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Axial Dispersion in Pressurized Water Distribution Networks—A Review

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Abstract. A review of recent findings on axial dispersion in pressurized water distribution networks is presented. Solutions, with axial dispersion via a two-dimensional advection-diffusion-reaction model and without dispersion using a one-dimensional advection-reaction model, are compared. Axial dispersion turns out to be an important transport process in laminar and transitional flows. The effects of stochastic water demand on solute spreading are discussed. Expressions for the time-averaged rates of axial dispersion are presented. An Eulerian-Lagrangian scheme is combined with a network numerical Green's Function technique, applied to a network with stochastic water demands and then compared against the EPANET model and field observations. Both models achieve similar results at locations where turbulent flows prevail. However, the dispersion model provides better agreement with field observations at locations where laminar flows dominate.

Keywords: Drinking water quality modeling, water distribution networks, dispersion, contaminant transport, chlorine decay

1 Introduction

Because of physical, chemical and biological processes, water quality deteriorates in a water distribution system during transport between the points of treatment and consumption. Since it is not feasible to monitor water quality throughout a network, nor is it possible to sample all possible operation scenarios, water-quality engineers and system designers often employ computer-based mathematical models to predict

the spatio-temporal distribution of constituents in water distribution networks. Such models can be used to analyze water quality degradation problems, assess alternative operational and control strategies for improving and maintaining water quality, design water-quality-sampling programs, optimize disinfection processes and evaluate the water quality aspects of distribution-network improvement projects.

Axial (or longitudinal) dispersion of fluid flowing through a pipe is defined as a mass transport process in which a solute spreads in the axial direction while moving downstream due to a non-uniform velocity distribution over the pipe's cross-section. Most distribution network water quality models including the widely used, public-domain EPANET [28] and commercial codes [37] apply a one-dimensional advection and reaction scheme (1D-AR) that neglects axial dispersion. These transport models perform satisfactorily when used for analyzing pipes in which turbulent flows dominate, but they tend to be less reliable when used for pipes in low flow zones, such as dead-end zones, which are common in municipal water-distribution systems. Depending on the time of day, low-flow conditions may predominate in 20-50% of a water distribution network having pronounced diurnal demand patterns [7].

In the presence of laminar flow, axial dispersion can be an important factor when predicting water quality. For example, the travel time of water through a distribution system is often assumed as nominal hydraulic residence time (volume/flow) or estimated as the residence time using a water-quality model like EPANET. In either case, the computed travel time does not take dispersion into account. However, the fact is that a part of a reactive disinfectant will move further along the supply pipe under conditions of advection-dispersion (A-D) transport than it does under pure advection transport conditions. Similarly, under A-D transport some fraction of the disinfectant will *not* move as far along the supply pipe as expected in pure advection. These differences in residence times could have ramifications when the supply system requires expeditious and accurate disinfection. In addition, when dispersive transport is neglected, utilities may over-dose the disinfectant to achieve certain residual concentrations at remote points in distribution network. Using dispersion transport model, on the other hand, may help utilities to fine-tune their disinfectant doses.

For these reasons, the next generation of network water quality models should account for axial dispersion. This paper presents the summary of recent research on the subject of axial dispersion in water distribution networks.

2 Background

Classical works on axial dispersion, conducted five decades ago (Taylor's theory [29]), laid the foundations that have been examined ever since and applied to chemical and industrial processes for laminar and turbulent flows. However, these theoretical and experimental findings have not been integrated into water quality models for pressurized water distribution systems. Transport of a conservative chemical tracer moving in steady laminar flow through a pipe is described by the two-dimensional advection-diffusion equation:

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial x^2} \right) - 2U \left(1 - \frac{r^2}{a^2} \right) \frac{\partial C}{\partial x} - KC \quad (1)$$

where: $C=C(r, x, t)$ is the solute concentration at any point in the cross section, D is the molecular diffusion coefficient (diffusivity) of the solute in water, U is the mean velocity in the axial direction, K is the first-order reaction rate constant for bulk decay (no wall decay is considered), a is the pipe radius, r is the radial position, x is the axial position, and t is time.

