

VOL. 57, 2017



Guest Editors: Sauro Pierucci, Jiří Jaromír Klemeš, Laura Piazza, Serafim Bakalis Copyright © 2017, AIDIC Servizi S.r.l. **ISBN** 978-88-95608- 48-8; **ISSN** 2283-9216

# Modeling Chlorine Decay in Drinking Water Distribution Systems using Aquasim

## Vhutshilo A. Madzivhandila, Evans M.N. Chirwa\*

Water Utilisation and Environmental Engineering Division, Department of Chemical Engineering, University of Pretoria, Pretoria 0002, South Africa evans.chirwa@up.ac.za

The main purpose of drinking water distribution systems or networks is to supply water of impeccable quality to consumers according to their demand. Problems relating to declining water quality in natural water bodies have been on the increase around the world. In many countries, Chlorine is the most widely used disinfectant in water and wastewater treatment. It is mostly used to destroy pathogens, control nuisance microorganisms and for oxidation. A lot of research on the decay of Chlorine within a water distribution network has been done. This paper aims to present an alternative method of modeling Chlorine decay in water distribution systems.

## 1. Introduction

Problems relating to declining water quality in natural water bodies have been on the increase around the world. The problems are worsened by high nutrient inputs from agricultural land runoff and unregulated municipal wastewater discharges into natural water bodies (Barakat et al., 2005). In South Africa, problems relating to declining water quality in water supply bodies have included high turbidity, algal infestation and taste and odour problems (Chirwa and Bamuza-Pemu, 2010). Most water bodies in various regions have been classified as hyper-eutrophic, meaning that they experience perpetual algal blooms and poor water quality all year round (Das et al., 2008).

In many countries, Chlorine is the most widely used disinfectant in water and wastewater treatment. It is mostly used to destroy pathogens, control nuisance microorganisms and for oxidation. As an oxidant, Chlorine is used in iron and manganese removal, for destruction of taste and odour compounds and in the elimination of nitrogen containing compounds. Chlorination, especially in large water treatment networks; relies on a balance between the dosing of Chlorine and the amount of residual Chlorine that remains within the system until the treated water reaches the next dosing station or its destination. Hence, a control system to maintain these two important variables (Chlorine dosing and Chlorine residual) is essential to ensure that the desired water quality is met throughout the network.

A lot of research on the decay of Chlorine within a water distribution network has been done (Robescu et al., 2008, Li Xin et al., 2003, Rossman et al., 1994, Georgescu and Georgescu, 2012) One of the contributions that standout was the development of EPANET (Rossman. 1994); a tool to help us understand the movement and fate of drinking water constituents within distribution systems. This paper aims to introduce an alternative methodology that can be used on AQUASIM to predict the movement of water constituents, i.e. Chlorine, in water distribution systems.

A small scale literature example (Robescu et al., 2008) was used to test the methodology, which will later be applied on a larger scale at the Sedibeng Water Distribution System based in South Africa.

## 2. Theoretical overview

EPANET was designed to be a research tool for improving our understanding of the flow, degradation (or decay) and distribution of drinking water constituents within distribution systems. It can be used for many different kinds of applications in distribution systems analysis. Sampling program design, hydraulic model calibration, chlorine residual analysis and consumer exposure assessment are some examples. EPANET can

also help assess alternative management strategies for improving water quality throughout a system. These can include:

- Altering source utilization within multiple source systems
- Altering pumping and tank filling/emptying schedules
- Use of satellite treatment, such as re-chlorination at storage tanks
- Targeted pipe cleaning and replacement

AQUASIM on the other hand is a computer program mainly used for the identification and simulation of aquatic systems. Its original purpose was to support Environmental Scientists in finding an adequate model of the system they are investigating. The platform allows users to perform (among others) simulations using different models, estimate parameter values and perform sensitivity analysis. AQUASIM has been successfully used in water-treatment plants for biofilm modeling, parameter estimation and troubleshooting amongst other uses.

