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DYNAMIC PLUG FLOW REACTOR NETWORK MODEL FOR CONTAMINANT TRANSPORT IN WATER DISTRIBUTION SYSTEMS

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Abstract

We present a network water quality model that idealizes the distribution system as a network of ideal flow reactors, namely plug flow reactors. The plug flow reactors are linked together through an assumption of complete mixing at the network nodes. The resulting system of coupled 2-D (space - time) partial differential equations are discretized spatially using a finite difference scheme, and solved by numerical integration. The model will be evaluated with regard to its prediction capabilities, relative to previous modeling efforts.

Introduction

Recent studies have demonstrated that significant spatial and temporal water quality variations can exist in urban water distribution systems. Just as hydraulic network models have played an important role in designing water distribution systems for hydraulic performance criteria, it is expected that contaminant transport network models will be needed if water quality criteria are to be included in the water distribution system design process. We present a combined hydraulic and water quality model that has been developed for single species transport and production/decay in water distribution systems. First, the hydraulic model equations are briefly reviewed. Next, the network water quality model equations are discussed along with solution procedures.

Water Distribution System Hydraulic Model

The hydraulic modeling of distribution systems has been studied extensively, beginning with the work of Shamir and Howard [1968] that prefaced the modern approach to net-

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work modeling. Assuming a constant density fluid, conservation of fluid mass at each of the network nodes can be expressed in matrix-vector form:

$$\mathbf{RIM} \cdot \mathbf{q} + \mathbf{w} = 0 \tag{1}$$

where: **RIM** is the reduced incidence matrix of the network, **q** is the vector of pipe flow rates, and **w** is the vector of nodal demands (fluid sinks). The (i,j)*th* element of **RIM** equals +1 if flow in arc j is assumed to flow into node i, -1 if such flow is assumed out of node i, and 0 if arc j is not connected to node i.

Energy in the distribution network is conserved if the loss in fluid potential between any two nodes is independent of the path. If energy is measured as the total hydraulic head, **h**, then conservation of energy for one-dimensional pipe flow in a network can be defined:

$$\mathbf{LOOP} \cdot \Delta\mathbf{h} + \Delta\mathbf{E} = 0 \tag{2}$$

where: **LOOP** is the loop matrix of the network, $\Delta\mathbf{h}$ is the vector of hydraulic head losses or gains in each pipe, and $\Delta\mathbf{E}$ is the vector of energy differences between the loop end points.

The head losses or gains in each pipe are modeled using the Darcy-Weisbach formula for pipe flow friction losses and a quadratic relationship between pump head and discharge. The friction factor is assumed to depend on the roughness and the pipe Reynolds number. Eqs. (1) and (2) are combined and solved for the unknown pipe flow rates **q** using Newton's method.

The pipe flow rates defined by eqs. (1-2) are continually varying because of continuous changes in the nodal demands, **w**, and in the fluid elevations at the fixed grade nodes, **E**. This dynamic hydraulic behavior is modeled approximately by solving a system of ordinary differential equations (o.d.e.'s) for conservation of fluid mass at the FGN's. This common method of approximate dynamic modeling, known as extended period simulation (EPS), is described by Rao and Bree [1977]. Conservation of mass for a constant density fluid is written at the fixed grade nodes:

$$\frac{dV_i}{dt} = -q_{j\to i}(\mathbf{w}(t), \mathbf{V}(t)); \qquad V_i(t_o) = V_i^o; \qquad i = 1,\ldots,nfgn \tag{3}$$

where V_i is the volume of fluid in the *ith* FGN, **V** is the vector of all FGN fluid volumes, $q_{j\to i}$ is the flow in pipe j that is connected to FGN i, and *nfgn* is the number of fixed grade nodes. By convention, all pipes connected to FGN's are assumed to flow *out of* the FGN, hence the flow $q_{j\to i}$ appears with a minus sign. The FGN elevations, **E**, are related to the storage volumes through the tank geometry.

