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PREDICTION OF CHLORINE AND DISINFECTION BYPRODUCT CONCENTRATION IN WATER DISTRIBUTION SYSTEMS USING KYPIPE AND TTHM REGRESSION MODELS: APPLICATION TO TWO SYSTEMS IN KENTUCKY

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THESIS

A thesis submitted in partial fulfillment of the
requirements for the degree of Master of Science in the
College of Engineering
at the University of Kentucky

By
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2023

ABSTRACT OF THESIS

PREDICTION OF CHLORINE AND DISINFECTION BYPRODUCT CONCENTRATION IN WATER DISTRIBUTION SYSTEMS USING KYPIPE AND TTHM REGRESSION MODELS: APPLICATION TO TWO SYSTEMS IN KENTUCKY

The main objective of this research is to study if the hydraulic and water quality models can be used for water quality analysis of chlorine decay and TTHM formation at various locations across a water distribution system. This is particularly important because it is not always easy or economical to take multiple field samples and analyze them in the laboratory. In this study, models of two different water distribution systems (one more urban and efficiently managed system located in a relative flat topography, and other more rural and less efficiently managed system located in a mountainous topography) were developed in a commercial software package. These models were then calibrated and successfully applied to predict water age, and chlorine residual values.

Furthermore, these models are used to incorporate water age and chlorine demand based regression relationship to predict TTHM values throughout the distribution system. Regression models based on water age and chlorine decay approach can simplify the TTHM prediction by lowering the number of parameters involved in the water quality analysis. Both water age and chlorine demand can be useful in prediction of TTHM in water distribution systems, but their accuracy depends on available data and decency of the model calibration.

Based on the investigation of possible operational changes using these models, it appeared that both the change in demand and plant chlorination can have significant impact in the chlorine residual and TTHM formation in the system. The reduction in system demand after controlling the water loss can cause significant decrease in the chlorine residuals in the distribution system as the flow velocity decreases and the time to reach the consumers increases allowing enough time for chlorine decay and for TTHM formation.

KEYWORDS: [Water Distribution System, Water Treatment, Plant Chlorination, Disinfection By-products, Chlorine residuals, Water Quality Modeling]

Yogesh Gautam

04/12/2023

Date

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Date

DEDICATION

Dedicated to my parents, who are already in their seventies and missing their youngest living 8000 miles away.

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I would like to express my sincere gratitude to my professors, thesis committee, department of civil engineering staff, KWRRI team, fellow students, water utilities staff and my family members without whom this research work could not be completed.

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1. INTRODUCTION

1.1 Background

Water is known as the liquid of life as no life has ever existed without water, but on the other hand the use of contaminated water has become one of the major causes of serious health issues and deaths thought the history of mankind. Today, in the United States, approximately 90% of the population is provided safe drinking water from over 148,000 public water systems(USEPA, 2021a). In Kentucky, about 97% of the population receives their drinking water from more than 435 public systems.

Untreated raw water supplies may have some amounts of physical, biological, chemical, or even radiological contaminants that can be harmful to human health (EPA, 2022a). Scientists and engineers have tried various ways to remove or deactivate these harmful contaminants from drinking water to make it safe. These practices include coagulation, settling, filtration and disinfection. The most common form of disinfection still used today involves compounds containing chlorine. Drinking water disinfection using chlorine has effectively controlled the spread of contagious waterborne diseases from our drinking water systems for over 100 years after its introduction in Europe and America (Galal-Gorchev, 1996).

Because of the relatively low cost and effectiveness as a disinfectant, chlorine remains the most commonly used disinfectant throughout the globe. However, the process of disinfection can produce negative side effects. Chlorine is a powerful oxidant and highly reactive. At higher concentrations it can also be a skin or respiratory irritant. As a result, USEPA places limits on the maximum levels of chlorine in drinking water. A list of the

maximum contaminant limits goals (MCLG) and maximum contaminant limits (MCL) for common chlorine-based disinfectants is provided in Table 1-1.

Table 1-1 Regulatory Limits for Disinfectants (United States Environmental Protection Agency, 2022)

Disinfectant	MCLG (mg/L)	MCL (mg/L)	Potential Health Effects	Sources of Contaminant
Chloramines (as Cl_2)	MRDLG=4	MRDL=4.0	Eye/nose irritation; stomach discomfort, anemia	Water additive used to control microbes
Chlorine (as Cl_2)	MRDLG=4	MRDL=4.0	Eye/nose irritation; stomach discomfort	Water additive used to control microbes
Chlorine dioxide (as ClO_2)	MRDLG=0.8	MRDL=0.8	Anemia; infants and young children: nervous system effects	Water additive used to control microbes

Excessive chlorine in drinking water can also precedent the formation of disinfection byproducts (DBPs). DBPs are formed when chlorine reacts with natural organic matter (NOM) present in the source water. Over last several decades, more than 600 different kinds of DBP's have been detected in disinfected drinking water (Richardson et al., 2007).

DBPs occurring at the household tap depend on several factors, including the amount of NOM in the source water, the concentration of the chlorine residual leaving the plant, the time it takes for the treated water to reach the home, the temperature of the water, and the presence of pipe deposits or biofilm that may affect the chlorine residual (Calderon, 2000).

Several DBPs have been linked to severe health issues such as cancer of the internal organs such as kidney, liver, and intestine, as well as developmental and reproductive problems (Boorman et al., 1999). Due to their association with ongoing health issues, regulating bodies have placed a greater emphasis on the amount of DBPs formed in the water supply system including the distribution networks. Many countries, including the U.S., now regulate the concentrations of two of the common types of DBPs Trihalomethanes (THMs) and Halo acetic acids (HAAs) in drinking water. The U.S. Environmental Protection Agency (EPA) Stage II Disinfection Byproduct Rule known as DBPR II and implemented in 2003, strengthened regulations on these two groups of regulated DBPs. Maximum contaminant levels (MCL) are kept below 80μg/L for TTHM and 60 μg/L for HAA. Also, the sampling and reporting requirements for utilities were made stricter. Public water utilities in the US are now required to provide a rolling annual average concentration based on quarterly sampling for different distribution system areas with severe DBP levels. Many utilities, particularly the smaller ones, have been facing difficulty in satisfying the new rule as the utility is forced to maintain a delicate balance between providing adequate disinfection while not exceeding the DBP limits. While most of the drinking water systems reliably serve safe drinking water to their customers, some face several difficulties in their ability to achieve and maintain system water quality requirements and sustainability. The field assessment of the DBPs at all segments of the distribution system is not always an easy task. Some of these small systems lack operational expertise and financial resources to operate and maintain such systems. Utilities unable to meet basic requirements of operation are susceptible to violating these regulations. A list of MCLs and MCLGs for common disinfection by-products is provided in Table 1-2.

Table 1-2 Regulatory Limits for Selected Disinfection by-products

Contaminant	MCL (mg/L)	MCLG (mg/L)
TTHM	0.08	Chloroform (0.07) Bromodichloromethane (0.0) Dibromochloromethane (0.06) Bromoform (0.0)
HAA5	0.06	Monochloroacetic acid (0.0) Dichloroacetic acid (0.0) Trichloroacetic acid (0.0)

A summary of the number of health-based violations of the US EPA water quality requirements from 1982 to 2015 is provided in Figure 1-1. These violations were based on an assessment of 17,900 community water systems across the United States (Allaire et al., 2018).

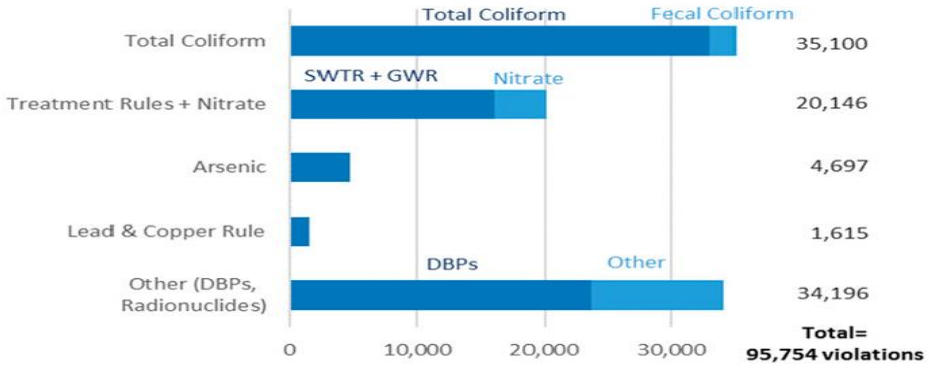

Figure 1-1 Number of Health-based Violations, 1982–2015, by Contaminant Type (Allaire et al., 2018).

This figure shows that the DBPs continue to be a major source of violations for many systems. This reflects the continuing challenge of balancing adequate disinfection while not exceeding the current DBP limits. This is because of the fact that DBP assessment and control can be an arduous task requiring greater vigilance and higher cost than regulating conventional pollutants (R M Clark & Boutin, 2001).

1.2 Research Hypothesis

This research seeks to determine if the process of managing chlorine residuals and DBP concentration could be facilitated through the use of computer models of water distribution systems. To test this hypothesis, water quality models of two distribution systems will be developed and calibrated and then used to explore whether such models can be used to improve the operational strategies for use in maintain compliance with both chlorine and DBPs. If successful, the developed methodology could then be extended to other systems.

1.3 Research Objectives

The goal of the proposed research project is to assist water utilities to predict and regulate DBP concentrations at any point in their distribution system. In order to achieve this goal, this research will focus on the following objectives.

1. The first objective of the proposed research is to review the relevant scientific literature to identify the possible factors that influence the decay of chlorine and formation of DBP concentrations. Potential factors include pipe material and age, pipe flowrate and velocity, source water quality, treated water quality, water age, water temperature, chlorine residuals, and chlorine demand.
2. The second objective is to develop and calibrate hydraulic models for two systems based on available distribution data. This model developed in KYPIPE will be used for water age and chlorine decay analysis.

3. The third objective of the proposed research is to develop and implement a sampling protocol and use it to obtain relevant chlorine and DBP data from multiple water distribution systems in Kentucky.
4. The fourth objective of the proposed research is to develop a mathematical model for DBP prediction using a regression model. Potential independent variables to be considered will include water temperature, water age, conductivity, turbidity, chlorine residuals and chlorine demands. The regression model will be calibrated and validated against actual water quality sample results from two different water distribution systems in Kentucky (i.e., Lebanon Kentucky and Martin County Kentucky).
5. Once a final regression equation for DBP has been developed, the fifth objective will be to embed the model within a commercially available hydraulic/water quality network model (i.e., KYPIPE).
6. The sixth objective of the proposed research will be to demonstrate whether the composite model can be used to successfully predict DBP concentrations for the two water distribution systems.
7. The seventh and final objective of the research will be to investigate whether the model can be used to identify any potential operational strategies that can decrease the formation of the DBPs within the system while still meeting the water quality requirements.

1.4 Utilities of Interest

In order to test and validate the proposed DBP transport models, the model will be applied to two different distribution systems, the Lebanon Water Utility in Marion County,

Kentucky and the Martin County Water System in Martin County, Kentucky. The Lebanon Water Utility was chosen because it represents a well-run utility with minimal water quality violations and because of the availability of data on the infrastructure system (both physical and topological) and water quality data (TOC) from associated with the surface water and water quality data (TTHMs and HAA5) collected from the distribution systems. The Martin County system was selected because it represents a system with significant problems (e.g., greater than 70% water loss) and a history of significant water quality violations. Similar to the Lebanon system, data on the physical infrastructure as well as past water quality data were also readily available, however, in the case of Martin County additional field data was also collected.

1.5 Organization of the Thesis

This thesis is divided into the following chapters.

Chapter 1. Introduction: this chapter provides background information on the need for DBP analysis research in water distribution systems.

Chapter 2. Chlorine Chemistry and Disinfection Byproducts: this chapter reviews previous research on the topic of water quality in the distribution systems. This includes a review of different contaminants as well as strategies for their assessment and control.

Chapter 3. Distribution System Water Quality Modelling: this chapter reviews previous research on the topic of water quality in the distribution systems. This includes a review of different contaminants as well as strategies for their assessment and control.

Chapter 4. Water age and Chlorine Demand Assessment Using Field Based Modified (KYPIPE) Hydraulic Models: This chapter is divided into hydraulic modeling and water quality modeling sections. They hydraulic modeling section includes development and calibration of hydraulic models. The water quality section includes prediction of water age and chlorine residuals and their verification using field data.

Chapter 5. Prediction of Disinfection Byproducts in Water Distribution System by Developing Regression and Computer Models and Study of Operational Changes in their Formation: This chapter will summarize the application of regression models in exploring possible strategies for improving DBP formation. DBP. This chapter will summarize the approach related to the collection of DBP data for modeling purposes. It describes the methods associated with the development and application of regression and computer models for DBP prediction.

Chapter 6. Discussion and Conclusions: this chapter discusses the summary of the research along with its conclusions.

Chapter 7. Recommendations For Future Research.

Appendix A, this section contains details of the MOR Database used in the research.

Appendix B, this section contains tank level data used in hydraulic calibration.

Appendix C, this section contains the data collected from field sampling for both systems.

Appendix D, this section contains standard operating procedures for collecting the DBP samples and measuring chlorine concentrations.

