DEVELOPMENT OF AN INTEGRATED WATER QUALITY PREDICTION TOOL FOR DRINKING WATER DISTRIBUTION SYSTEMS **

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Background
Given Arizona’s growing population, new communities have the unique opportunity to establish water supply and distribution infrastructures upon innovative concepts that not only seek to satisfy water demands in quantity, but also anticipate the future needs for an integral service to customers. Issues such as improving water aesthetics, reducing hazardous byproducts of disinfectants, and responding promptly to public health emergencies due to ingestion of contaminated water are part of increasingly stricter requirements for water providers. As seen, these concerns are all related to understanding water quality transformations as water travels from the treatment plants to the multiple points-of-use. Computer models of the piping system and its operation rules are widely used as water quality prediction tools. However, such models are still unable to represent the spread of constituents as a water volume moves along a pipe (axial dispersion) and only consider that constituents travel at the same speed as the water parcel (advection). Thus, in the simplest flow configuration, a tracer pulse of short duration injected at the upstream location of a long pipe is incorrectly predicted to travel for miles without changing its shape at all. Though this assumption is based on the ground of prevailing turbulence in pipes of large diameter, recent developments in water system modeling tend to include smaller pipes where low flows occur. Because dispersion predominates over advection in such instances, slow/stagnant/intermittent flows found near the households and peripheral areas aggravate the inaccuracy of the current water quality models.

Another critical oversimplification of water quality solvers is related to how solutes are assumed to mix as cross junctions. In this subject, two adjacent inflows of unequal quality interact fully to produce two outflows of equal quality, i.e. mixing is complete. Several research efforts addressed this assumption from elucidating its potential for erroneous predictions to developing a solver that accounts for incomplete mixing at cross and other 4-way junctions (Fowler and Jones, 1991; van Bloemen Waanders et al., 2005; Romero-Gomez et al., 2006; Romero-Gomez et al., 2008, Austin et al., 2008, Choi et al., 2008; Song et al., 2009). Particularly, a solver called AZRED developed at the University of Arizona is based upon experimental data in multiple 4-way junctions (Choi et al., 2008). We intend to develop a second generation of such solver, AZREDII, which is in addition capable of fully and accurately representing the axial dispersion of constituents in water (Figure 1). The objectives were achieved through the application of three consecutive methodologies:

(i) the development of axial dispersion coefficients in single long pipes under constant flows,
(ii) the corresponding experimental verification and
(iii) the integration of the axial dispersion effects and incomplete mixing at junctions (Figure 1).

** Research funding was provided by Technology and Research Initiative (TRIF) Fund 2009/2010, Water Sustainability Graduate Student Fellowship Program at the University of Arizona.
The broad research goal of this work aimed at expanding the capabilities of the current water quality prediction tools. With our methodology, such improvement proceeded from micro-scale model development toward macro-scale development with its corresponding experimental/field verifications. To make a contribution, this study began with a series of axial dispersion experimental runs in a single long pipe, which shows how the inlet concentration/flow conditions (experimental input data) give rise to a concentration pulse at the pipe outlet. Next, these same experimental input data are fed into Computational Fluid Dynamics simulations in order to thoroughly map out the spatio-temporal solute distribution along the pipe. When an acceptable agreement between the two approaches exists, the CFD technique then becomes a feasible way to characterize the axial dispersion rate, $E$, as a function of flow, solute properties and travel time. Further verifications of the developed model determine its applicability to represent axial dispersion in laminar pipe flows.

**Methods**

**Experimental study of axial dispersion**

The experimental setup was constructed at the Real-Time Sensor Testing Laboratory of the Water Village, an experimental facility at the University of Arizona, Tucson, AZ. Figure 2 depicts the components of the water conditioning system and the main pipe section. Municipal tap water was run through five water filters connected in series in order to remove particles of sequentially decreasing sizes. Following filtration, a reverse osmosis system removed most of the salts contained in the tap water (about 90%) and increased the efficiency of an additional two-tank deionizer unit. In this way, only the salt tracer injected in the pipe section affected the conductivity sensor readings. A frequency inverter controlled the centrifugal pump delivered the main water source into a PVC pipe (15.6 mm diameter, ½” nominal diameter). A programmable peristaltic pump injected pulses of tracer solution from a beaker. A turbine-type flow sensor the flow rates, which were controlled with a needle valve. A four-ring potentiometric probe, combined with a conductivity transmitter measured the inlet conductivity data (upstream detection point). Another unit was used to measure the conductivity values of grab samples taken at the downstream detection point. Sensor readings at various tracer solutions determined the relation between conductivity and salt concentration. Flow rates and upstream solute concentrations were recorded every second using a data logger.

The development of the axial dispersion model was based on a set of experimental runs that targeted mean flow velocities ($U_0$) ranging from 8.37 to 12.88 cm s$^{-1}$ in a 6.5 m-long pipe and subject to 10 second-long injection pulses. Another set of experimental runs was used for verifying the developed model in both a 6.5 m- and a 12.5 m-long pipe.