The system of o.d.e.'s in eq. (3) is solved by a simple, explicit Euler method:

$$V_i^{k+1} = V_i^k - \Delta t_h \cdot q_{j\to i}(\mathbf{w}^k, \mathbf{V}^k), \qquad i = 1,\ldots,nfgn \tag{4}$$

where the superscripts $k, k+1$ denote the time level, and Δt_h is the hydraulic time step.

Water Distribution System Water Quality Model

The dynamic transport of a single dissolved species through the distribution system is described mathematically by conservation of mass relationships at each network node and in each pipe. Starting at the contaminant sources, the dissolved species is advected and dispersed through the distribution system, and in addition may decay or be produced according to a process rate relationship. Advection is by the bulk fluid velocity in each pipe, which can have great variation both spatially and temporally. It is common for flows in certain pipes to reverse direction on a regular basis (notably those pipes connected to storage tanks), in response to temporal water demand fluctuations. Dispersal of the species mass occurs not

only because of concentration and velocity gradients within each pipe, but also on a perhaps larger scale due to mixing of fluid at the network nodes. In addition, storage tanks with large volumes are typically present in urban water distribution systems, and the operation of such tanks can have a significant affect on the network contaminant transport dynamics. For at least these reasons, mass transport in distribution systems is complex.

Others have modeled transport in water distribution systems using flow routing techniques [Males et al., 1988, Clark et al., 1988, Clark and Coyle, 1990]. The simulation model presented here builds on these original works by: 1) formally linking the simulation models for fluid flow and species mass transport, 2) describing the species mass transport in a standard mathematical way that is flexible and that makes results in other fields (e.g., numerical analysis) more accessible, and 3) using modern numerical methods to solve the resulting initial value problems.

Each pipe is assumed to be a plug flow reactor (PFR). This assumption is likely a good one if the pipe flow regime is turbulent, and is less accurate for laminar flow. From a balance on mass in a volume element of pipe, the well-known partial differential equation (p.d.e.) describing a PFR without axial dispersion is:

$$\frac{\partial C_i}{\partial t} = -\frac{4\, q_i}{\pi\, D_i^2}\frac{\partial C_i}{\partial x} + r_i \tag{5}$$

where: C_i is the species concentration in pipe i, (x,t) are axial distance and time, respectively, and r_i is a process production or decay rate in pipe i. The effects of axial dispersion are not included in the current model, and we have no experience with the effects of axial dispersion on transport in networks. The present modeling framework could, however, incorporate the dispersive flux, using spatial discretization techniques developed specifically for solving the resulting parabolic equations [Wong, 1988].

The hyperbolic equations in eq. (5) are solved by a standard p.d.e. solution technique called the method of lines (MOL) [Aiken, 1985]. The MOL is a technique whereby all but one of the independent variables are discretized, thus approximating the p.d.e. by a system of o.d.e.'s. The o.d.e.'s are then solved by numerical integration methods. We have used the backward difference approximation in the present model, so as to avoid oscillatory solutions:

$$\frac{\partial C_{i,j}}{\partial t} = -\frac{4\, q_i}{\Delta x_i \pi\, D_i^2}(C_{i,j} - C_{i,j-1}) + r_{i,j} \qquad j = 1,\ldots,m_i \tag{6}$$

where: $C_{i,j}$ is the species concentration at pipe node j in pipe i, $r_{i,j}$ is the process rate at pipe node j in pipe i, Δx_i is the distance between pipe nodes in pipe i, and $m_i \cdot \Delta x_i$. equals the pipe length. The term "pipe nodes" is used to distinguish these nodes that result from discretizing eq. (5) from the "network nodes" that occur at pipe junctions.

Eq. (6) is equivalent to modeling the transport by a series of continuous flow stirred tank reactors (CFSTR's), where the volume of each CFSTR is identical and equal to $4/(\Delta x_i \pi\, D_i^2)$. As the number of CFSTR's becomes large ($\Delta x_i \rightarrow 0$), then of course the behavior of eq. (13) approaches plug flow. Even for finite Δx_i, we prefer the view that the pipes are PFR's and that the disretization approach is an approximation to that ideal. Better discretization methods would yield better approximations for a given Δx_i.