Appendix E, this section contains the list of model files used in various analysis.

2. CHLORINATION CHEMISTRY AND DISINFECTION BYPRODUCTS

2.1 Water Quality

The term water quality refers to the suitability of water for a particular purpose, in this case its suitability for primary (consumption) and secondary household uses (cooking, bathing etc.) (Boyd, 2015). Maintaining and predicting water quality in distribution systems has become a major area of interest in analysis of water distribution networks.

2.2 Water Quality Parameters

Water quality parameters are the set of physical, chemical and biological properties of water that can be measured, and monitored for maintaining desired quality in drinking water at the consumers tap (YSI Inc., 2022). These parameters include temperature, turbidity, total organic carbon, dissolved oxygen, pH, conductivity, oxidation-reduction potential (ORP), chlorine concentration, metals(e.g.: iron), and bacteria and viruses etc. (Omer, 2012). The USEPA currently has set legal limits on more than 90 contaminants in drinking water (USEPA, 2021b). These contaminants can be lumped into several categories including:

Micro-organism contaminants (bacteria e.g., E. coli, parasites, and viruses)

Radioactive contaminants (including uranium and radium)

Disinfectants (including chlorine)

Disinfectant by products (including bromate, chlorite, TTHMs and HAA5s)

Inorganic compounds (including arsenic, lead and copper)

Organic contaminants (including benzine, trichloroethylene, and vinyl chloride)

In addition to these primary contaminants, the EPA also provides guidance on several other contaminants that may cause cosmetic effects (skin or tooth discoloration) or aesthetic effects such as taste, odor, or color.

These regulated parameters can be measured directly in the field using standard sampling techniques or they can be measured in the laboratory form collected samples. Today, highly sensitive and user-friendly optical sensors (OS), microelectronic mechanical systems (MEMS) and biosensors are widely used sensing techniques for detecting water quality parameter (Bhardwaj et al., 2015).

2.3 Chlorination Chemistry

Gaseous chlorine and hypochlorite have been utilized for drinking water treatment ever since they were first used in 1908 because of their low cost and potent disinfectant properties. Chlorine has the ability to kill the bacteria by disrupting their cellular membranes. When chlorine is added to drinking water, it undergoes a series of reactions and decays over time (Deborde & von Gunten, 2008). First, chlorine gas (Cl_2) hydrolyzes in water to produce hypochlorous acid and H^+ and Cl^- ions as shown in the following reaction:

$$Cl_2 + H_2O = HOCl + H^+ + Cl^- \quad \text{(2-1)}$$

The hypochlorous acid formed from the above reaction dissociates in aqueous solution as it is a weak acid:

$$HOCl = H^+ + OCl^- \quad \text{(2-2)}$$

The quantity of hypochlorous acid, hypochlorite ion (i.e., OCl^-), or any other molecular chlorine in the drinking water that is readily accessible for disinfection is referred to as the "free available chlorine.". Some of the chlorine is used up in disinfecting

pathogens present in water, while some of it combines with ammonia (NH3) and ammonium ion (NH4+) to form various substances called chloramines (e.g., monochloramine (NH2Cl), dichloramine (NHCl2) and nitrogen trichloride (NCl3)).

$$NH_3 + HOCl = NH_2Cl + H_2O \quad \text{……..(2-3)}$$

$$NH_2Cl + HOCl = NHCl_2 + H_2O \quad \text{…… (2-4)}$$

$$NHCl_2 + HOCl = NCl_3 + H_2O \quad \text{……. (2-5)}$$

This amount of chlorine is not available as immediate germicide and is known as combined chlorine.

In addition to chlorinating ammonia, chlorine also reacts with ammonia and oxidizes it to chlorine free products (e.g., nitrogen gas and nitrate) as shown below.

$$3Cl_2 + 2NH_3 = N_2 + 6H^+ + 6Cl^- \quad \text{…….…… (2-6)}$$

$$4Cl_2 + NH_3 = NO_3^- + 9H^+ + 8Cl^- \quad \text{……. (2-7)}$$

2.4 Break-Point Chlorination

For many years, the concept of breakpoint chlorination has been used to produce a concentration of "free" chlorine residual in drinking water for use in continuing to maintain a chlorine residual as the water continues to move through the distribution system. Breakpoint chlorination is the point where the level of the chlorine is enough to overcome the oxidation demand associated with any pathogen or ammonia in the water and there is enough chlorine left to develop a free chlorine residual. Free chlorine is the remaining chlorine that is readily available for disinfection. This process is illustrated in Figure 2-1.

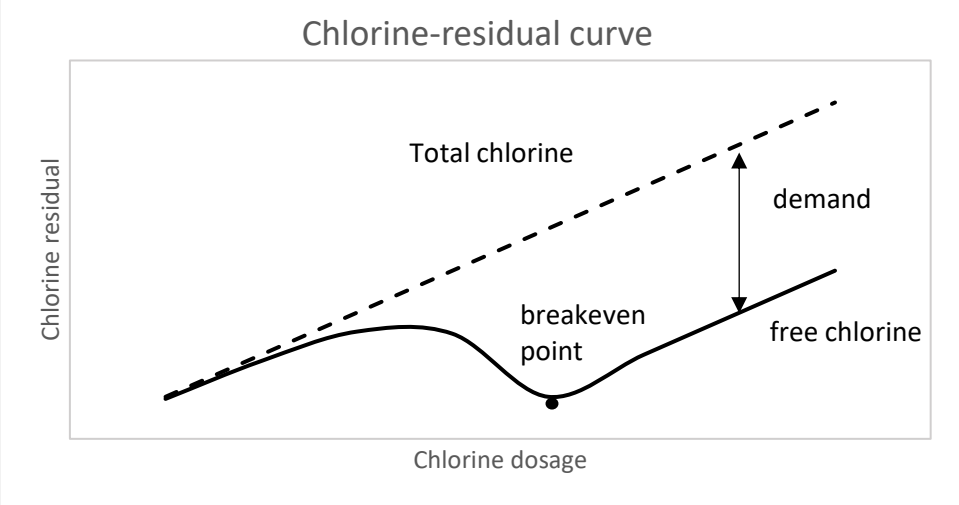

Figure 2-1 Chlorine Residual Curve

The presence of free chlorine in water indicates that enough chlorine was added to the water to oxidize any bacteria or ammonia in the surface water and the potential to oxidize any bacteria or ammonia that might be encountered as the water moves through the distribution system. It is therefore a major factor in preserving the potability of water after treatment in the plant. Free chlorine can be as high as the total chlorine if there is no chlorine demand or if the chlorine has not yet had time to react with pathogens or ammonia in the water. However, the free chlorine available for disinfection decreases as the chlorine demand increases in the distribution system.

2.5 Formation of Disinfection By-Products

When chlorine is added to the treated source water, it can also interact with other compounds in the water in addition to pathogens and ammonia. The results of these interactions are commonly called disinfection by-products (DBPs). They are undesirable chemicals formed in the conventionally treated drinking water due to the reaction between the natural organic matters and chlorine used for treatment process. DBPs have been found to be associated with various health issues such as cancer of the kidney, liver, and intestine,

as well as reproductive and developmental issues (Li & Mitch, 2018). More than 600 DBPs have been identified thus far but only some of them are regulated by the EPA. These include: Bromate, Chloride, Total trihalomethane (TTHM), and 5 Haloacetic acids (HAA5)(USEPA, 2021b). Trihalomethanes are chemical compounds in which three of the four hydrogen atoms of methane have been replaced by halogen atoms (e.g., Cl, Br, F). Regulated total trihalomethanes include chloroform, bromodichloromethane, dibromochloromethane, and bromoform. Haloacetic acids are carboxylic acids in which a halogen atom takes the place of a hydrogen atom in acetic acid (i.e., CH3COOH) such as in monochloroacetic acid (i.e., $ClCH_2COOH$). The five regulated haloacetic acids, also known as HAA5, are: monochloroacetic acid, dichloroacetic acid, trichloroacetic acid, monobromoacetic acid, and dibromoacetic acid(US Environmental Protection Agency, 2016). The possible factors that influence the formation of disinfection by products are also related to the factors that influence the decay of the chlorine residual. Potential factors include pipe material and age, pipe flowrate and velocity, source water quality, treated water quality, water age, water temperature, chlorine residuals, and chlorine demand.

Disinfection By-Product Formation

In distribution systems, chlorine reacts with a reducing agent such as natural organic matter (NOM) present in source water to form DBPs. This is schematically shown in Figure 2-2.

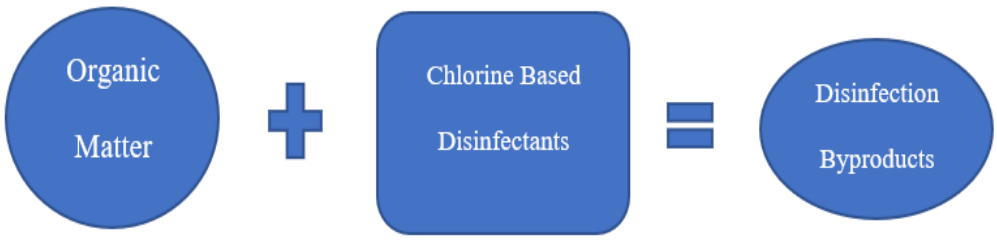

Figure 2-2: Formation of Disinfection By-products

The exact mechanism for formation of disinfection byproducts varies with various precursors and disinfection conditions. A general chart for the process is provided in Figure 2-3 where R' and R" represent hydrocarbon chains (R M Clark & Boutin, 2001; Hua & Reckhow, 2008b).

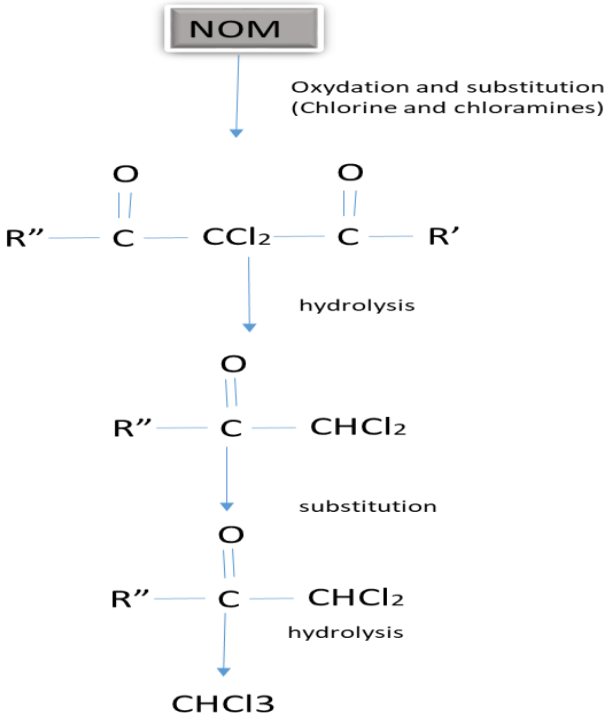

Figure 2-3 Simplified View of Major Chlorine and Chloramine Reaction Pathways Leading to the Formation Of Trichloromethane (I.E. Chloroform) (Hua & Reckhow, 2016)

Precursors of the DBPs are the substances that exist in the water during disinfection and react to form the byproducts. It has been determined that the formation of DBPs in chlorinated water may vary largely based on the chlorine dose, bromide levels, and the total organic carbon (Zazouli & Kalankesh, 2017). The formation of DBP in water also depends on the source water quality (i.e., the amount of NOM), and the efficiency of water treatment process, the method of disinfection, the chlorine doses, chlorine decay rate, and other disinfection conditions. Various studies have tried to quantify the effect of each of the following precursors in the formation of disinfection by products.

Natural Organic Matters

Organic matter in source water typically comes from plants (e.g., leaves) and animal waste. The characteristics of the NOM can vary depending upon its type and source. The ability of NOM to react with chlorine and form DBPs also differ according to their hydrophobicity, polarity, nature of functional groups presents, aromaticity etc. (Tak & Vellanki, 2018). When chlorine is added to the water containing NOM, a series of oxidation reduction reactions takes place. The rate of these reactions depends on various factors.

The Effect of the Water Treatment Process

DBP formation can be decreased if the source water NOM concentration can be reduced prior to chlorination. This will typically depend upon the efficiency of the water treatment process (i.e., coagulation, settling, filtration). In general, final disinfection should normally take place at the end of the treatment process, however, operators may sometimes treat the source water prior to filtration to minimize the formation of the biofilms on the filter beds.

Method of Disinfection

Various methods of water treatment have varied potential of forming disinfection byproducts. An experiment conducted by Guanghui Hua and David Reckhow showed a significant reduction in the rate of DBP formation by using ozonation followed by chlorination than just using the chlorination (Hua & Reckhow, 2007). This result suggests that the rate of formation of the DBPs varies with the method of disinfection.

Chlorine Dose

The doses of chlorine applied for disinfection vary seasonally and even daily based on source water quality. DBPs formation is likely to show a general increasing trend as the

disinfectant dose of chlorine and chloramine is increased (Hong et al., 2013).