**Determination of axial dispersion rates**

The experimental runs supplied the inlet boundary conditions (flow rate and inlet concentration data) needed to simulate the solute mass transport using Computational Fluid Dynamics (CFD) techniques. The approach consists of numerically solving a set of conservation equations that fully describe the velocity field and solute distribution in pipe flows under prescribed initial/boundary conditions. Although the CFD approach to solving for axial dispersion is computationally intensive for real-world applications, analyses of selected cases provide a detailed portrayal of the mass transport phenomena taking place as the solute moves along a single pipe. The approach follows three steps: pre-processing (defining pipe geometry),
numerical setup (modeling assumptions and solving conservation equations) and post-processing (obtain the time series of solute concentration at various distances). Next, we determined axial dispersion models via PDE-constrained parameter optimization. The optimization formulation sought to minimize an error occurring between the solute concentrations predicted by the 1D-ADR equation ($C_S$, Equation 1) and the results obtained by the CFD-simulation upon the application of dispersion coefficients $E_f$ and $E_b$, which thus became the decision variables. In other words, we want to get as close as possible to the CFD predictions by systematically manipulating $E_b$ and $E_f$ in Equation 1, as they correspond to the sought dispersion coefficients valid for hydraulic and quality conditions found in drinking water systems.

\[
\frac{\partial C_S}{\partial t} = \frac{1}{\Delta x} \left( \phi_b - \phi_f \right) - U_0 \frac{\partial C_S}{\partial x} \quad (1)
\]

**Initial Condition**
\[C_S(x,0) = 0\]

**Boundary Conditions**
\[C_S(0,t) = C_o(x); \quad \left. \frac{\partial C_S}{\partial x} \right|_{x \to \infty} = 0 \quad t > 0\]

where:
\[
\phi_b = -E_b \left. \frac{\partial C}{\partial x} \right|_b \quad \text{and} \quad \phi_f = -E_f \left. \frac{\partial C}{\partial x} \right|_f
\]

**Development of an integrated water quality prediction tool**

In order to evaluate the impact of dispersion coefficients $E_b$ and $E_f$, we computed predictions of chlorine concentrations over a small exemplary network (Figure 3). An EPANET toolkit/C++ routine (US EPA, 2000) was used to obtain the system’s hydraulic information, which then served as the primary input data to implement incomplete mixing and to solve for the 1D-ADR model (Equation 1). Predicted concentrations computed with the new modeling assumptions were then compared to those computed without those assumptions. Whereas the incomplete mixing at junctions was computed by using AZRED (Choi et al., 2008), axial dispersion was solved via a finite difference method applied to the 1D-ADR model (Equation 1). The latter procedure has been thoroughly described by Romero-Gomez and Choi (2010). This intermediate step of implementing axial dispersion enabled us to identify sequential steps that are relevant to using the hydraulic and water quality solver efficiently to achieve our ultimate goal.

Net1 of the EPANET examples (Figure 3) consists of 12 pipes, 9 nodes, a water source, a pump, and an elevated tank. The base demands are subject to a transient pattern throughout a simulation period of 24 hours. The remaining characteristics are readily accessible for downloading from the EPANET software package (US EPA Website). In order to achieve prevailing laminar flows in the network, some of the original features of the model were modified. The water demand at node 22 (cross junction) was set equal to zero. In order to ensure that most flows are subject to laminar conditions, all base demands were divided by 100, and pipe diameters were divided by 2. Likewise, pipe lengths were divided by 20 in order to make dimensionless travel times (as calculated by average mean flow velocity at each pipe) less than 0.01. Additionally, the status of the pipe connecting to the tank was set to “close,” while initial nodal qualities were set to zero, and both global bulk and wall reaction coefficients were set to zero. The time option settings were as follows: total duration = 48 hours, hydraulic time step = 1 min and quality time step = 1 min.
Key findings

The first stage in the development of the axial dispersion model entailed validating the results from CFD-simulations against the experimental readings of solute concentration. To accomplish this, we introduced a 10 s-long injection pulse of a sodium chloride solution at a flow rate equal to 30 ml min\(^{-1}\). All experimental data points presented in this work were obtained with duplicate runs conducted at the same (or nearly same) flow velocity in order to guarantee repeatability during data collection. All downstream concentration featured lower peak values as well as a stretched curve in comparison to the upstream signal. Nevertheless, such expected characteristics were quantitatively distinct depending upon the approach. The CFD-simulated results and experimental results showed an acceptable correlation over time \((0.81 < R^2 < 0.96)\) for various runs (not shown for brevity, but summarized in Romero-Gomez and Choi, 2010). These results demonstrate the ability of CFD tools to accurately represent the axial dispersion transport in pipe flows. Because CFD poses the advantage of providing time series of concentration not only at the pipe outlet, but also at any location before and after, then we proceeded to determine axial dispersion coefficients by applying parameter optimization techniques. In doing so, we determined that coefficients \(E_b\) and \(E_f\) in Equation 1 took the following form:

\[
E_b = E_b(0)\exp(-16T) + \beta_b(T)E^* \]

\[
E_f = E_f(0)\exp(-16T) + \beta_f(T)E^* \]