According to the Taylor's classical theory for dispersion, Eq. (1) can be simplified to the one-dimensional advection-dispersion equation, provided a certain initialization period has elapsed:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = E \frac{\partial^2 C}{\partial x^2} - KC \quad (2)$$

where: C is now the average concentration in the cross section and E is the axial dispersion coefficient, considered as constant. A dispersion process with a constant dispersion coefficient is known as *steady dispersion*. Expressed in dimensionless time T , the initialization condition is $0 < T < 0.5$, where $T = Dt/a^2$. Because of the small value of the diffusivity ($D=10^{-5}$ cm²/s for water) and the constantly changing flow in water distribution networks, the dispersion process is always in the initialization period, i.e., it is *unsteady dispersion*, and Taylor's theory is not valid. Accordingly, Gill and Sankarasubramanian (G/S, [14]) extended Taylor's theory and obtained an exact dimensionless expression for the unsteady instantaneous rate of dispersion in steady laminar flow.

A few previous studies of mass transport in single pipes under steady flow conditions indicate that axial dispersion is an important factor in laminar flow zones. Using analytical solutions of one-dimensional models in a steady flow, Axworthy and Karney [4] studied water quality under low-velocity and high-dispersion flow in a water distribution system. They concluded that the advective transport model with a continuous step input of solute significantly underestimates the nodal concentrations obtained by solving the advection-dispersion equation under low flow velocity. Their research implies that water quality models should incorporate dispersive transport in low-flow pipes.

Starting with a two-dimensional model and laboratory experiments that stressed the influence of dispersion, Ozdemir and Ger [22, 23] used a single equation to express bulk decay, radial diffusion and the subsequent pipe-wall reaction of chlorine and then converted the equation into a one-dimensional model. In subsequent studies, Ozdemir and Ucak [24] and Ucak and Ozdemir [36] embedded that equation into a computer program designed to analyze dynamic water quality in drinking water distribution networks.

In formulating a model for steady-state dispersion, Biswas *et al.* [6] argued that radial diffusion is the only important dispersion mechanism for chlorine concentration decay, and they compared it to field data.

One of the first attempts to numerically model the dispersion in water distribution networks is presented by Islam and Chaudhry [15]. However, their work did not consider unsteady dispersion and dispersion between pipes at network junctions.

Basha and Malaeb [5] applied an Eulerian – Lagrangian method for simulating the advection-dispersion-reaction process of constituent transport in water networks. In their study, the dispersion term in the governing equation is approximated using finite differences, and the resulting first-order partial differential equation is integrated using the method of characteristics. However, their model neglects the dispersion effects present between pipes at network junctions, which may lead to inaccurate results in networks where such effects are significant.

3 Recent Advances

3.1 Dispersion in Steady and Random Intermittent Laminar Flow

Since the exact G/S expression [14] for the time dependent dispersion coefficient is somewhat cumbersome to use, Lee [16] derived the following, well-fit approximation to the G/S equation with a correlation that exceeds 99.9%:

$$E(t) = E^* \left[1 - \exp\left(-\frac{t}{\tau_0}\right) \right] \quad (3)$$

where: $\tau_0 = a^2 / 16D$ is a Lagrangian time scale reflecting molecular diffusivity D across the pipe radius a . Lee [16] also presents an expression for estimating the time-averaged dispersion coefficient in steady flows as

$$\overline{E(T)} = \beta(T) E_T \quad (4)$$

where: $\beta(T) = 1 - \frac{1 - \exp(-16T)}{16T}$ and E_T is the Taylor dispersion coefficient in a steady flow [29].

Equation (2) is restricted to steady flow; however, flow in a water-distribution system fluctuates over time due to changing consumer demands. Because of the sporadic and stochastic nature of water demands, the flow (besides laminar) in water distribution pipes at the network periphery is often intermittent [7, 8, 11], giving rise to an even stronger dispersion transport. As a starting point (Buchberger *et al.* [8]), analyzed dispersion in intermittent laminar flow under the assumption of achieving an instantaneous laminar velocity profile during the periods when flow occurs, and concluded that the value of the time-averaged dispersion coefficient in intermittent laminar flow is larger than that given by Taylor's formulae for dispersion in steady laminar flow. Later, using principles from the linear systems theory Lee [16] studied unsteady dispersion in random, intermittent laminar flow and derived explicit expressions for the instantaneous rate of dispersion $E(t)$ resulting from an arbitrary sequence of laminar flow pulses. The study reveals that $E(t)$ is the sum of two

factors: the dispersion memory derived from previous pulses and the nonlinear excitation derived from the current pulse. During periods of stagnation, active dispersion ceases and the memory of previous dispersion decays exponentially.

Based on the Eq. (4) (Li *et al.* [18]) estimated the spatially averaged dispersion coefficient using the travel time in a pipe with laminar flow as:

$$E_i(t^n) = \frac{[aU_i(t^n)]^2}{48D} \left\{ 1 - \left(\frac{\tau_0}{t_i^r} \right) \left[1 - \exp\left(-\frac{t_i^r}{\tau_0} \right) \right] \right\} \quad (5)$$

where: t_n is current time at time step n ; $U_i(t^n)$ is averaged flow velocity in pipe i within time step n ; t_i^r is the travel time in pipe i with flow velocity $U_i(t^n)$.