Chlorine Decay Rates

The chlorine decay rate depends on different physical conditions prevailing in the distribution system. Since residual chlorine is directly related to the initial chlorine concentration in the distribution system so mostly chlorine decay is typically modelled as a first order reaction (Vasconcelos et al., 1997; World Health Organization, 1996) using the following equation:

$$C=C_0 e^{-kt} \quad \text{..... (2-8)}$$

Where, k is the bulk reaction rate coefficient and C_0 is the initial chlorine concentration.

While moving through a distribution system, chlorine is consumed for bacterial disinfection and oxidation of substances present in the bulk water as well as in the pipe walls. The consumption of chlorine within the bulk aqueous phase is computed using a bulk decay rate(k_b) of chlorine. Since chlorine is a strong oxidizing agent, it may also react with the materials in the wall of the pipes in the distribution system or the attached biofilm and accumulated sediment. This consumption of chlorine is typically modelled using a separate decay rate known as wall decay(k_w) (Mostafa et al., 2013).

Chlorine demand is a measure of the potential of dissolved organic matter to react with chlorine. Chlorine demand is the difference between the chlorine applied and the residual chlorine in the distribution network at any given point of time. The concentration of DBPs formed in a particular point in a water distribution system has been found to be correlated to the level of chlorine demand at that point (Robert M Clark, 1998; Zhao et al., 2018). The chlorine demand can typically be estimated as the difference between chlorine

concentration leaving the plant and the measured free chlorine concentration at a particular point in the system.

Disinfection Conditions

The various environmental and distribution conditions that exist in the water treatment plant and distribution network are referred to as disinfection conditions. These may include pipe material and age, pipe flowrate and velocity, water age (chlorine contact time), water temperature, pH, etc. (Hua & Reckhow, 2008a). The effect of each disinfection criteria will vary depending upon the characteristics of the actual distribution system.

Pipe material and age are important aspects of water quality analysis as they are directly related to the wall reaction coefficients of the distribution system. The physical and biological materials that are embedded in the pipe walls (e.g., corrosion products and biofilms) as shown in Figure 2-4.

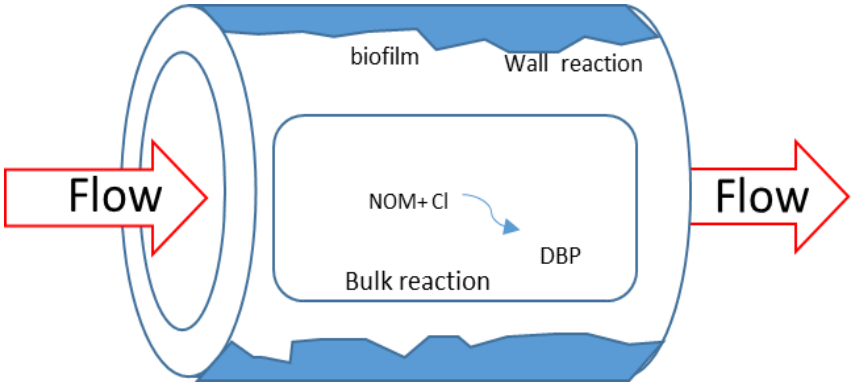

Figure 2-4: Schematics of Wall and Bulk Reactions in Pipe

The embedded materials can create significant chlorine demand which is typically modeled using either a global or pipe specific chlorine decay coefficient. Pipe age can also be correlated to the wall reaction rate since older pipes are typically more susceptible to water quality degradation. The flowrate and velocity in the pipe are dependent on the

diameter and roughness of the pipe. The effective diameter of the pipe can decrease over time (due to tuberculation buildup) while the roughness of the pipe increases over time, so the flow capacity decreases. This can affect the overall hydraulics and flow characteristics of the distribution system which can affect the water age and the associated water quality. The temperature of the water can also affect the rate of chlorine decay and any associated DBP formation. In general, the chlorine decay rate and DBP formation rate are directly correlated with the water temperature. As a result, all things being equal, higher DBP formation will normally occur in the warmer months of the year than in the colder months.

2.6 The Relationship between Water Age and Chlorine Demand and Disinfection By-Products

The water age refers to the time that water spent in the distribution system before being used by the consumer. The longer the water remains in the distribution system the longer will be the time available for chemical reactions and DBP formation. This indicates that the DBP values at a particular node are directly related to the age of water at that node.

Chlorine demand at a particular node in the distribution system is the difference between chlorine applied at the treatment plant and the chlorine residuals observed at the node. The chlorine demand is higher at the peripheral nodes as the chlorine has more time to decay on its way. From the rigorous studies from the past, it has been concluded that DBP formation can be demonstrated as a function of chlorine demand in the distribution system (Robert M Clark, 1998; Sohn et al., 2004).

Therefore, DBPs concentration in the distribution system can be modeled as a function of the water age or chlorine demand.

2.7 The Impact of Temperature and Seasons on DBP Formation in the Water Distribution System

With the change in seasons, the temperature of the surrounding environment changes and it results in the change overall demand in the distribution system. The flow rate and velocity of water changes with change in the demand which results in different mixing patterns in various mixing zones. DBPs may rise during summer months when water temperatures are greater because higher temperatures cause chemical reactions to occur more quickly and thoroughly. Additionally, higher water temperature frequently results in a greater chlorine demand, necessitating a larger disinfectant dose and increasing the likelihood of DBP formation (American Water Works Association, 2002).

3. DISTRIBUTION SYSTEM WATER QUALITY MODELLING

In order to model the water quality in a distribution system, two different types of models are necessary: 1) a hydraulic model, which simulates the transport of water through the water distribution system over time, and 2) a water quality model, which simulates the transport and decay of the chemical constituents (e.g., chlorine residuals) over time. Each of these are briefly discussed below:

3.1 Hydraulic Modeling

A water distribution network consists of an arrangement of pipes, fittings, reservoirs, tanks, pumps, hydrants, valves, etc., for supplying treated drinking water from the treatment plant to consumers. For modeling purposes, such systems are typically characterized as a network of links and nodes as shown in Figure 3-1. In this case the links are used to represent distinct pipe segments and the nodes are used to represent points in the system where the diameter of a pipe changes or the locations of different pipe elements such as tanks, reservoirs, pumps, and valves. For most modeling applications, the distribution of water withdrawals along a pipe segment due to individual service connections are typically simplified by aggregating the demands and allocating 50% of them to the upstream and downstream nodes respectively.

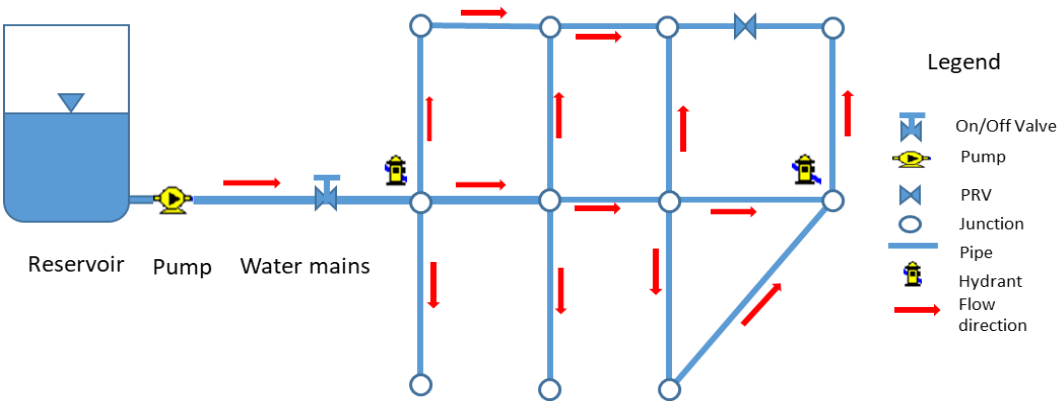

Figure 3-1. Schematic of a Typical Water Distribution Model

It is not always feasible nor economic to collect water quality samples across the full network on a daily basis, so modelling can be used to predict such values in response to different operating conditions. Modelling can make prediction easier than collecting samples and analyzing them in a laboratory. Water distribution hydraulic and water quality models are frequently used to plan, design, and operate the network in order to provide safe and potable drinking water. In applying to such models, it is crucial to analyze the hydraulics of the distribution system to achieve reliable and optimum performance in quality simulation. Various network analysis methods such as the Hardy cross method (Cross, 1936; L.N. & Weinberg, 1957), the simultaneous node method (Martin & Peters, 1963; Shamir & Howard, 1968), simultaneous loop method (Epp & Fowler, 1970; Jeppson, 1976), linear method (simultaneous pipe method) (D.J Wood & Charles, 1972), and the gradient method (i.e., the simultaneous network method (Todini, E. and Pilati, 1987) have been used to analyze the hydraulic network since the emergence of the "computer age" in 1957 (Ormsbee, 2007). Several of these methods have been incorporated into different commercial software packages for use in analyzing water distribution systems. These include: KYPIPE (KYPipe LLC, 2022), EPANET (EPA, 2022b), WaterGems (Bently, 2022) and Infoworks (Autodesk, 2022).

Such methods essentially solve two basic sets of equations 1) conservation of mass at each of the junction nodes in the system, and 2) conservation of energy around any loop or path in the network. While the conservation of mass equation is linear, the conservation of energy equation is nonlinear and thus must be solved iteratively, typically using a gradient based approximation approach such as the Newton-Raphson method. For water quality simulations, these set of equations must be solved repeatedly for each time step in

the simulation (typically a day), where the head boundary conditions for each solution are typically obtained using a Eulerian projection of flows over the previous time step to obtain the new head boundary conditions (i.e., tank levels). The boundary conditions associated with the conservation of mass equations are explicitly updated at the beginning of each time step based on a user specified distribution of spatial and temporal demands at each junction node. The equation of conservation of mass for each junction node can be expressed as:

$$Q_{in} - Q_{out} = d \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3\text{-}1)$$

Where, Q_{in} is the sum of all flows entering at the node and Q_{out} is the sum of all flows flowing out through the node and 'd' is the demand at the node.

When applied across a path of pipes, the conservation of energy equation for two nodes i and j can be expressed as:

$$H_i - H_j = \Delta E \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3\text{-}2)$$

Where, H_i is head at the upstream node, H_j is head at downstream nodes and ΔE is head loss in the pipe connecting the two nodes.

When applied around a particular loop (see Figure 3-2) of pipes in a network, the conservation of energy equation can be expressed as:

$$H_{ij}-H_{jk}-H_{kl}-H_{li}=0\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3\text{-}3)$$

Where, H_{ij} is head difference between the upstream and the downstream node

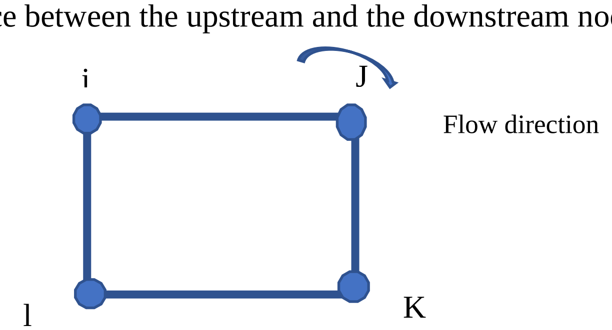

Figure 3-2: Pipe Loop

Historically, the headloss in a given pipe segment (e.g., Hij) has been modeled using either the Darcy-Weisbach Equation along with an explicit equation for friction f, or with the Hazen Williams Equation. Each of these are briefly summarized below:

Darcy Weisbach Equation

The Darcy Weisbach Equation calculates the headloss in a pipe segment due to friction throughout its length. The relation to calculate frictional headloss is

$$\text{Frictional head loss } (H_f) = f * \frac{L}{D} * \frac{V\text{^}2}{2g}$$

Where, f= coefficient of friction or friction factor.

v= flow velocity (ft/s)

L= length of pipe (ft)

D= Diameter of the pipe (ft)

g= Acceleration due to gravity (32.2 ft/sec^2)

Hazen Williams Equation

The Hazen-Williams equation calculates the headloss in a pipe segment using following relation:

$$\text{Frictional head loss } (H_f) = \frac{4.72L * Q\text{^}1.852}{C^{1.852} * D\text{^}4.87}$$

Where, f= coefficient of friction or friction factor.

Q= flow (ft^3/s)

L= length of pipe (ft)

D= Diameter of the pipe (ft)

C= Roughness coefficient

3.2 Water Quality Modelling

In order to model water quality within distribution systems, the concentration of modeled substance must be predicted at every location as it travels through the system from the point of entry. Researchers have developed various approaches to predict chlorine and DBPs concentrations in the distribution system. These approaches have been embedded into several commercial software packages for use in modeling water age and the transport of both conservative (e.g., fluoride) and non-conservative (e.g., chlorine) compounds throughout the distribution system. The quality of water at the source and major points of interest can be obtained from field or lab observations. This data can be used to calibrate the model for determining water quality at other points of the network.

When chlorine is used as a disinfectant it is essential to model chlorine content throughout the distribution system. EPANET software is the most widely used open-source software used for water quality analysis that uses flows from hydraulic simulation to track the movement of contaminants in the distribution system. EPANET uses a Lagrangian time-based method to trace the outcome of discrete volume of water as they travel through pipes and mix together at junctions (Rossman, 2000). In this formulation, each pipe section is divided into discrete cells, whose size (i.e., volume) change over each time step in response to changes in the velocity of the flow in each pipe (see Figure 3-3).