#### 3. Methodology

#### 3.1 Formulation

The methodology was inspired by the nature of one of the reactor compartments (units) found in AQUASIM, i.e. the Advective-Diffusive reactor compartment. This reactor compartment is generally used to describe onedimensional Advective-Diffusive transport of substances in a flow-through reactor and substance transformations (Reichert, 1998). The governing equation that describes the behaviour of substances transported in the compartment is given by equation 1 at the absence of lateral inflows and outflows.

$$\frac{\partial C_i}{\partial t} = -\frac{1}{A} \frac{\partial}{\partial x} (QC_i) + \frac{1}{A} \frac{\partial}{\partial x} \left( AD \frac{\partial C_i}{\partial x} \right) + r(C_i)$$
(1)

Where,

 $C_i$  = concentration of the substance "i" being transported Q = volumetric discharge through the compartment A = cross sectional area of the compartment D = coefficient of longitudinal diffusion or dispersion  $r(C_i)$ = transformation process experienced by the transported substance t = time x = length of the compartment

Equation 1 is similar to the one-dimensional conservation of mass equation for a dilute concentration of total free substance in water flowing through a section of a pipe developed by Rossman et al. (1994) as per equation 2.

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - KC$$

Where,

$$K = k_b + \frac{k_w k_f}{r_h(k_w + k_f)}$$

K = overall decay constant  $k_b = bulk decay constant$   $k_w = pipe wall decay constant$   $k_f = mass transfer coefficient$   $r_h = hydraulic radius$ u = flow velocity in the pipe

With the assumption that dispersion in water distribution networks is negligible due to high flow rates experienced, equation 1 can be reduced to equation 2. Below is a summary of how the Advective-Diffusive

(3)

(2)

reactor compartment on AQUASIM can be used to simulate a given pipe flow network. Please note that a hydraulic model is required to determine the volumetric flow rates within the individual pipes of the network.

Step 1: Calculate the residence time of water in all the individual pipes within the network as shown by equation 3 and identify the pipeline with the shortest residence time.

$$RT_i = \frac{L_i}{u_i} \tag{3}$$

Where,

RT<sub>i</sub> = residence time of water within pipeline i  $L_i = length of pipe i$  $u_i =$  flow rate of water within pipe i

Step 2: Divide the pipelines into smaller segments as shown by equation 4. The reason for dividing the pipelines into smaller segments is to normalize the flow through all pipelines (off different dimensions in most cases) in terms of flow through the pipeline with the shortest residence time. In other words, it makes it easier to visualize the residence time of all pipelines as a multiple of the pipeline with the least (shortest) residence time. This in-turn helps in determining which pipelines would affect certain nodal (connection between 2 or more pipelines) conditions first by simply counting the number of segments.

$$S_i = \frac{V_i}{Q_i R T_{min}} \tag{4}$$

### Where, S<sub>i</sub> = number of segments in pipeline i $V_i$ = volume of pipeline i $Q_i$ = volumetric flow rate through pipeline i

These segments will then be represented by Advective-Diffusive reactors on AQUASIM. Please note that  $S_i$ can be a decimal. A more logical value to represent the number of segment is given by equation 5. Please note that the original Si should not be discarded as it is used in step 3.

$$LS_i = ceiling(S_i)$$

## Where, LS<sub>i</sub> = logical number of segments

Step 3: Determine the unit length of the segments that make up the individual pipelines as shown by equation 6.

$$L_{seg_i} = \frac{L_i}{S_i}$$

Where,

#### L<sub>seg</sub> i = unit length of a segment in pipeline i

An example to elaborate how steps 2 and 3 work is given below:

#### Given

 $L_i = 10$  and  $S_i = 2.2$ 

The following can be calculated:  $LS_i = \text{ceiling}(S_i) = 3$ 

This means that there will be 3 segments in the given pipeline. The unit length of the segments in this pipeline can then be calculated using equation 6 as shown below.

(5)

(6)

 $L_{seg_i} = L_i/S_i = 10/2.2 = 4.545$ 

This means that this pipeline will have 3 segments with lengths; Segment 1 = 4.545, Segment 2 = 4.545 and Segment 3 = 0.2\*4.545. The sum of these segments gives us the original length of 10.