Buchberger and Lee [9] proposed a simple analytical method for estimating dispersion in steady and unsteady laminar flow with no initialization time. Using a Lagrangian dispersion model to simulate water quality and the dispersion predicted by that analytical method, they suggested a method for integrating dispersive transport phenomena into water-quality models.

3.2 Assessment of the Importance of Dispersion in Water Distribution Network Modeling

Using analytical solutions for a non-conservative solute, Lee [16] suggested that dispersion is important in laminar flows when the dimensionless group, $KE/U^2 > 0.11$ and proved that the advection-reaction (AR) model significantly under-predicts the non-conservative constituent concentration.

Through theoretical and numerical approaches, Li and co-workers [17, 20] analyzed the relative importance of the three basic mechanisms (advection, dispersion and reaction) with respect to the overall transport process in laminar flow. The significance of longitudinal dispersion in conjunction with a step input of reactive solutes in steady flows was first investigated analytically and compared theoretically in order to obtain the relative importance of the terms in one-dimensional governing equation under different conditions.

To further study the conditions under which dispersion becomes important for accurate water quality modeling, numerical solutions for a two-dimensional advection-diffusion-reaction (2D-ADR) model and a 1D-AR model were then used to investigate and to corroborate dispersive behaviors with unsteady flows or unsteady solute source profiles [17, 20]. The differences between the water quality results obtained by the 2D-ADR model and those obtained by the 1D-AR model were identified. It was demonstrated that mass dispersion is an important factor of a conservative solute with an instantaneous injection source or a sinusoidal injection source, but it may not be important to the regions not affected by the concentration front for the linearly increasing source and the step injection source. These results are governed by the potential driver of dispersion, the second-order derivatives in Eq. (2), which are greater than zero for instantaneous injection and sinusoidal injection but

approach zero for regions unaffected by concentration front of the other two injection sources.

The effects produced by time scales, pipe sizes, flow velocities, water-demand pulse, arrival rate and the time history of flows on unsteady dispersion were also analyzed [17, 20]. It was concluded that the importance of dispersion in water quality modeling increases as pipe diameter increases for laminar dominated flows. Dispersion in water quality modeling plays a more important role for conservative contaminants. With an increase in reaction rate, dispersion becomes relatively less important for unsteady solute sources. Flow patterns and time scale do not appear to produce any obvious effect on the importance of dispersion. However, the time-averaged dispersion decreases greatly with the occasional bursts of turbulent or transitional flows, which most likely occur with small time scales. Therefore, a large time scale may lead to an overestimation of the dispersion rate because it masks the turbulent or transitional flow regimes in low flow zones

3.3 Numerical Methods

Numerical solutions for the 2D-ADR Eq. (1) in steady and random intermittent and unsteady laminar flow are presented by Buchberger and Li [10], Lee [16], Li [20] and Li *et al.* [17]. A Lagrangian-Eulerian numerical scheme was implemented by splitting Eq. (1) into two equations, one for molecular diffusion and another for advection. Each advected point retains its radial position but is translated downstream by an amount equal to the travel distance, which is computed as the product of the flow velocity and the time step. Radial and axial diffusion are computed with an Eulerian approach. In intermittent flow, during a busy period, only radial diffusion is considered using a Crank-Nicholson scheme, because axial diffusion is negligible compared to advection. During idle times, both axial and radial diffusion are simulated by applying an unconditionally stable alternating-direction implicit scheme and using two half steps to advance one full time step.

Because large water distribution systems often contain hundreds of dead-end stems serving thousands of consumers, it is impractical to use a 2-D transport model to simulate water quality in all the branching pipes of a municipal network considering the massive computational cost. Consequently, most network water quality models simulate solute transport with pipe hydraulics based on 1-D flow. Furthermore, to promote compatibility with existing models, the approximation for unsteady laminar dispersion is merged with a 1-D transport model in order to obtain an equivalent dispersion coefficient E for intermittent unsteady laminar flow [16], [17], [20].