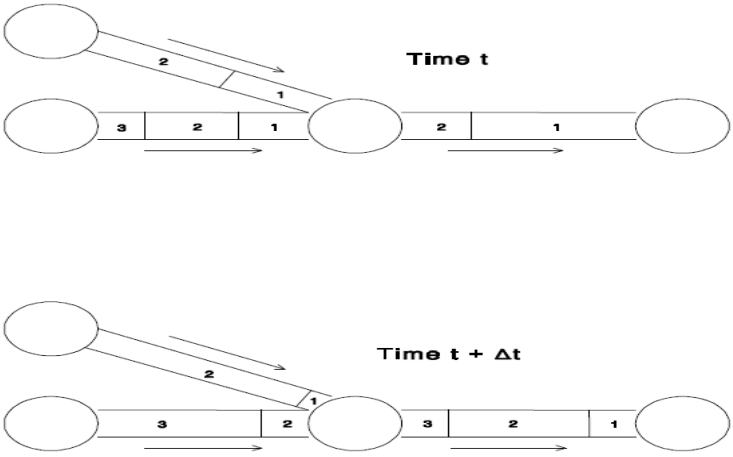

Figure 3-3 Behavior of Segments in the Lagrangian Solution Method (Rossman, 2000)

In this method the dissolved substance is assumed to move downstream of the section at as the same velocity of the transporting water. As a result, no intermixing is considered except at the junction nodes and storage facilities. The concentration within link i, C_i (x, t), at any point x (in the positive flow direction) and time t is given by:

$$\frac{\partial C_i}{\partial t} = -u_i \frac{\partial C_i}{\partial x} + r(C_i) \text{.....(3-4)}$$

where:

C_i= concentration (mass/volume) in the pope I as a function of distance x and time t

u_i= flow velocity (length/ time) in pipe i

r(Ci)= rate of reaction (mass/volume/time) as a function of concentration

3.3 KYPIPE For Modelling Water Quality

The KYPIPE software package, originally developed by researchers at University of Kentucky, provides a powerful tool for hydraulic analysis of the distribution system (KYPipe LLC, 2022; Don J. Wood & Rayes, 1981). This software also has the ability to perform water quality modelling through an internal interface with EPANET (Rossman, 2000). Together the two models can be used to determine pressure and flows across the distribution system as well as to estimate water age and chlorine residuals, although when

performing water quality calculations, KYPIPE utilizes the EPANET program to perform the associated hydraulic calculations. In this regard, the KYPIPE program simply provides its own customized user interface for the EPANET program.

Water Age Prediction Using KYPIPE

The water age at any point in the distribution system is the total time the water chemically treated in the treatment plant takes to reach a point in the distribution system. It is one of the major factors responsible for the water quality worsening in the water distribution system. Water age mainly depends on system layout, water demand, system operation, and system design. Practically, it is the residence time of the chemical applied for disinfection purpose. The major problem associated with increased water age are decay of the disinfectant and formation of the disinfection byproducts (American Water Works Association, 2002). Similar to other water quality parameters, EPANET calculates water age at various points in the distribution system using a Lagrangian time-based approach to track discrete parcels of water as they move through the distribution system. The average expected water age at any point in the system can then be approximated by running the model over an extended number of days until the water ages reach an equilibrium value. This is necessary to balance out the contributions of water ages from different sources to the system (e.g., water storage tanks).

Residual Chlorine Prediction Using KYPIPE

Residual chlorine at each junction and time step is determined based on the time of chlorine application and the rate of the chlorine decay in the system. Instead of manually entering a distinct chlorine decay rate for each pipe, normal practice is to assume a global value for both the bulk and wall reaction rates for all pipes. When using KYPIPE for water

quality analysis, the user inputs the appropriate model parameters into a KYPIPE graphical user interface, which then calls EPANET as a subroutine for subsequent water quality analysis. Once the results of EPANET are obtained, they are then passed back to the KYPIPE modeling environment for subsequent retrieval and display (EPA, 2022b; KYPipe LLC, 2022).

Disinfection By-product Modeling Using KYPIPE

The KYPIPE user interface was modified to allow for the input of a user defined regression relationship between DBP and chlorine demand or DBP concentration and water age as developed from measured field data from the modeled water distribution system or from literature. The mathematical concept of DBP formation as a function of either chlorine demand or Water age in the distribution system can be applied into KYPIPE. Depending on the nature of the regression relationship, the user is allowed to provide up to twenty coefficients for use in representing the function via a customized input table.

4. WATER AGE AND CHLORINE DEMAND ASSESSMENT USING FIELD BASED MODIFIED (KYPIPE) HYDRAULIC MODELS: APPLICATION TO TWO WATER DISTRIBUTION SYSTEMS IN KENTUCKY

4.1 Abstract

The water quality in a water distribution system can typically be assessed or predicted by measuring the amount of residual chlorine in treated water at different points in the distribution system or by predicting the age of the water at the same locations. The former can be assessed using field measurements while the later can be predicted using a calibrated computer model of the distribution system (e.g., KYPIPE or EPANET). When such data are combined, a functional relationship (i.e., an inductive model) between chlorine residual and water age can be developed which can then be used to predict the chlorine residual as a function of water age. Measured chlorine residual data can also be used to calibrate a chlorine decay model (i.e., a deductive model) of the distribution system (e.g., EPANET), which can then be used to predict chlorine residuals for each junction node in the system under different operational conditions.

In this study, models of two different water distribution systems were created in KYPIPE, a commercial software package for modeling water distribution hydraulics. Once developed, the hydraulic parameters of each model (e.g., pipe roughness and nodal demand factors) were adjusted to match (as close as possible) observed tank levels over a 48-hour period. Once calibrated, the models were then used to predict the water ages at each node in each system. The models were then calibrated to predict observed chlorine residual values and then used to predict chlorine decay throughout the distribution system.

Each analysis was first accomplished using KYPIPE which links with EPANET, another software package developed by EPA for use in modeling water age and the transport of both conservative and non-conservative constituents (such as chlorine) through the distribution system. EPANET requires both bulk decay and pipe wall decay coefficients for each pipe in the water distribution system although each coefficient is typically assumed to be the same for all pipes in the system. The bulk decay coefficients for each system were estimated from bulk-decay experiment using samples of treated water which were collected from each system. Initial estimates of the wall decay coefficients were obtained from literature and adjusted through model calibration using observed chlorine values at selected sampling locations within the system.

Once calibrated and validated, the models were used to explore new operational strategies for the purpose of minimizing the water age while maintaining a necessary chlorine residual (to protect against pathogen formation).

4.2 Introduction

Basic topographic data associated with the vast majority of water distribution systems in the state of Kentucky can be obtained from the Kentucky Water Resources Information System (WRIS) portal which is managed by the Kentucky Infrastructure Authority. The portal contains a collection of layout information (in ArcGis shapefiles) for most of the water utilities in the state of Kentucky, including data for Lebanon Water Works, Kentucky and Martin County Water District (Kentucky Infrastructure Authority, 2022). These existing layouts of water distribution systems for the city of Lebanon and Martin County Water District (MCWD) were first downloaded from WRIS portal and then uploaded into the KYPIPE modeling environment where they were converted into

hydraulic models for use in the proposed research. Various components of the distribution system were verified with field observation and onsite interviews with the system operators. These components include pumps, tanks, on/off valves, pressure reducing valves and master meters.

For reliable modeling, daily and monthly operation data, telemetry data and water quality data for the two systems were also needed. This information was collected from various online sources, utility office records and through field samplings. Additional data essential for thesis analysis were obtained from monthly operating reports (MORs) from Kentucky Department of Environmental Protection and from actual water distribution system sampling. The MOR dataset used in this research is presented in Appendix A.

4.2.1 Lebanon Water Works

The city of Lebanon Kentucky and its associated- water works (LWW) system is located in the Marion County, Kentucky (see Figure 4-1). It serves a town having a population of approximately 6,500 people and sells water to wholesale customers in Marion System.

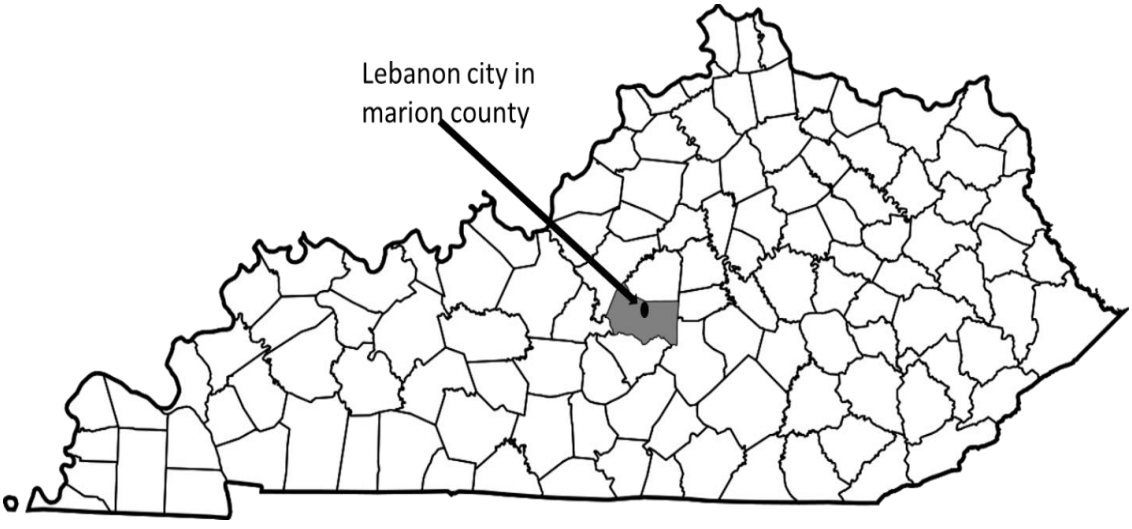

Figure 4-1 Location of Lebanon Water Works System

The LWW extracts its water from the Rolling Fork River and the Fagan branch reservoir and then treats it for distribution. While the treatment plant has a design capacity of 5.2 MGD, the average daily production during 2021 was approximately 2.6 MGD. Fagan branch reservoir is a small reservoir with a surface area of about 140 acres which is used to provide water to the system when the Rolling Fork River is unable to meet the total demand. The water utility also buys a portion of its water from the nearby city of Campbellsville which gets blended within the distribution system (Lebanon water works, 2021). During 2021, LWW purchased 61 million gallons from the Campbellsville system. The LWW sells some of its potable water to Marion County water system through ten distinct points in the distribution system. During 2021, they sold approximately 514 million gallons. Reports from past years do not reveal any major water quality issues but do show moderate TTHMs or HAAs concentrations without any violations.

The city is supplied from a looped system that consists of a treatment plant, two pump stations, three overhead tanks (two of which are located next to each other in the middle of the system, i.e., the Old Calvary Road tanks, which were modeled as single tank) and approximately 1000 pipe segments. A schematic of the system is provided in Figure 4-2.

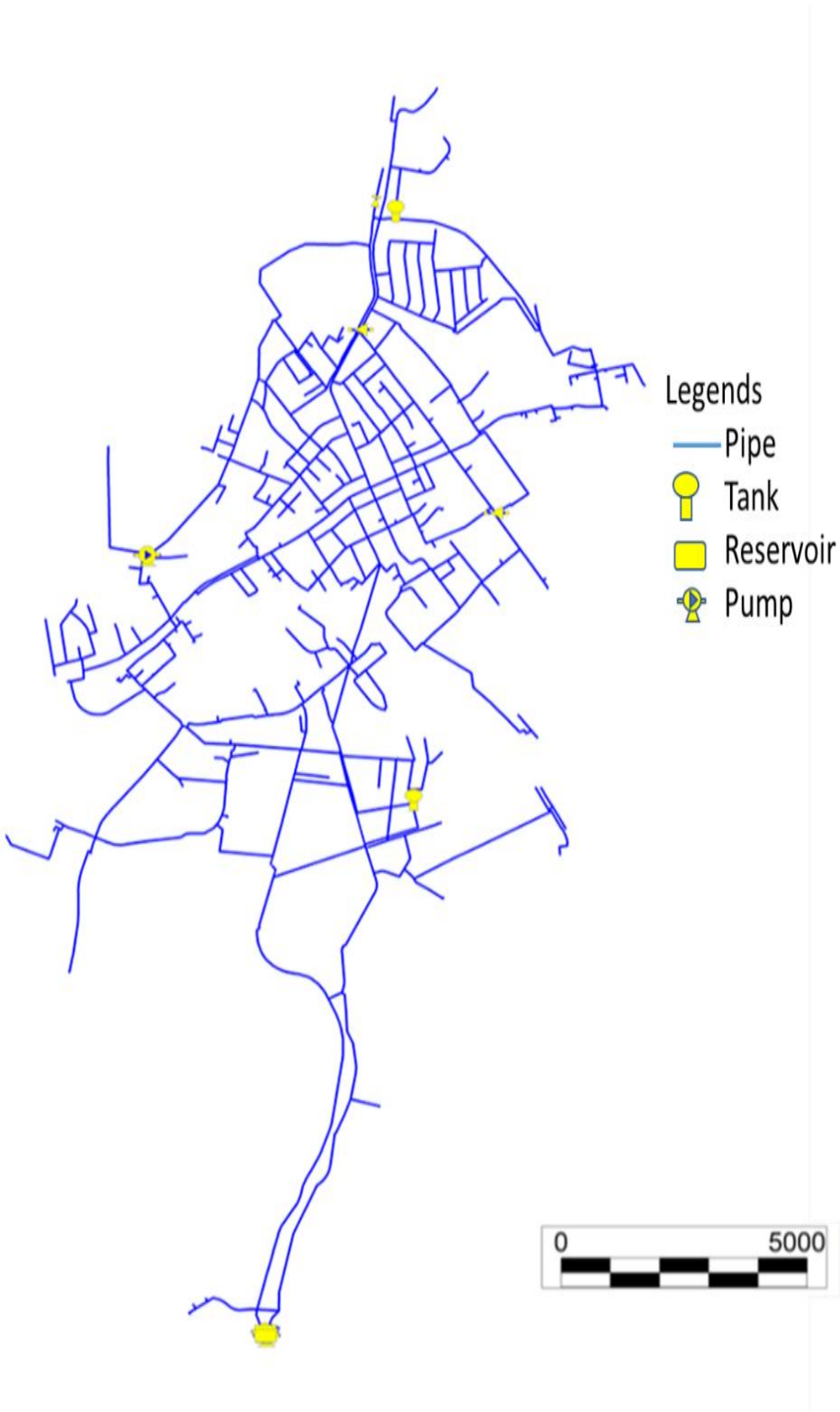

Figure 4-2 Schematics of the Lebanon Water Works Water Distribution System

4.2.2 Martin County Water System

The Martin County Water District (MCWD) is located in Martin County, Kentucky. Martin County is a mountainous county in the Appalachian region of eastern Kentucky (see Figure 4-3).