Step 4: The individual pipelines can then be connected on AQUASIM using Advective-Diffusive compartment reactors as pipeline segments with the cross sectional area given by the diameter of the pipeline and the End point of the compartment reactor (Reichert, 1998) given by the length of the segment ( $L_{seg_{.}}$ ). Detailed information on how variables and processes for the reactor compartment are defined on AQUASIM can be found on the AQUASIM 2.0 manual (Reichert, 1998).

#### 3.2 Application

A literature small scale example (Robescu et al., 2008) was adopted to test the developed model. Details of the example are given below.

The water distribution system adopted is situated in the Ramnicu-Valcea area in Romania. The distribution system is composed of the following:

- A raw water pipeline with a length of 8574 m and a diameter of 1200 mm that brings water from Bradisor Artificial Lake.
- A drinking water treatment plant (DWTP) located in Valea lui Stan village with a production of 5.76 ML/h and an Chlorine concentration of 1.14 mg/L.
- Treated water distribution pipeline to Ramnicu Valcea (carbon steel 36625 m length, 1200 mm diameter and 12 mm thickness pipeline).
- The water flows by gravity from the DWTP to Ramnicu Valcea
- Water supply to Brezoi (54000 m<sup>3</sup>/h) and Pausa (468000 m<sup>3</sup>/h) communities from the network.

Figure 1 shows the layout from the DWTP to Ramnicu - Valcea.



🔪 Ramnicu Valcea

Figure 1: Layout of the water distribution system from the DWTP to Ramnicu Valcea

The sampling points were at the 4 locations shown in Figure 1. Further of the system is given below: <u>Pipe flow rates</u>

The pipeline was viewed as a 3 link pipe with the link flow rates given below:  $DWTP \rightarrow Brezoi (Link 1) = 0.65 \text{ m/s}$   $Brezoi \rightarrow Pausa (Link 2) = 0.64 \text{ m/s}$  $Pausa \rightarrow Ramnicu (Link 3) = 0.52 \text{ m/s}$ 

#### Kinetics

It mentioned in the article by Robescu et al. (2008) that the pipe system was cleaned using COLBACH patented technology prior to the test run. This means the biofilm on the pipe walls could be neglected, i.e.  $k_w$  in equation 2 is almost zero. This reduces equation 2 to equation 7.

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - k_b C \tag{7}$$

The value of  $k_b$  was then determined to be 0.55 d<sup>-1</sup>. The model was first evaluated at steady state to determine what the concentrations at the 4 locations of interest would be after a long period of operation at the given conditions. This evaluation was followed by a dynamic evaluation to determine the changes in concentration with time at the 4 locations of interest for an operating period of 15 hours.

#### 4. Results and Discussion

The methodology was applied on AQUASIM as elaborated in section 3. The summary of results, as per the methodology is given below:

Step 1: the residence times of the individual links are Link 1 = 2.49 h, Link 2 = 6.36 h and Link 3 = 8.61 h Link 1 was determined to have the shortest water residence time; hence our critical link for further calculations.

<u>Step 2:</u> The number of segments per link (equation 4) was calculated to be  $S_1 = 1$ ,  $S_2 = 2.55$  and  $S_3 = 3.45$ . The corresponding logical number of segments, as per equation 5, were  $LS_1 = 1$ ,  $LS_2 = 3$  and  $LS_3 = 4$ . The unit length of the segments within the links were  $L_{seg_1} = 5846$  m,  $L_{seg_2} = 5751$  m and  $L_{seg_3} = 8996$  m. This means that links will be segmented as follows on AQUASIM:

- Link 1 will have 1 segment with the length of 5846 m.
- Link 2 will have 3 segments with lengths 5751 m, 5751 m and 0.55\*5751 m.
- Link 3 will have 4 segments with lengths 8996 m, 8996 m, 8996 m and 0.45\*8996 m. •

This information was used in AQUASIM, with link segments represented by Advective-Diffusive compartment reactors and the information defined as per the AQUASIM 2.0 manual (Reichert, 1998). Figure 2 shows the experimental data (little diamonds) and theoretical data (little squares) of Chlorine concentration throughout the pipeline. Although other conditions were fixed for the sampling period, the concentration recorded at the DWTP varied as shown by the little diamonds in Figure 2; hence various concentrations were also recorded downstream. It should be noted that for the purpose of model evaluation, the concentration at the DWTP was fixed at 1.14 mg/L. It is evident from Figure 2 that the predicted downstream values are within range of experimental data recorded during sampling. The downstream concentrations achieved by the model, with the fixed concentration at the DWTP, were 1.02 mg/L, 0.71 mg/L and 0.25 mg/L for Brezoi, Pausa and Ramnicu Valcea respectively as shown by the little squares in Figure 2.