Having:

\[
\beta_f = \beta_b = \beta = 3.705T \quad (2)
\]

where \(E_b(0)\) and \(E_f(0)\) are the initial dispersion coefficient values, \(E^* = \frac{a^2U_0^2}{48D_{AB}}\) and \(T = \frac{4D_{AB}f}{d^2}\). In these expressions, \(E^*\) is known as Taylor’s dispersion (1953), \(D_{AB}\) is the molecular diffusivity, \(d\) is the pipe diameter and \(a\) is the pipe radius. Thus, equation 2 is the central finding of the present study.

A battery of experimental was run in order to verify the axial dispersion formula for solving various combinations flow velocity \((U_0)\) and pipe lengths \((L)\). Figure 4 illustrates the dispersion effect in a 6.5 m-long pipe whereas the ones at the bottom depict the outcomes of runs at corresponding (or nearly corresponding) flow velocities in a 12.5 m-long pipe. As expected, the inlet pulse disperses considerably more in longer pipes. Figure 4 exhibits an acceptable agreement between the experimental measurements and the 1D-ADR predictions made by the newly-developed dispersion coefficients, \(E_b\) and \(E_f\). The largest discrepancies were observed at peak concentrations for runs at \(U_0 = 11.12\ \text{cm s}^{-1}\) and at \(U_0 = 11.27\ \text{cm s}^{-1}\). These were underestimated by the modeling approach; however, this discrepancy is a consequence of the optimization formulation in which we primarily emphasized the model’s ability to predict the solute arrival time over its ability to reproduce other features. The duplicate experiments (run 1 and run 2) produced downstream concentration readings that complemented each other.

Outcomes in Figure 4 make evident the improvement in quality predictions with the coefficients found in the present study. To evaluate the combined effect of incomplete
mixing/axial dispersion over a network, we conducted quality simulations of a tracer injection in the exemplary network shown in Figure 3. The injection of a soluble tracer occurred at 2 am and lasted for two hours (injection period from 2:00 – 4:00) at node 11. The tracer molecular diffusivity \( D_{AB} \) was \( 10^{-9} \text{ m}^2 \text{s}^{-1} \). This rectangular injection pulse had a high concentration of 100 mg L\(^{-1}\). The traveling pulse is subject to transient conditions over the entire simulation period, giving rise to distinct concentrations at the downstream nodes.

Figure 5 shows the curves of the tracer concentration vs. time obtained from EPANET (complete mixing/advection-only transport) and with new modeling elements (incomplete mixing/advective-dispersive transport). Differences in solute distribution over time manifest even at nodes closest to the injection location (nodes 12 and 21), e.g. a more spread-out curve with lower peak concentrations, as compared to EPANET outcomes. In fact, at those locations, tracer pulses essentially mimic the injection pulse, but only at posterior times. The further travel times required to reach nodes 13, 32 and 23 amplify the discrepancies between outcomes from both models. Though EPANET predictions did show extended solute arrival over time, they still exhibit stepwise distributions, as opposed to the smooth dispersion shown by the improved predictions. It is essential to remark that the procedure followed here is capable of handling this exemplary network only. A future development must seek to apply both improved assumptions in any piping network. A fundamental reason to seek a full implementation of incomplete mixing/axial dispersion into EPANET is justified by the long computational time required to obtain quality predictions, even for the presented small network. Approximately 25 minutes was required to run the toolkit/C++ routine on a personal computer (with an Intel Core 2.33 GHz, 1.99 GB of RAM). The advantage gained from shortening this computational effort should, by itself, provide enough motivation to pursue an efficient, yet accurate development of AZRED II.

**Outcomes and outputs**

- **Outcomes**
  - Development of dispersion rate formulas relevant for conditions in drinking water systems
  - Application of new coefficients into a piping network model

- **Outputs - these are given in terms of publications where the present work is detailed.**
  - “Axial dispersion coefficients in laminar flows of water distribution systems” manuscript submitted to American Society of Civil Engineering Journal (Journal of Hydraulic Engineering)

**References**


Distribution System Analysis Symp., Kruger Park, South Africa. Also, note the website http://cals.arizona.edu/~cchoi/AZRED.


Figure 1. Development of an integrated water quality prediction tool
Figure 2. Experimental setup for the
Figure 3. Net1 from EPANET package example networks was modified
Figure 4. Experimental verification of the developed axial dispersion coefficient model at various Reynolds numbers. The inlet concentration pulse (bold line, —) gives rise to downstream concentrations at L = 6.48 m and L = 12.50 m by several approaches: 1D-ADR with dispersion rates developed in the present study (continuous line, —) and experimental measurements ((1st run, ●; 2nd run, ○)).
Figure 5. Solute concentration at downstream nodes, as calculated by EPANET (---), AZRED (\---\---), and AZRED II (—)