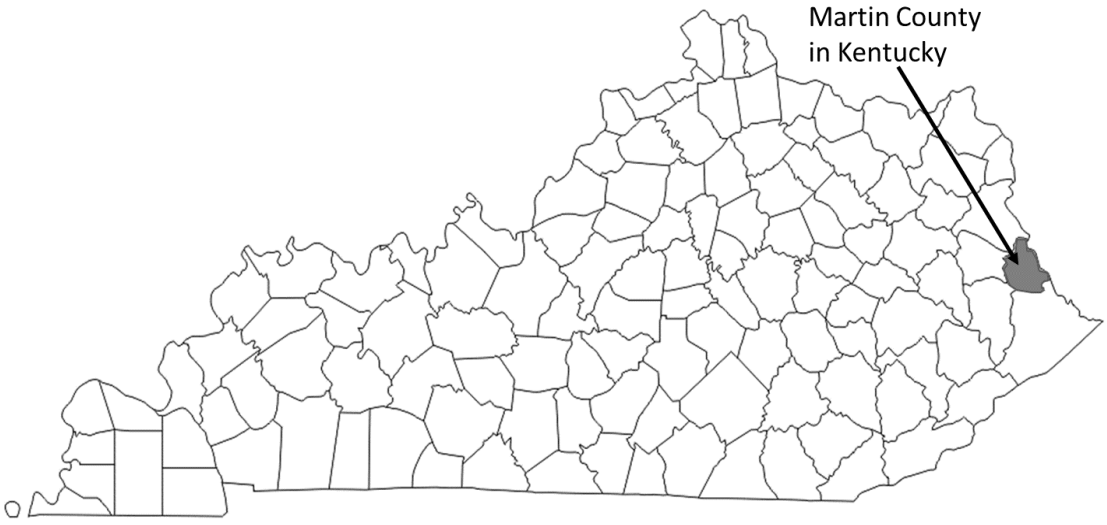

Figure 4-3: Location of Martin County Water System

Martin County has approximately 11,000 residents resulting in approximately 3,500 customers. The MCWD serves rural households but has a history of failing infrastructure and has struggled to meet the regulatory requirements for DBPs. The system currently experiences water losses greater than 70% in nearly all of its demand management areas (i.e., areas of the system isolated by master meters) (Kentucky Infrastructure Authority, 2022).

Martin County Water District treats surface water withdrawn from Curtis Crum Reservoir which is fed from natural drainage as well as from water pumped from the Tug Fork River. Crum Reservoir has a maximum storage capacity of 3.1 million gallons and receives natural drainage from about 672-acre watershed that is mainly forested. Water

from the reservoir flows by gravity into the water treatment plant which has a maximum treatment capacity of 2.0 MGD. Primary treatment is accomplished using three combined settling tank/filter units.

Contaminants that are likely to be present in Martin County source water are natural organic matters, microbial contaminants, inorganic contaminants, and chemical contaminants. The Martin County Kentucky Community-Engaged Drinking Water Health Pilot Study conducted in 2019 by University of Kentucky Center for Appalachian Research in Environmental Sciences (UK-CARES) observed 28 cases of instantaneous EPA MCL exceedances for TTHMs and 10 for HAA5 (Unrine, 2020). While these did not constitute an official water quality violation (because the DBP water quality standards are based on an annual moving average of four quarterly samples) they raise some questions about potential DBP issues in the system. The main source of DBP formation appears to be associated with the natural organic matter (NOM) or bromide compounds in the water. The study also determined that THM concentrations tend to be higher when using water from Tug Fork as opposed to water exclusively from the Curtis Crum watershed. This was found to be correlated with higher levels of conductivity and bromide in Tug Fork.

This utility supplies treated drinking water through a branched network of approximately 700 pipe segments that include a treatment plant, 16 pump stations, and 16 storage tanks. Being a widely spread system, some of the components were in maintenance phase and not fully functional during the study period. A schematic of the pipe network is provided in Figure 4.4.

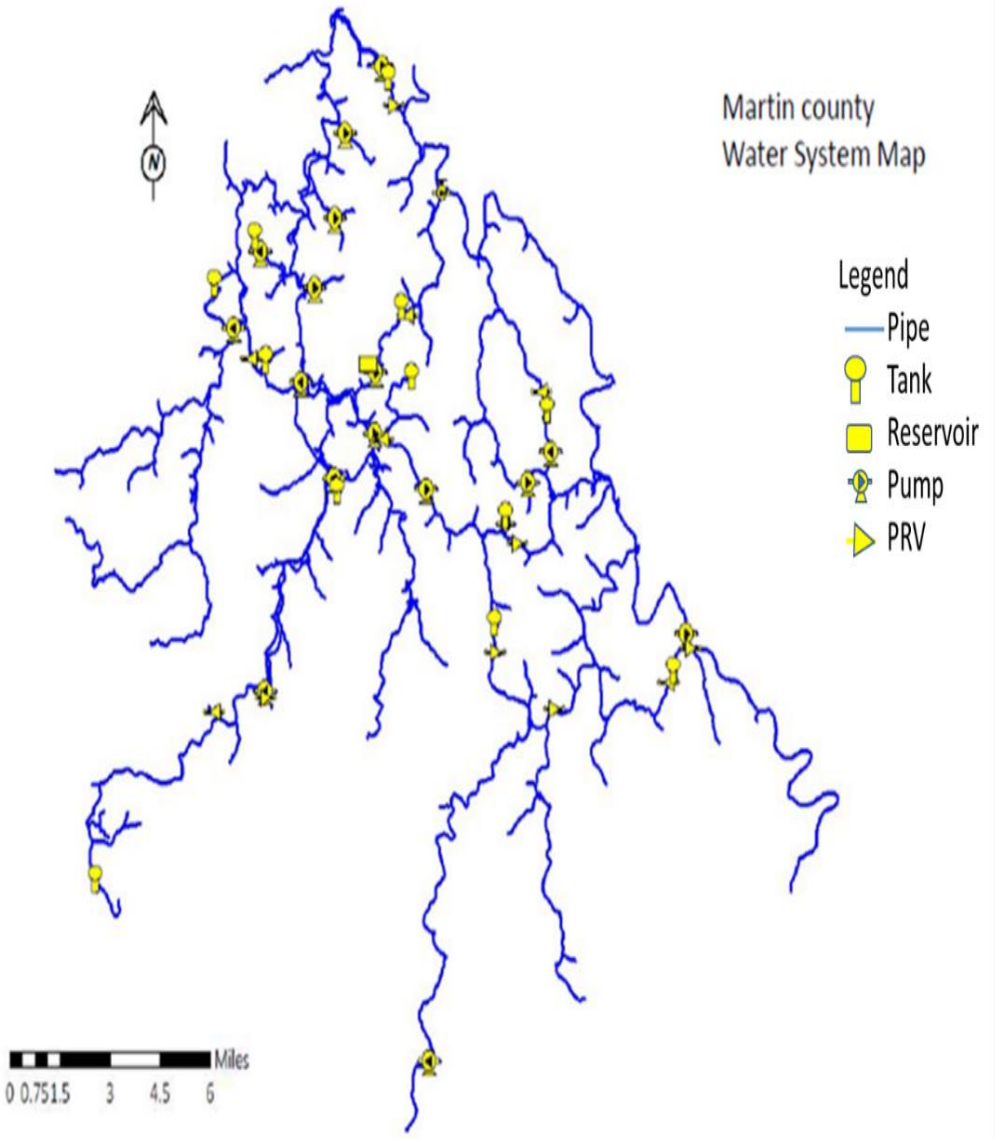

Figure 4-4. Schematic of the Martin County Water Distribution System

4.3 Hydraulic Model Development and Calibration

Hydraulic models for both of the systems were created using the KYPIPE interface with data from WRIS online database. To be useful, the developed hydraulic models should generate results that match the field results as closely as possible. For this purpose, hydraulic model calibration is necessary. Model calibration is the process of comparing model results with real measurements taken from the system and modifying a particular set of model parameters to decrease the differences between the observed and predicted results. The process of model calibration can also help to identify any latent discrepancies between the model topology and the actual system. In this study, the model calibration process involved two sequential steps: Steady state calibration and extended stated calibration. Normally, steady state calibration is used to adjust the roughness parameters (e.g., Hazen Williams roughness coefficients) associated with each pipe (or group of pipes). This is typically required when dealing with systems with ductile iron or cast-iron pipes, since the pipe can slowly accumulate tuberculation on the pipe wall which can change the pipe roughness over time. When the headloss associated with individual pipe fittings (typically called minor losses) are not explicitly modeled, these effects are also frequently modeled by further adjusting the Hazen Williams coefficients. These coefficients are normally adjusted to match the observed flow and pressures in the system, typically in response to a fire-hydrant flow test. However, in both the Lebanon and Martin County systems, most of the pipes were made from PVC material, which historically does not experience tuberculation problems (although it may accumulate biofilms). As a result, for the purpose of this modeling effort, conservative estimates of pipe roughness (e.g., C-100 to C-150) were used for all pipes (to reflect the possible impacts of fitting losses and

past hydrant flow tests), and the calibration process proceeded with the extended period simulation calibration.

As part of the extended period simulation calibration, the boundary conditions (i.e., pump status: on or off, tank levels, pressure regulating valve settings, etc.) during a particular sampling event were obtained from utility personnel and then entered into the model. Total demand was then distributed amongst the individual nodes in the model using the automatic demand distribution feature of KYPIPE. Next, the water levels for each tank in the system were obtained for the day on which field sampling was conducted. The hydraulic model was then run and the predicted and observed tank levels were compared. The system demands were then adjusted to minimize the deviation between the observed and predicted tank levels. To assess the accuracy of hydraulic calibration Root Mean Squared Error, RMSE was calculated for both MCWD and LWW tank levels.

Lower RMSE values are deemed good. In this study RMSE values are below 5 feet except for one season. This case might have high error due to system complexities and uncertainties about the quality and accuracy of tank data. The tank level data used in calibration and RMSE calculation are presented in Appendix B.

Hydraulic Calibration of the Lebanon Water Works

The Old Calvary Road tanks (T1) and Springfield tank (T2) are the main tanks pressurizing the system. The tank level data recorded by utility in December was used as typical for the winter season, and that for June was used as typical for summer. Comparison of the observed and predicted water levels over a two-day simulation period for both winter and summer are provided in figures 4-5 through 4-8. The associated R squared values for each simulation are also shown in the figures. As shown by the figures and the RMSE

values, the simulated tank levels were similar with the Springfield Tank levels showing a better correlation than the Old calvary road Tank.