Species mass conservation at the *ith* network node is defined:

$$\sum_{j \in IN_i} |q_j| \cdot C_{j,m} = \sum_{j \in OUT_i} |q_j| \cdot C_{j,0} - w_i \cdot C_i^* \tag{7}$$

where: IN_i is the set of all pipe indices for which flow is directed *into* node i, OUT_i is the set of all pipe indices for which flow is directed *out of* node i, and C_i^* is the network node

concentration at node i. Combining eqs. (6–7) result in a differential–algebraic system of equations that describes the dynamic mass transport in the network. These equations are not well–posed, however, since the number of mass balance equations is less than the number of unknowns. The unknowns consist of the concentrations at the pipe nodes, $C_{i,j}$, $i = 1,\ldots,narcs$, $j = 1,\ldots,m_i$, the concentrations at the network nodes, C_i^*, $i = 1,\ldots,nn$, and the concentrations corresponding to the pipe boundary conditions, $C_{i,0}$, $i = 1,\ldots,narcs$. The ill–posedness of eq. (8–9) results because the mixing process that occurs at the network nodes is undefined. The approach used in the previous cited studies, and here as well, is to assume complete and instantaneous mixing of all source streams at each network node, although there is little evidence to support this claim. This assumption is equivalent to assuming each network node is a CFSTR with zero volume. With the assumption of complete mixing, eq. (7) becomes:

$$C_i^* = \frac{\sum_{j \in IN_i} |q_j| \cdot C_{j,m}}{\sum_{j \in OUT_i} |q_j| - w_i} \tag{8}$$

where C_i^*, the network node concentration, now equals the concentration at the boundary for all pipes j, $C_{j,0}$, such that $j \in OUT_i$. It is apparent that eqs. (6) and (8) now constitute a well–posed differential–algebraic system, with the unknowns being the network and pipe node concentrations.

Solution of eqs. (6) and (8) requires that the concentrations at the network boundaries be a known or computable function of time. These network boundary conditions may correspond to the effluent concentrations from treatment facilities, or to the concentrations in storage tanks that are emptying. If the boundary is at a treatment works, then the boundary concentration is a specified function of time If the boundary is at a storage tank, then the boundary concentration is a function of the initial tank concentration, the mixing characteristics of the fluid, the species decay or production rate, and the time history of mass entering and leaving the tank. Presently, all FGN's are modeled as CFSTR's.

If the *ith* FGN is emptying, then conservation of mass for complete mixing is:

$$\frac{dC_i^{BC}}{dt} = r_i^{BC} \tag{9}$$

where: C_i^{BC} is the concentration in the *ith* FGN (the *ith* network boundary condition), and r_i^{BC} is the process rate in the *ith* FGN. If the *ith* FGN is filling, then conservation of mass for a completely mixed tank becomes:

$$\frac{dC_i^{BC}}{dt} = \frac{-q_{j\to i}}{V_i}(C_{j\to i,m} - C_i^{BC}) + r_i^{BC} \tag{10}$$

where $C_{j\to i,m}$ is the concentration in pipe j connected to FGN i, at the pipe node m that is adjacent to the FGN. It should be noted that this concentration is a function of time. Depending on whether the FGN is a fluid source or a fluid sink for the network, either eq. (9) or eq. (10) provides the basis for computing the time dependent network boundary concentrations

The pipe flow, pipe and network node concentration, and network boundary concentration simulations are performed separately and combined by a coordinated algorithm. The hydraulic simulation is performed as described in the previous section. This procedure yields a time series of pipe flow rates and FGN fluid volumes that are constant for the duration of each hydraulic time step, Δt_h. These results are then used to simulate the dynamic species

mass transport through the network. Following we describe the transport simulation that is done during each hydraulic time step.

