t} = \sum_{j=1}^{m}\left(A_j D_j\frac{\partial C}{\partial x} + Q_j C - K_j A_j C\frac{dx_j}{2}\right) - q_j C \tag{2.2}$$

where m = number of pipes connected to the node; A_j= cross sectional area of pipe j; Q_j = flow rate in pipe j; D_j= dispersion coefficient of pipe j; K_j= first order decay constant of pipe j; and q_i= flow rate abstracted at the node. For the case where two pipes of equal characteristics meet at the node and q_i=0, the equation 2.2 reduces to the equation 2.1 if dx_j and dt tend to be infinitesimally small.

d) Mass balance at the storage tanks connected to the network:

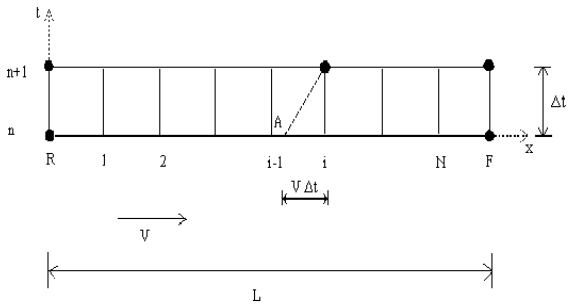

Figure 3.1: Discretization in a pipe

3. Numerical solution. In order to numerically solve eqn 2.1 for each pipe with the given boundary conditions at the network nodes, a two-stage Eulerian-Lagrangian solution is employed [2]. The space-time domain (x, t) of each pipe is discretized in a rectangular grid with time step Δt_q and gridsize Δx. The interior points are numbered from 1 to N, and the two pipe ends are called *rear node*, R, and *front node*, F (Figure 3.1). For each time segment considered in the numerical solution, the values of C for the points on the time level t^n are known and the values of C for the points on the time level t^{n+1} are to be computed. The differential equation 2.1 is split in two parts, an advective part and a dispersive part, and numerically solved in each time step in two stages.

3.1. Lagrangian stage. In the first (Lagrangian) stage the advective (or advective-reactive) part of the equationn 2.1, i.e.,

$$\frac{C^a - C^n}{\Delta t_q} = -\left(u\frac{\partial C}{\partial x}\right) \tag{3.1}$$

is solved for each pipe. The backward method of characteristics is used [5]. The points of the level t^{n+1} are projected backwards in time on the characteristic lines that pass through them until the characteristic lines cross the time level t^n. For the point i shown in Figure 3.1, for example, the projected point is A. Because of the pure advection nature of eqn 3.1, the value of C for point i at time t^{n+1} will be the same as that for point A, and can be found by interpolation between the known values for the time level t^n. The solution obtained is denoted by C^a.

This procedure is used to compute C^a for points 1 to F within each pipe. To compute C^a for the point R (the rear end of the pipe), the mass balance of the inflowing pipes connected to the same point (which is a network node) is considered assuming complete mixing. Thus the concentration at a network node i, C_i, is computed as:

$$C_i^a = \frac{\sum (QC_F^a)}{\sum Q_{out} + q_i} \tag{3.2}$$

where q_i = flow rate abstracted at the node; Q_{out} = flow rate in a pipe outflowing to the node; C^a = concentration computed in the advection stage; (QC_F^a) = flow rate in an inflowing pipe multiplied by the value of C^a for the front pipe end, F. To simulate the effect of a tank connected to the network, the concentration inside the tank is computed assuming complete mixing of the inflowing mass and considering bulk water decay.

3.2. Eulerian stage. The dispersion term is considered at this stage by numerically solving the differential equation:

$$\frac{C^{n+1}-C^a}{\Delta t_q}=\left(uD\frac{\partial^2 C}{\partial x^2}\right)^{n+1} \tag{3.3}$$

using the values of C^a calculated in the Lagrangian stage as initial conditions. Several well established numerical methods exist for the solution of eqn 3.3 in a single domain. Little attention has been given nevertheless to the application of these methods to interconnected domains such as pipeline networks. The direct application of a finite difference approximation to eqn 3.3 in a network of pipes produces a non banded system of linear equations, not amenable for an efficient numerical solution. This problem is aggravated when the network is large. Additionally, the condition given by eqn 2.2 has to be met. The application of known numerical solutions to problems in networks addresses these two difficulties with some *ad hoc* and particular procedure, due to the lack of a general approach. To overcome these difficulties, [1] proposed an approach for the consideration of the boundary conditions and for an efficient numerical solution of boundary value problems in networks, called *the numerical Green's function technique*. This technique is applied here in order to obtain an efficient numerical solution.