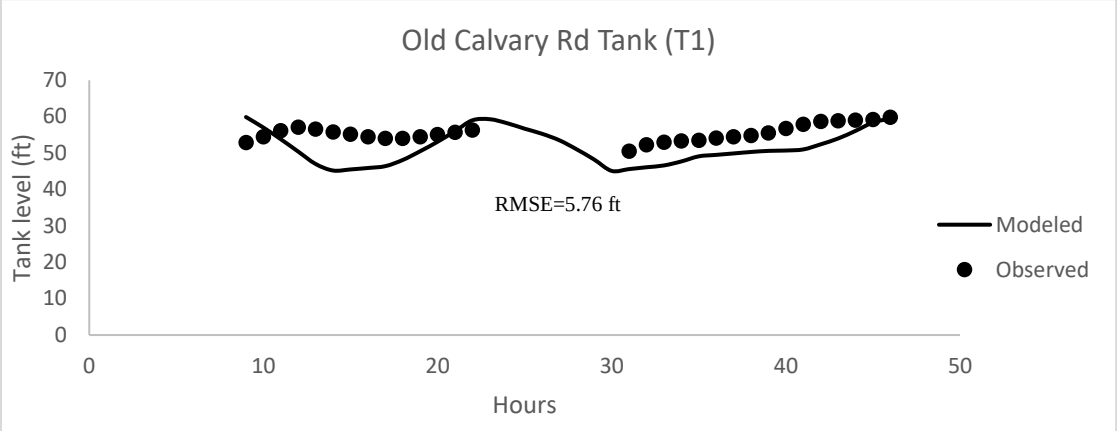

Figure 4-5: Old Calvary Tank Level Changes on Typical Summer Days

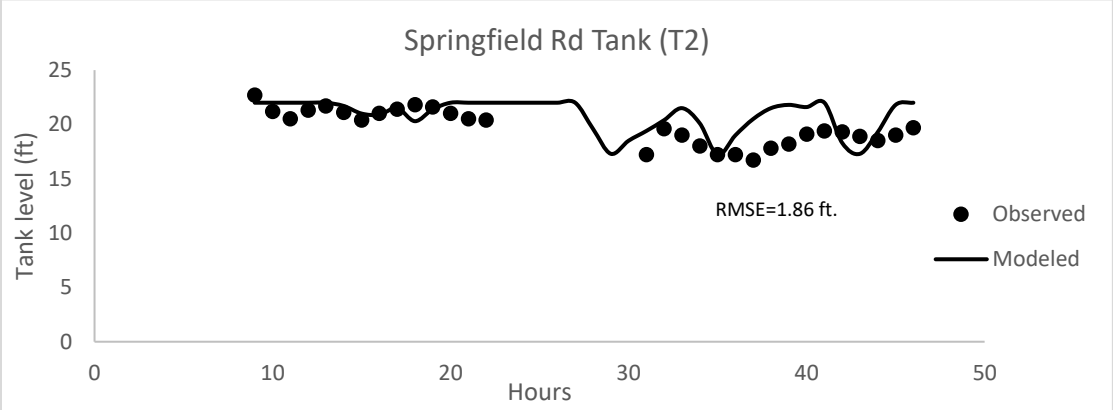

Figure 4-6: Springfield Field Tank Level Changes on Typical Summer Days

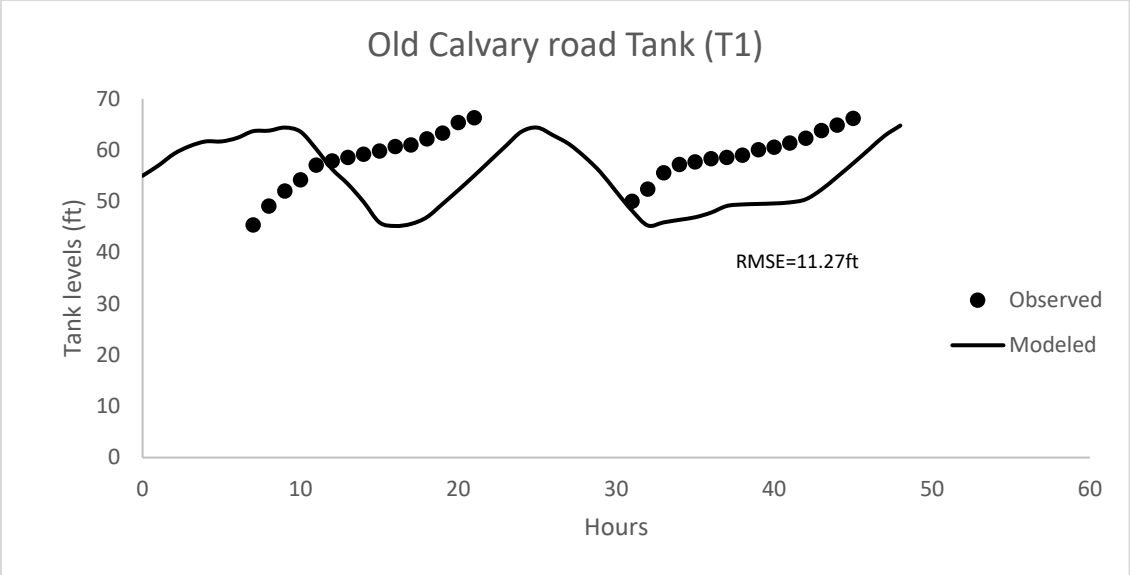

Figure 4-7: Old Calvary Tank Level Changes on Typical Winter Days

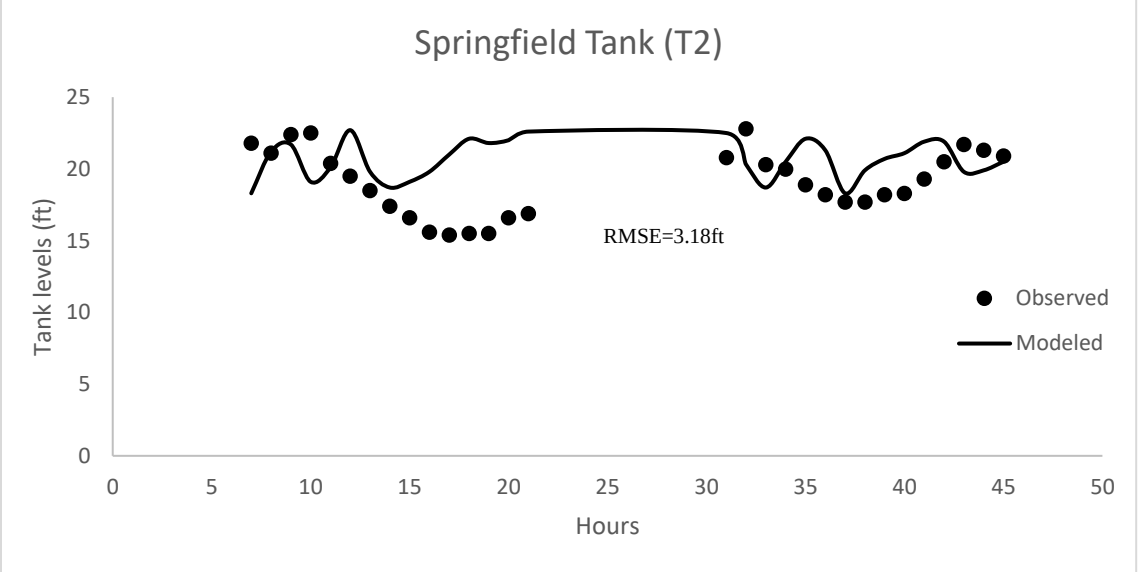

Figure 4-8: Springfield Tank Level Changes on Typical Winter Days

Hydraulic Calibration of the Martin County Water System

Out of the 16 tanks in MCWD, operational data of four representative tanks were studied and compared with their modeled tank levels. Comparison of the observed and predicted water levels over a two-day simulation period (for May 24 and May 25, 2022)

are provided in Figures 4-9 through 4-12. The associated RMSE values for each simulation are shown in the respective figures. As shown by the figures and the R squared values, the tank levels were similar for all four tanks with the Rock Castle tank being the best and the Turkey Tank being the worst. It appears the observed and the predicted values for each tank are slightly out of phase with the modeled values. This could be associated with an unknown error in the telemetry data, pump operation time or errors in the assumed temporal distribution of demands. Also, the utility also has been suspicious about water leakage, some of them are being discovered at present. Given the complexity of the system and continued data uncertainties with Martin County System, these results were deemed to be acceptable.