Figure 2: Experimental and predicted results for residual chlorine concentrations at the 4 locations of interest

The dynamic state (concentration vs time) of the model was also evaluated for 15 hours with the focus on the 4 locations of interest as shown in Figure 3. Node 1, Node 2, Node 3 and Node 4 represent the DWTP, Brezoi, Pausa and Ramnicu Valcea locations respectively. The concentration at Node 1 was again assumed to remain constant at 1.14 mg/L for the entire period of evaluation (15 hours) for simplification purposes. It is evident from Figure 3 that the concentrations of Nodes 2, 3 and 4 start at 0 mg/L and increase to their steady state concentrations of 1.02 mg/L, 0.71 mg/L and 0.25 mg/L respectively with time. This confirms the results obtained during the steady state evaluation of the model as shown in Figure 2. It should be emphasized that the dynamic evaluation can only be done for predetermined (chosen) locations on the pipe system to provide additional boundary conditions to solve equation (7). The results (concentrations) are expected to approach steady state results (concentrations) with time, provided the initial conditions are fixed for the period of evaluation.



Figure 3: Dynamic evaluation of the model at the 4 locations of interest

## 5. Conclusion

An alternative methodology to model water distribution networks on AQUASIM was presented. The PFR nature of the Advective-Diffusive compartment reactor was demonstrated to show easy tracking of the Chlorine concentration along the pipe system for steady state conditions. The model also allows for evaluation of the dynamic state of the system to determine the changes in Chlorine concentration with time for predetermined locations in the pipe system. The methodology however requires hydraulic data such as volumetric flow rates within pipelines as inputs. Further evaluation of this methodology on a larger scale at the Sedibeng Water Distribution System in South Africa is currently underway.

#### Acknowledgments

We would like to acknowledge the support from the Sedibeng Water not only for funding the project, but also for trusting our ability and giving us an opportunity to work on a project of such magnitude. Many thanks.

#### References

- Barakat M.A., Tseng J.M., Huang C.P., 2005, Hydrogen peroxide-assisted photocatalytic oxidation of phenolic compounds. Applied Catalysis B: Environmental, 59, 99-104.
- Chirwa E.M.N., Bamuza-Pemu E.E., 2010, Investigation of Photocatalysis as an Alternative to Other Advanced Oxidation Processes for the Treatment of Filter Backwash Water, Water Research Commission, WRC Report No 1717/1/10, Gezina, South Africa.
- Das S.K., Routh J., Roychoudhury A.N., Klump J.V., 2008, Major and trace element geochemistry in Zeekoevlei,South Africa: A lacustrine record of present and past processes, Applied Geochemistry, 23 (8), 2496–2511.
- Georgescu A., Georgescu S., 2012, Chlorine concentration decay in the water distribution system of a town with 50000 inhabitants, U.P.B. Sci. Bull, 74 (1), 103–114.
- Reichert P.,1998, AQUASIM 2.0 User manual, Computer program for the identification and simulation of aquatic systems, Swiss Federal Institute for Environmental Technology (EAWAG), Switzerland, ISBN: 3-906484-16-5.
- Robescu D., Jivan N., Robescu D., 2008, Modelling chlorine decay in drinking water mains, Environmental Engineering and Management Journal, 7(6), 737-741.
- Rossman L.A., Clark R.M., Grayman W.M., 1994, Modeling chlorine residuals in drinking-water distribution systems, J. Environ. Eng., 120, 803-820.
- Xin L., Da-Ming G., Jing-yao Q., Ukita M., Hong-bin Z., 2003, Modeling residual chlorine in water distribution systems, Journal of Environmental Sciences., 15 (1), 136-144.