By definition, a Green's function is a one parameter P function that obeys the given differential equation, having the value of 1 at point P and value zero at the boundaries. It is common to denote a Green's function as $G(\xi, P)$ where ξ is the running coordinate and P is the point of application of the unit load. The reader is referred to [9] or [6] for a formal definition and theory of the Green's functions.

Using Green's functions, the sought solution of eqn 2.2 inside each network pipe, can be expressed as

$$C(\xi)=H(\xi)+G(\xi,R)C_R+G(\xi,F)C_F \tag{3.4}$$

where C_R and C_F is the (still unknown) concentration at the two pipe ends R and F respectively, $H(\xi)$ is a function that obeys eqn 3.4 with C_R=0 and C_F=0 (the so called *homogenous solution*), $G(\xi,R)=G(\xi,0)$ is the rear end Green's function and $G(\xi,F)=G(\xi,L)$ is the front end Green's function. $C(\xi)$, given by by eqn 3.4, is the sought solution of eqn 3.3 because each of the functions $H(\xi), G(\xi,R)$ and $G(\xi,F)$ obeys eqn 3.3 (the sum of any number of particular solutions of a linear differential equation is also a solution), and their sum satisfies the boundary conditions at the pipe ends. The first term on the right hand side of eqn 3.4 accounts for the initial conditions, and the other two for the boundary conditions.

$H(\xi), G(\xi,R)$ and $G(\xi,F)$ are easy to obtain numerically in each pipe. Expression 3.4 is then substituted in the balance condition at the network nodes (such as eqn 2.2) resulting in a system of equations for the values of C at the network nodes. After obtaining the values of C at the network nodes from the solution of this system, the values of C at the interior points are computed by eqn 3.4. This way the large system of equations produced by the finite difference scheme is decomposed into three easy-to-solve systems for each pipe and one (much smaller) system for the concentration at the pipe junctions.

The finite difference approximation for equation 3.3 for the interior points of a pipe can be written in the following form:

$$-\frac{\lambda}{2}C_{j-1}^{n+1}+(1+\lambda)C_j^{n+1}-\frac{\lambda}{2}C_{j+1}^{n+1}=b_j,\quad j=1,\ldots,N \tag{3.5}$$

where

$$\lambda=\frac{D\Delta t_q}{\Delta x^2};\quad b_j=\tfrac{\lambda}{2}C_{j-1}^a+(\lambda-1)C_j^a+\tfrac{\lambda}{2}C_{j+1}^a \tag{3.6}$$

Expression 3.5 represents a system of N equations with $N+2$ unknowns, that are the values of C at the points 1 to N, R and F. This system cannot be solved directly (separately) for each pipe because the number of unknowns is larger than the number of equations. Instead, the following procedure is used:

First, C is set to zero on the two pipe ends and the system of equations is solved numerically. The resulting solution vector represents *the homogeneous solution* $H(\xi)$ for the pipe and accounts for initial conditions. Then C is set to 1 on the rear reach end, C is set to zero on the front end, all b_j in eqn 3.5 are set to zero, and the system of equations is solved numerically. This way the rear end Green's function $G(\xi, R)$ is obtained. After that C is set to zero the rear reach end, C is set to 1 on the front end, all b_j in 3.5 are set to zero, and once again the system of equations is solved to obtain the front end Green's functions $G(\xi, F)$. Since 3.5 with b_j=0 is invariant under changing the order of the equations, the last two functions are symmetric, i.e., $G(\xi, R) = G(L-\xi, R)$, where L = pipe length; so the system needs to be solved only for one of them. Thus the desired solution for C 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, according to eqn 3.4, i.e.,

$$C_i = CH_i + GR_i C_R + GF_i C_F \quad i = 1, \ldots, N \tag{3.7}$$

where h_j = homogeneous solution for the point j; GR_j = the rear pipe end Green's function; GF_j = front pipe end Green's function; N = number of points inside the pipe, and C_R and C_F =unknown values of the desired solution for the rear and front pipe ends.

At each network node i, a unique and continuous value (the same for the ends of the pipes that join at that node) for C is supposed, say C_i. To obtain this value for the network nodes (and thus the values of C_R and C_F at the pipe ends) the equation 2.2 is used. The term $\sum_{j=1}^{m} Q_j C - q_j C$ in this equation is considered in the Lagrangian stage, so the equation can be written in finite difference form as:

$$\left(\sum_{j=1}^{m} \frac{dx_j}{2} A_j\right) \frac{C_i^{n+1} - C_i^a}{\Delta t_q} = \sum_{j=1}^{m} \left[\frac{A_j D_j}{2\Delta x_j}\left(C_{1,j}^{n+1} - C_i^{n+1} + C_{1,j}^a - C_i^a\right) - \frac{dx_j}{2} K_j A_j C_i^a\right] \tag{3.8}$$

where i denotes the network node; and $1, j$ denotes the discretization point of the pipe nearest to the network node i (which can be 1 or N depending on the numbering direction within the pipe). The value of $C_{1,j}^{n+1}$ in this equation is still unknown for each pipe j and can be expressed by eqn 3.7 thus involving the unknown values of C at the two pipe ends (which are two network nodes). Equation 3.8, written for each network node i in turn, provides a system of linear equations for the values of C at the network nodes. Once the system of equations is solved, the values of C for the intermediate points along the pipe are computed using eqn 3.7.