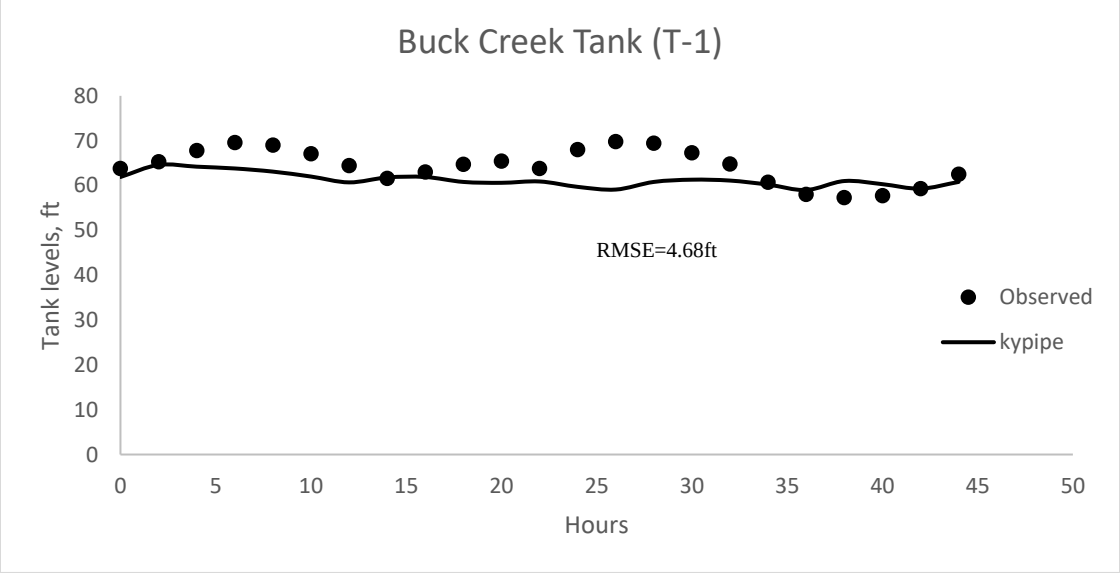

Figure 4-9: Buck Creek Tank Levels on May 24th and 25th May 2022

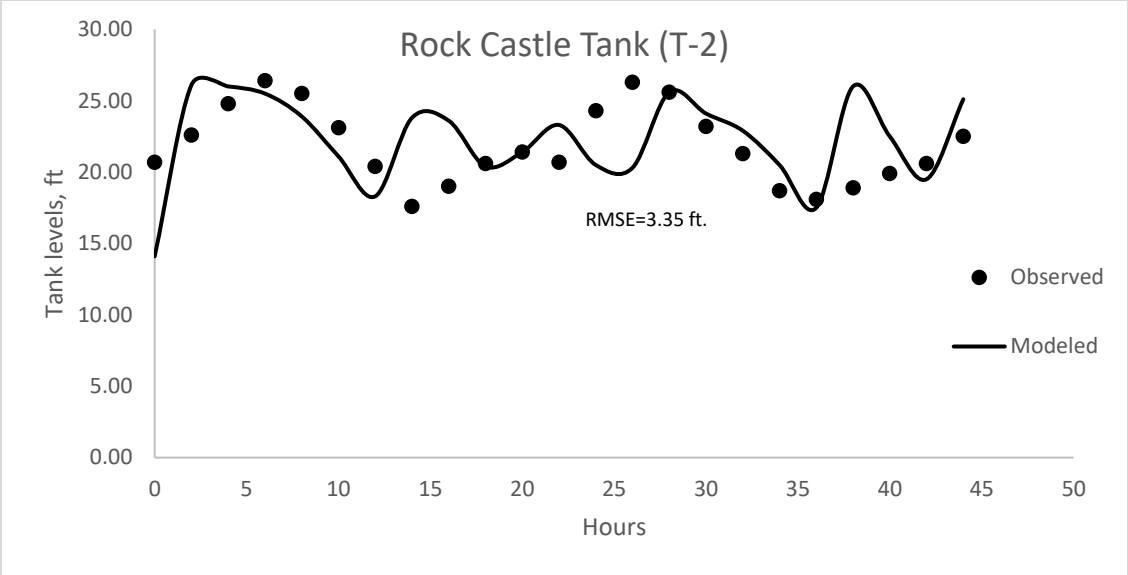

Figure 4-10: Rock Castle Tank Water Levels on 24th And 25th May 2022

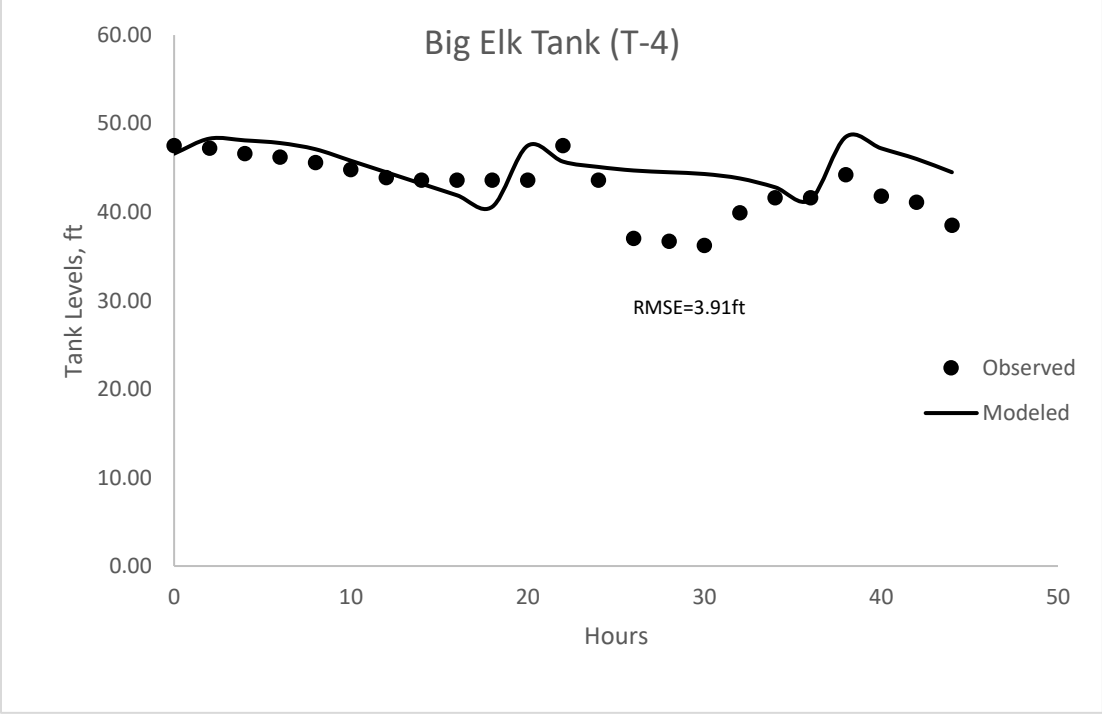

Figure 4-11: Big Elk Tank Levels on 24th And 25th May 2022

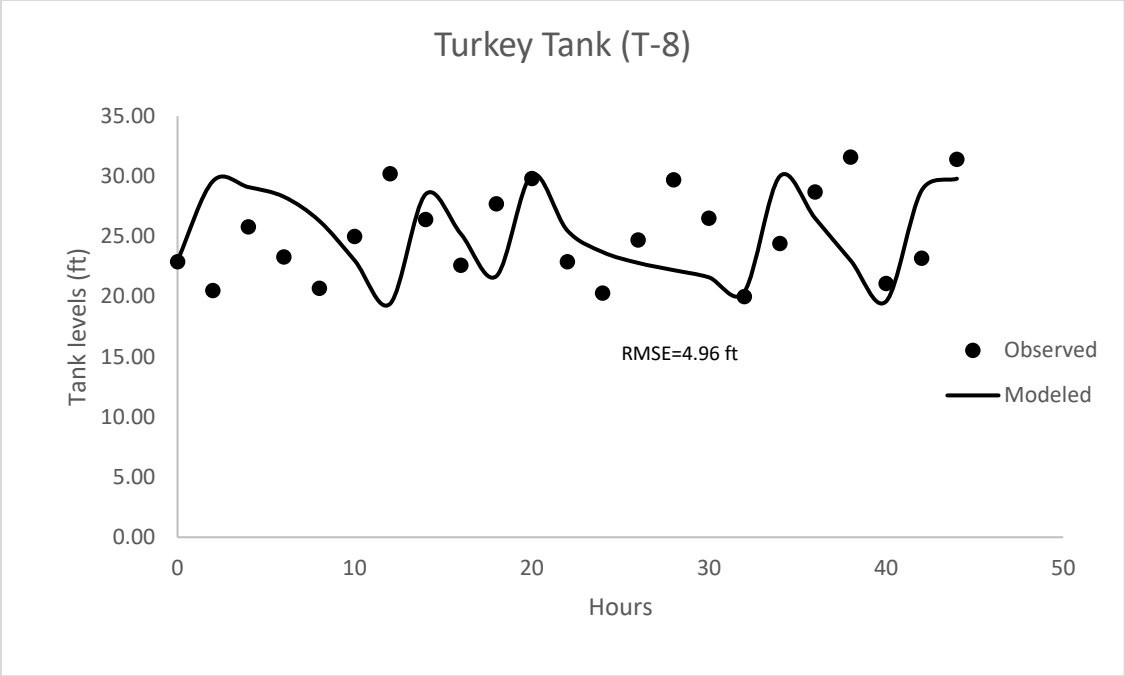

Figure 4-12: Turkey Tank Levels On 24th And 25th May 2022

4.4 Water Age Modeling Using KYPIPE

Once both the Lebanon System and Martin County System hydraulic models were calibrated, they were used to predict the average water age for each junction node in the respective system. KYPIPE interfaced with EPANET calculates water age at various points in the distribution system using a Lagrangian time-based approach to track discrete parcels of water as they move through the distribution system. The average expected water age at any point in the distribution system is approximated by running the model over an extended number of days until the water ages in the tank reached an equilibrium value. This is necessary to balance out the contribution of water ages from different sources to the system (e.g., water storage tanks). Maps showing the spatial distribution of average water ages (in hours) for each system are provided in Figures 4-13 and 4-14.

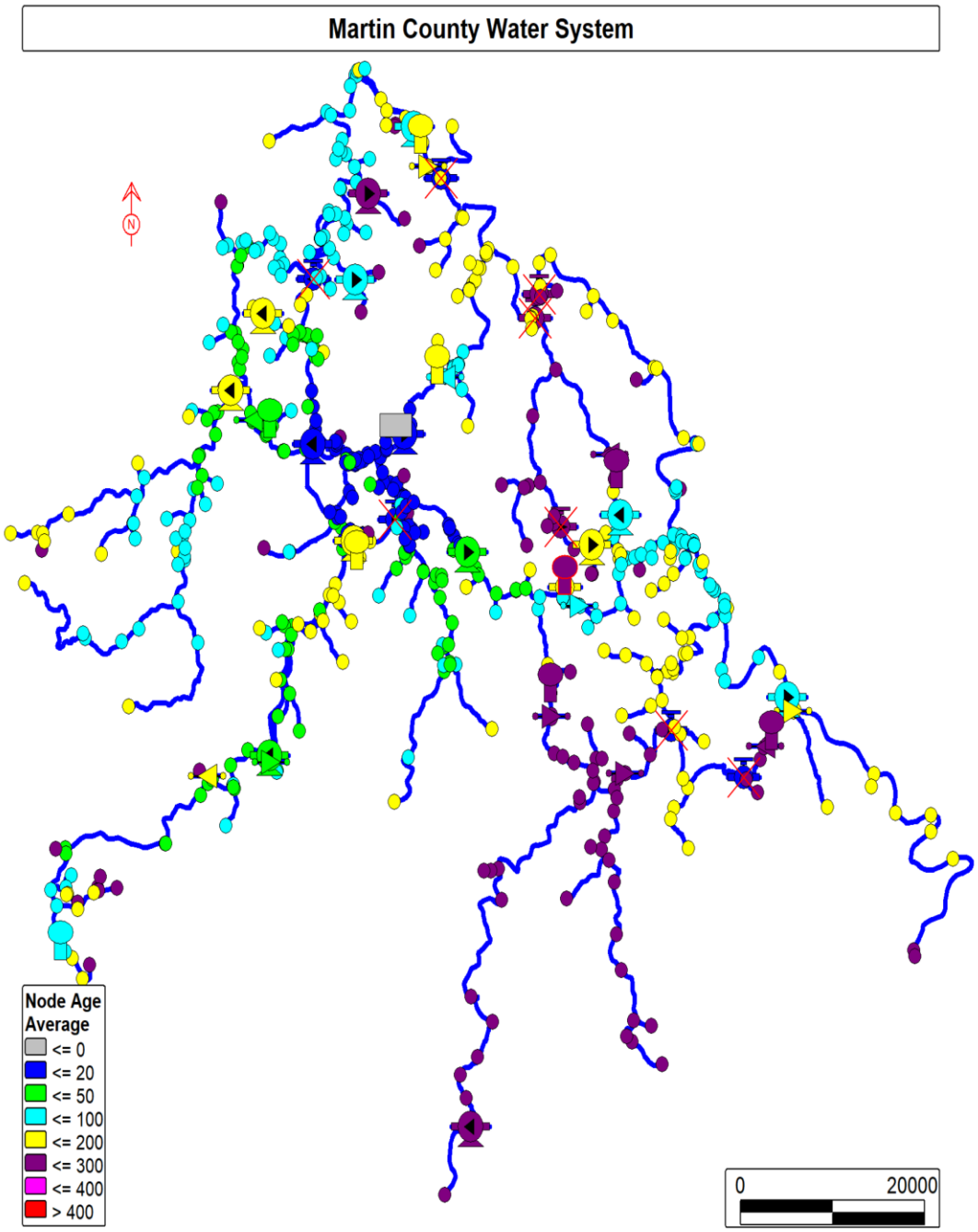

Figure 4-13 Spatial Distribution of Average Water Ages in hours (Fall-MCWD)

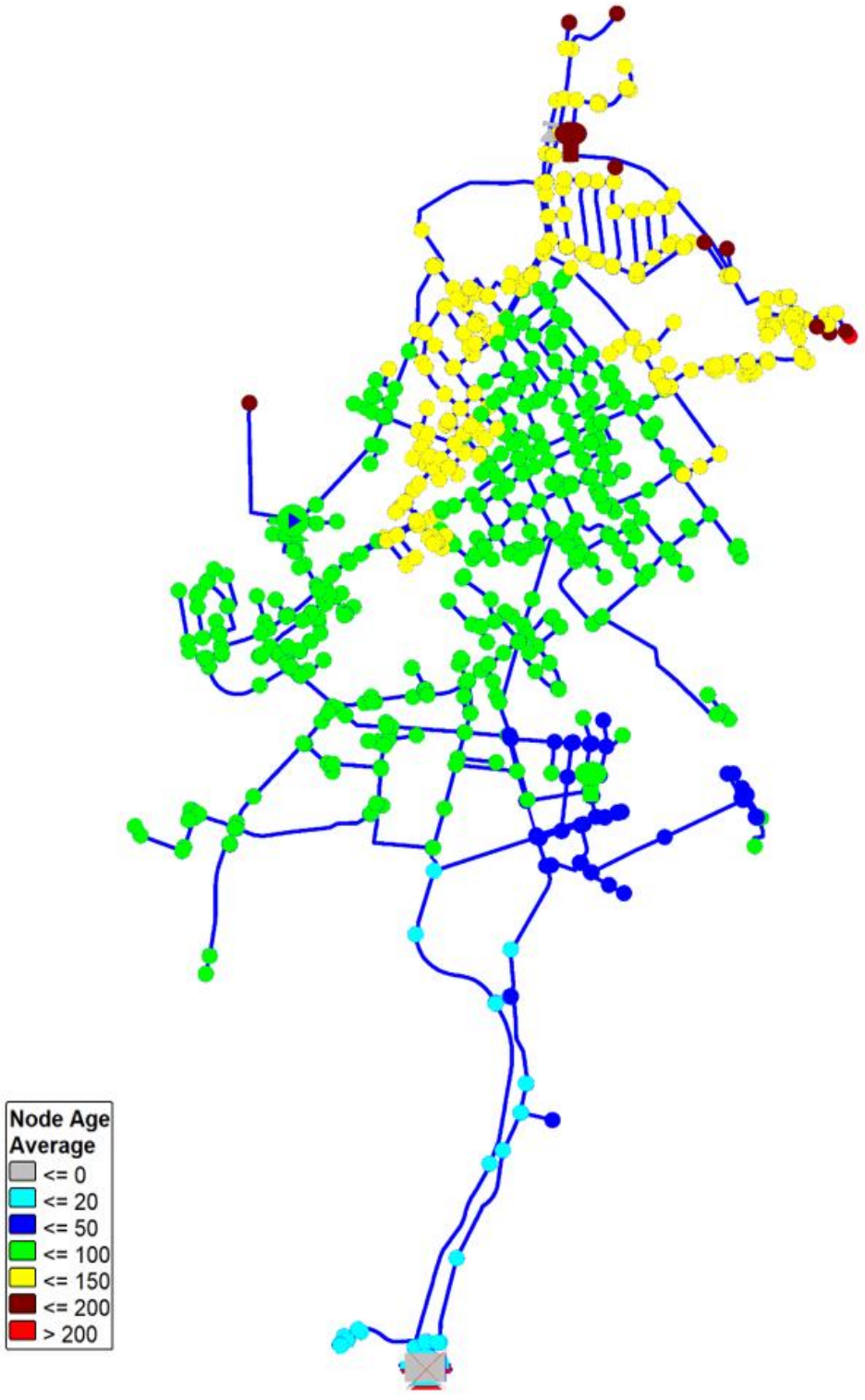

Figure 4-14 Spatial Distribution of Average Water Ages in hours (Summer-LWW)

4.5 Chlorine Decay Modeling and Calibration

Once the models were hydraulically calibrated to replicate the observed tank levels, the bulk and wall decay rates were first estimated and then applied to match observed chlorine values throughout the system. In the case of Lebanon System, reliable chlorine models (summer and winter) were developed using half of the available historic MOR data from the year 2021, and then validated using the other half of the historic chlorine values from same year. For Lebanon system, field data was also collected at the treatment plant and at four sampling locations across the system (see Figure 4-15).

For the Martin County system, field data were collected at the treatment plant and at four sampling locations across the system (see Figure 4-16) during two separate sampling periods (summer and fall) for use in model calibration exercise. MOR data available from the plant was then used for validation of the model. A summary of the data collected from field sampling for both systems is provided in Appendix C. The standard operating procedures used in collecting the samples and then for measuring their chlorine concentrations are provided in Appendix D.