In a piping network, Eq. (2) applies for each pipe, and the following boundary conditions hold at the network nodes:

- a) At some nodes, seen as constituent sources, the concentration C is prescribed.
- b) Mixing at the network nodes: a complete mixing has long been assumed in the network models, although recent works clearly demonstrated that this assumption needs to be revised [3], [25]. Recent studies [3], [25] show that pipes with different flow and constituent concentration may convey flow to a four way junction including a cross, a double-tee, or a tee-wye combination. Constituents are *mixed* at the node

and new concentration values are obtained based on the ratios of flow rates in upstream and downstream pipes.

c) Mass conservation at the network nodes: Tzatchkov *et al.* [32], by generalizing the derived Eq. (2) to include the case of a junction at which several pipes meet, obtained the following nodal equivalent of Eq. (2):

$$\sum_{j=1}^m \left(\frac{dx_j}{2} A_j \right) \frac{\partial C}{\partial t} = \sum_{j=1}^m \left(A_j D_j \frac{\partial C}{\partial x} + Q_j C - K_j C A_j \frac{dx_j}{2} \right) - q_i C \quad (6)$$

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 cases in which two pipes of equal characteristics meet at a node and $q_i=0$, Eq. (6) reduces to Eq. (2) if dx_j and dt tend to be infinitesimally small.

The numerical solution of the 1D-ADR equation in networks poses three main problems:

a) Boundary conditions at those nodes that are common to several domains have to be formulated and considered;

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

c) The difficulty increases when advection dominates over dispersion. Sharp concentration gradients are expected in this case, and an extremely fine discretization would be needed if Eulerian methods were to be applied. Because of the small values of the dispersion coefficient, contaminant transport in water distribution networks falls exactly in this category of advection-dominated problems.

To solve the advection-dispersion-reaction equation in pipe networks, Tzatchkov *et al.* [32] developed a numerical solution based on the domain decomposition strategy used to efficiently solve the resulting finite difference equations. A two-stage Eulerian-Lagrangian numerical scheme is applied [1]. Eq. (2) is split into two parts (an advective part and a dispersive part) and then numerically solved in each time step in two stages. In the first (Lagrangian) stage, the advective (or advective-reactive) part is solved for each pipe. The backward method of characteristics is used. In the Eulerian stage, an implicit numerical scheme is used, leading to a system of linear equations. To achieve computational efficiency in solving this system, a special technique that employs numerically computed Green's functions within each pipe is proposed [2]. 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 that correspond 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 at each end, and continuity balance relations are used to construct a system of linear equations for finding the values of the unknown quantities at the network nodes. Thus, the large system of equations that

represents the discretized network is decomposed exactly into three easy-to-solve tridiagonal systems for each pipe, and one low-order system to represent the concentration at the pipe junctions. This method can be applied to any type of network, branched or looped, and to advection-dominated and dispersion-dominated transport phenomena in order to handle a broad range of flow velocities that can be met in real distribution networks. More details can be found in [1], [30], [31], [32], [34], [35].

Tzatchkov *et al.* [33] extended the proposed advection-dispersion-reaction numerical model to include dispersion in intermittent laminar flow and variation of the dispersion coefficient during the initialization period. Li [20], Li *et al.* [18] and Li *et al.* [19] extended the method proposed by Tzatchkov *et al.* [32] to create a more complete computer model, ADRNET. The EPANET toolkit network hydraulic functions are incorporated and used as the hydraulic engine in order to simulate the extended period pipe flows in ADRNET based on time-averaged stochastic demands. The improvements made to the model are as follows: a) for better computational stability, a fully implicit difference format has been adopted to replace the Crank-Nicholson format; b) to achieve a more reasonable representation of network conditions, improved techniques for estimating the spatially-averaged dispersion coefficient have been utilized based on Lee' work [16]; and c) to more accurately simulate network water quality, stochastic water demands have been incorporated and examined.

3.4 Experimental and CFD Work

Cutter [12] conducted dispersion coefficient estimation experiments with a 15 cm diameter pipe. His results showed, as expected, that the dispersion coefficient increases with an increasing Reynolds number for $Re \leq 2400$ in laminar flow zone but decreases linearly with an increasing Reynolds number ($2400 < Re < 4000$) in transitional flow zone. In a turbulent flow zone, however, dispersion coefficients maintain a much lower level compared to those in laminar and transitional flow zones.