This way the homogeneous solution and the two numerical Green's functions in each pipe are computed from tri-diagonal systems of linear equations. The same matrix is used in each of them. The two Green's functions are symmetric, so only one of them needs to be computed. The matrix of the system of equations for the network nodes is symmetric and sparse, and reflects the structure of the network itself: for each network node there is a row in the matrix whose non zero elements correspond to the diagonal and to the nodes to which the current node is connected. Efficient sparse matrix algorithms can be applied to store and to solve systems of equations with this type of matrix. Thus the large non banded systems of equations that would otherwise produce the direct application of the finite difference scheme for the network, is decomposed in three easy-to-solve systems for each network reach and a

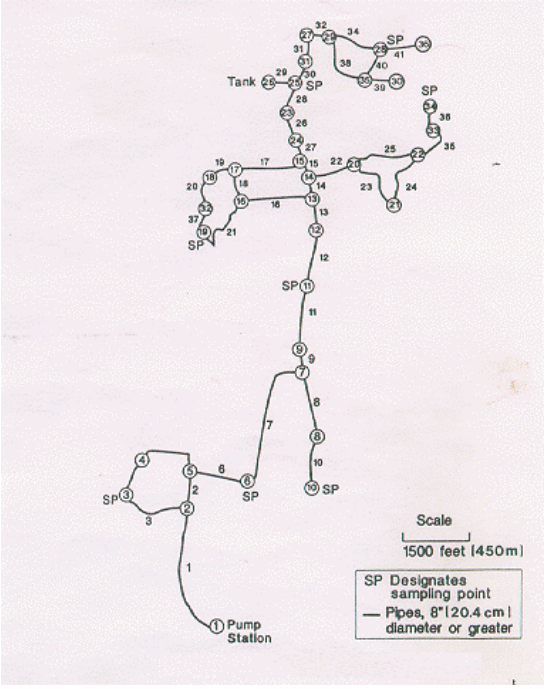

Figure 4.1: Node-link representation of the Brushy Plain-Cherry Hill networks

much smaller sparse system for the network nodes, and the solution can be computed more efficiently, especially for large networks.

4. Comparison with known models 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) [7]. The program uses an advection-reaction contaminant transport model. The proposed advection-dispersion-reaction model was applied to simulate the fluoride and chlorine transport in 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 the observed concentration with the predictions of the EPANET model [8]. Figure 4.1 shows the node-link representation of the network and the sampling points where fluoride and chlorine concentration was measured.

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 fails to represent correctly the trend of concentration evolution, as can be seen in the corresponding graphics presented by [8]. Figure 4.2 shows the results for sampling point 10 with a $D = 0.20$ m2/s in pipes 8 and 10. It is seen that the proposed advection-diffusion model represents more realistically the concentration evolution thanks to the inclusion of dispersion.

5. Summary and conclusions. An Eulerian-Lagrangian numerical solution for the non-steady advection-dispersion-reaction constituent transport in water distribution networks is proposed. The solution employs the numerical Green's function technique to efficiently solve the system of linear equations produced by the numerical scheme in the Eulerian

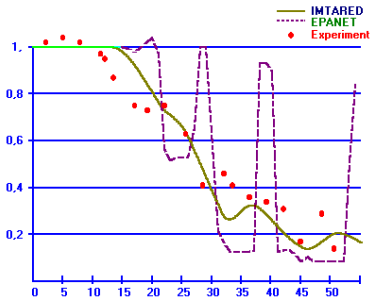

Figure 4.2: Concentration evolution obtained by the proposed model (IMTARED), the EPANET model and field measurements

stage. As a result of the application of this technique the large system of equations produced by the numerical scheme is decomposed in three tri-diagonal systems for each pipe and a smaller system of equations for the concentration at the network nodes. The numerical solution is applied to a real water distribution network for which results of simulations with the EPANET model and field observations are available. In the network pipes with medium and high flow velocities the two models give similar results. In pipes with low flow velocities the measured concentration evolution is represented better by the proposed model than by the EPANET model, due to the inclusion of dispersion.

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