The differential equations that define the network boundary conditions are integrated during each hydraulic time step using a simple explicit Euler method. If the *ith* FGN is emptying, then the Euler explicit update formula is:

$$C_i^{BC,k+1} = C_i^{BC,k} + \Delta t_c \cdot r_i^{BC,k} \tag{11}$$

While if the FGN is filling, then the update formula is:

$$C_i^{BC,k+1} = C_i^{BC,k} + \Delta t_c \cdot [r_i^{BC,k} - \frac{q_{j\to i}}{V_i^*}(C_{j\to i,m}^k - C_i^{BC,k})] \tag{12}$$

where the superscripts $k,k+1$ denote the time level, and Δt_c is the water quality time step for the boundary computations. These time levels are different from those in eq. (6), as Δt_c is different from the hydraulic time step. The water quality boundary condition time step is selected such that $\Delta t_h = n \cdot \Delta t_c$, where n is a positive integer.

The time step used in numerical integration of eqs. (6) and (8) is independent of the water quality time step, Δt_c, used to simulate the network boundary conditions. For simplicity, we assume the network boundary conditions to be constant for the duration of a water quality time step, and eqs. (6) and (8) are then integrated in time until the end of the water quality time step is reached. This process is repeated, alternately updating the network boundary concentrations and solving the network mass transport equations, until the end of the hydraulic time step. Figure 3 shows the main steps of the algorithm.

Eq. (6) is integrated in time by first substituting eq. (8) for each upstream pipe boundary condition. The resulting o.d.e. system is integrated using either an Adams–Moulton or a Gear Multi-Value (MV) method, as implemented in the widely used code LSODE [Aiken, 1985]. Both methods allow for automatic order and step size selection based on specified tolerances for local error control. We do not yet have extensive experience comparing the various methods of solution, but have had success with both approaches.

Both the Adams–Moulton and Gear MV methods are implicit methods, and hence require the solution of a system of (in general) nonlinear equations at each time step. These equations can be solved by either functional iteration or by Newton's method. Functional iteration is a technique suggested by the special form of the nonlinear equations, in which the unknowns (the concentrations at the next time step) appear both in general nonlinear terms and isolated. Thus the equations can be used in a simple updating scheme (functional iteration) that may save considerable computation. The drawback of functional iteration is that it may not converge, and in fact functional iteration itself places step size restrictions on the numerical integration that are similar to those associated with explicit methods. We have been successful in using functional iteration on all problems analyzed thus far, but then none of these problems were nonlinear.

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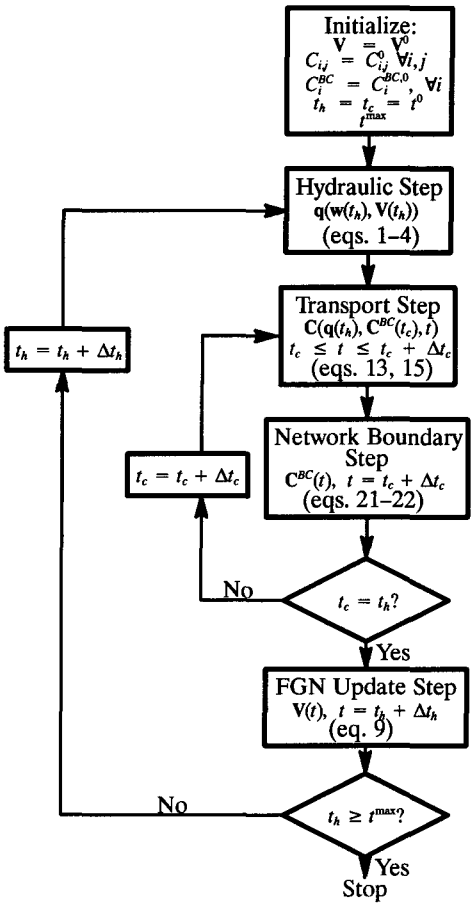

Figure 3. – Hydraulic and Transport Simulation Algorithm

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