Romero-Gomez *et al.* [26] conducted a series of experiments in an effort to compare the empirical results of an axial dispersion of a non-reactive tracer in a pipe under laminar and transitional flow conditions with the modeling outcomes obtained from EPANET, Computational Fluid Dynamics (CFD), and the 1D Advection-Dispersion (AD) model. The experimental setup was constructed at the Water Distribution Network Laboratory at the Water Village, an experimental facility at the University of Arizona, Tucson, AZ, U.S.A., and consisted of a 10 m-long PVC pipe with a 15.3 mm inner diameter (1/2 inch nominal diameter), mounted on a metal scaffolding. Tap water, pumped from a storage tank into the pipe, constituted the main water source, whereas a micro-pump was used to inject water taken from a beaker and containing a tracer (sodium chloride). The flow rate was both controlled and monitored by means of turbine type flow-rate sensors. The flow rate was controlled using pump controllers and the needle valve at the downstream end of the pipe. Tracer concentration was monitored with electrical conductivity sensors. Two 4-ring potentiometric electrical conductivity probes and transmitters were placed at the

upstream and downstream monitoring locations, 7.84 m apart, to measure tracer concentrations. Flow rate and concentration were observed in real time and recorded every second using a data logger.

The CFD simulations of the species transport in the pipe were carried out using FLUENT [13]. Two-dimensional, axi-symmetric, unsteady-state simulations were performed. The geometric extents of the circular pipe were $H = 0.008$ m \times $L = 1.6$ m, both numbers representing a 2D computational domain axi-symmetric about the x -axis. Therefore, a 100D-long pipe was simulated. A quadrilateral mesh was defined with 30,480 cells, of which 10,160 cells (8x1270) belonged to the boundary layer region that was defined at the pipe walls. The following boundary types were set at the domain edges: velocity inlet (left), outflow (right), wall (top), and axis (bottom). The material was set as a mixture of water and sodium chloride. The boundary conditions (BCs) at the inlet were obtained from the experimental readings of flow rate (used for velocity BC) and upstream concentration (used for species BC). Because the upstream concentrations are transient, a time dependent profile was created for the latter. The species transport equation, which was added to the solver, was taken to be uncoupled from the flow calculations.

CFD simulation results for laminar flows were in excellent agreement with the experimental data. Two distinct characteristics were observed: (i) the experimental and CFD-simulated maximum concentration at the downstream location is lower than those based on the “plug flow” for all the cases, and (ii) the downstream breakthrough time of the “plug flow” profile is always delayed as compared to the experimental and CFD-simulated time and this difference becomes shorter with higher Reynolds numbers. Thus, axial dispersion of a solute can be an important transport process in laminar and transitional flow regimes. The actual rate of dispersion can be estimated by using the method of moments and experimental tracer data obtained under any flow regime. The magnitude of the dispersion coefficient dropped quickly when the flow leaves the laminar regime and enters the transition regime, consistent with available theory and previous experimental results by Cutter [12].

3.5 Field Validation and Applications

Tzatchkov *et al.* [32] and Li *et al.* [19] applied advection-dispersion-reaction models 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 made by the EPANET model [27]. In those 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 more closely represented by the proposed model than by the EPANET model [30], [32], [34]. The proposed model that considers dispersion appears to provide a substantial improvement over predictions by EPANET using advection-reaction model in low pipe flow zones of the network.

Nilsson [21] used numerical Monte Carlo experiments to simulate a deliberate biochemical assault on the Cherry Hill Brushy Plains water distribution system. The attack was modeled as a steady 6-hour injection delivering 3600 g of a conservative contaminant to a single node on the main line. Advection, dispersion and reaction

were considered. The migration of the contaminant plume was tracked for 55 hours throughout the pipe network and the cumulative mass dose was computed at five target nodes. Combining the EPANET solver with a stochastic water demand generator the exercise was repeated for 1000 independent trials to establish a distribution of consumer dose exposures at the target nodes. A battery of simulation experiments was then performed to investigate how changes in system storage and demand patterns affect the baseline nodal dose loadings. Results for this case study show that the nodal dose distribution was extremely sensitive to the assumed system's operating conditions. When comparing different network configurations, the degree of system storage dominated the overall response. A relatively minor variability in water demands can lead to a broad range in the cumulative dose received at a particular node. In the case study, advective-dispersive transport did not have an appreciable effect on the total contaminant dose delivered to the target nodes. This could be due to the relatively small size of the network, the prolonged length of the attack, and/or the conservative contaminant modeled.

5 Conclusions

Solute dispersion is an important component of network water quality simulation, and it should be incorporated into the next generation of distribution network water quality models. The work presented in this paper should improve our fundamental understanding of solute transport and enhance our ability to model and predict water quality in municipal distribution systems. Improved water quality models capable of achieving accurate spatio-temporal axial dispersion patterns will be critical to efforts aimed at optimizing water quality sensor placement, assessing models for early warning systems, and generating the exposure information needed for quantitative risk assessment. Progress has been made, but the spatial evolution process of dispersion requires further research in order to determine the mass dispersion coefficient in network pipes under unsteady flow.

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