In order to achieve the project goal, the developed chlorine models should generate results that best match the chlorine values from field observation. For this purpose, water quality model calibration is necessary. The water quality model was used to simulate the performance of the system over time (typically several days) to establish equilibrium concentrations for chlorine in each of the storage tanks. Once these equilibrium values were obtained, they could then be used to predict the residual chlorine levels as each junction node. The calibration process then involved the adjustment of the water quality parameters (initial chlorine concentrations at the plant, bulk decay rates, and wall decay rates) until the

predicted values of the chlorine match as closely as possible with the observed value at the selected junction nodes.

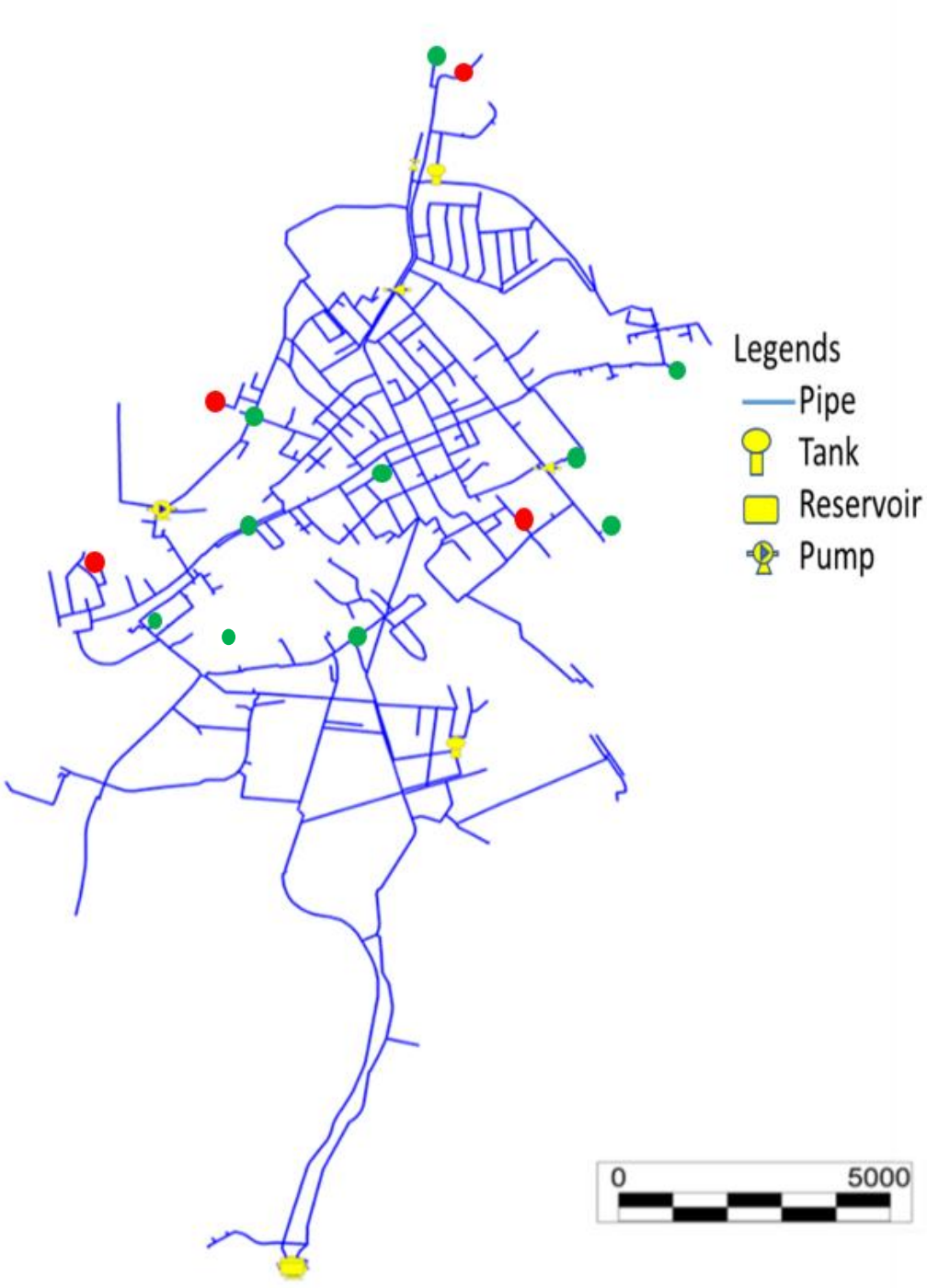

Figure 4-15 Locations of MOR data (Green dots) and Field Sampling Sites (Red dots) in LWW

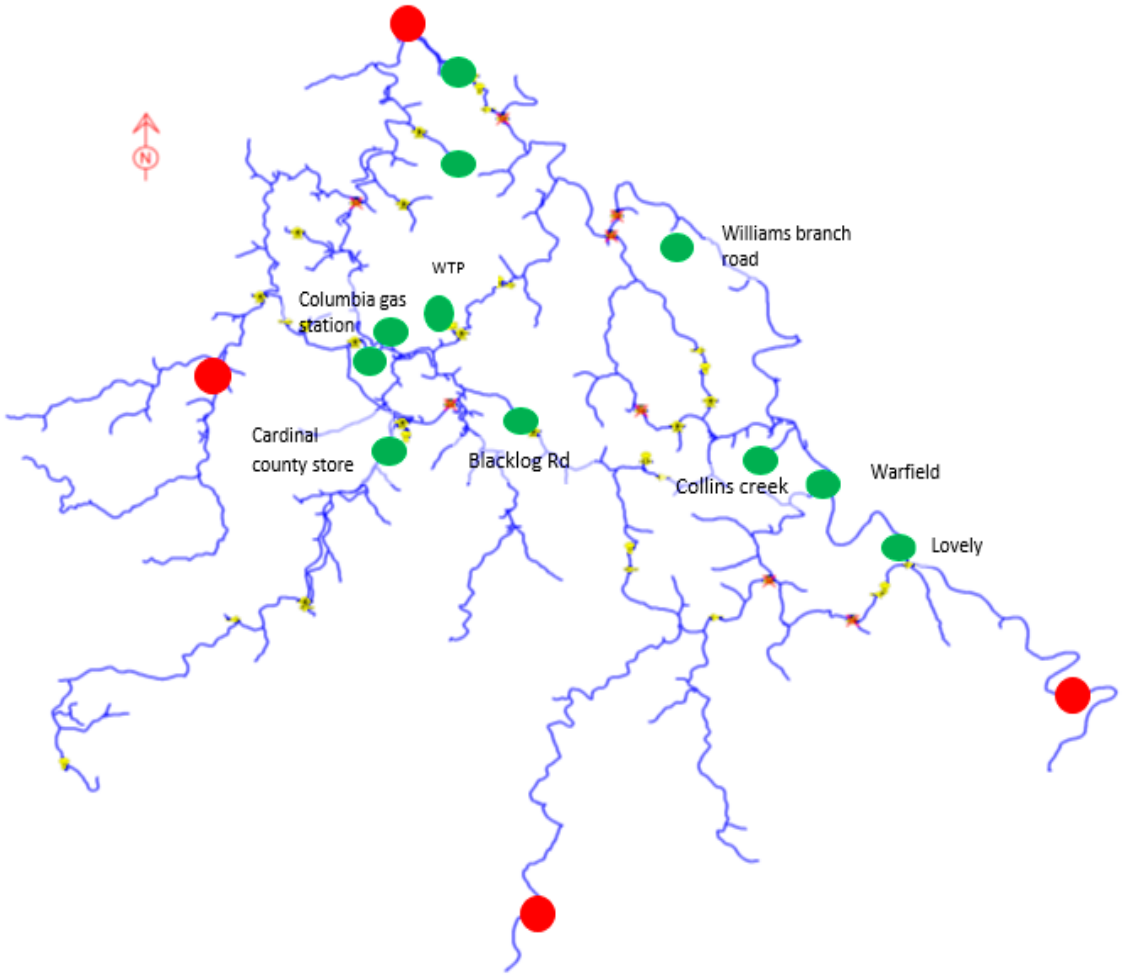

Figure 4-16 Locations of MOR data (Green dots) and Field Sampling Sites (Red dots) in MCWD

Determination of Bulk Decay Rates

For both the Lebanon and Martin County systems, initial estimates of the bulk decay rate were obtained from separate bulk decay experiments. In each case, samples of treated water leaving the treatment plants were placed in a series of clean glass bottles that were prepared to ensure no chlorine decay occurred from the interactions with the bottle material. These bottles were transported to the UK lab and placed at room temperature to match the field conditions. At a designed timestep (i.e., usually every 24 hours) a chlorine test was performed on the sample and any observed free and total chlorine was recorded.

The chlorine values for the Martin County system are summarized in Table 4-1. The free chlorine values observed for bulk decay experiment at the Lebanon samples are summarized in Table 4-2. The plots of the data for both systems are provided in figures 4-17 and 4-18.

Table 4-1: Free Chlorine Values from Bulk Decay Experiment (MCWD)

Date	Time	Time lapse (hr.)	Total chlorine	Free chlorine
10/24/2022	12:00:00 PM	0.00	1.87	1.69
10/24/2022	4:00:00 PM	4.00	1.51	1.42
10/24/2022	8:00:00 PM	8.00	1.51	1.45
10/25/2022	9:30:00 AM	21.50	1.25	1.17
10/25/2022	1:52:00 PM	25.87	1.18	1.11
10/26/2022	12:45:00 PM	48.75	0.87	0.72
10/27/2022	1:45:00 PM	73.75	0.82	0.72
10/28/2022	1:45:00 PM	85.75	0.61	0.44
10/30/2022	3:00:00 PM	147.00	0.52	0.36
11/1/2022	2:00:00 PM	194.00	0.33	0.30
11/2/2022	1:00:00 PM	217.00	0.30	0.20
11/3/2022	2:00:00 PM	217.00	0.15	0.10
11/8/2022	1:30:00 PM	361.50	0.05	0.01

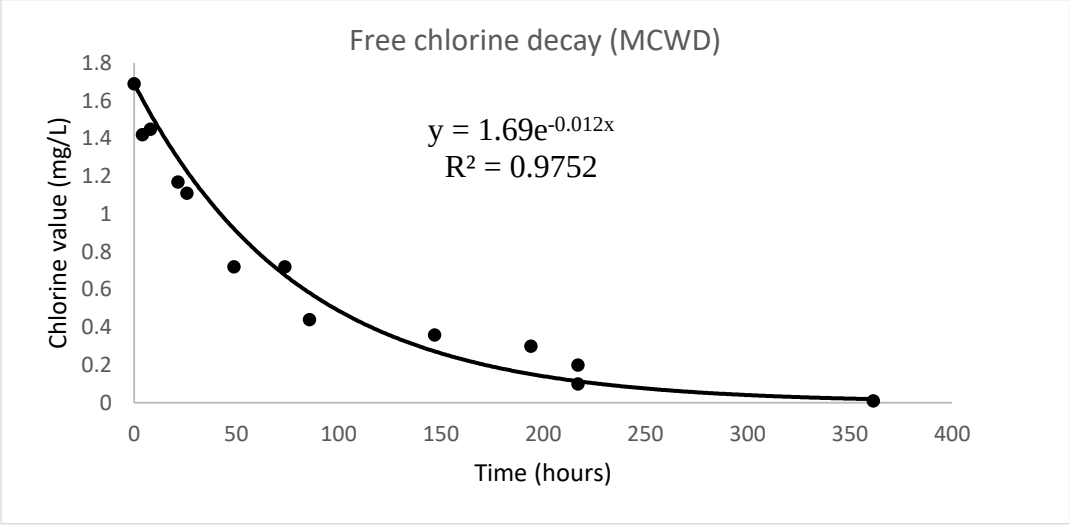

Figure 4-17: Free Chlorine Decay Result (MCWD)

Table 4-2: Free Chlorine Values from Bulk Decay Experiment (LWW)

Date	Time	Time lapse (hr.)	Total chlorine	Free chlorine
2/8/2023	7:46:00 AM	0.00	1.66	1.63
2/8/2023	11:44:00 AM	3.97	1.50	1.48
2/9/2023	10:22:00 AM	26.60	1.39	1.31
2/10/2023	11:50:00 AM	52.07	1.27	1.19
2/11/2023	1:20:00 PM	77.57	1.09	1.02
2/12/2023	1:24:00 PM	101.63	1.06	1.00
2/13/2023	10:25:00 AM	122.65	0.96	0.94
2/14/2023	11:35:00 AM	147.82	0.92	0.91
2/15/2023	1:10:00 PM	173.40	0.83	0.77
2/16/2023	11:50:00 AM	196.07	0.65	0.61
2/17/2023	2:15:00 PM	222.48	0.7	0.7
2/19/2023	4:50:00 PM	273.07	0.7	0.55
2/20/2023	2:30:00 PM	294.73	0.53	0.45
2/21/2023	12:00:00 PM	316.23	0.6	0.49
2/24/2023	2:10:00 PM	390.40		0.36
2/27/2023	3:30:00 PM	463.73	0.35	0.23
3/4/2023	1:30:00 PM	581.73	0.07	0.06

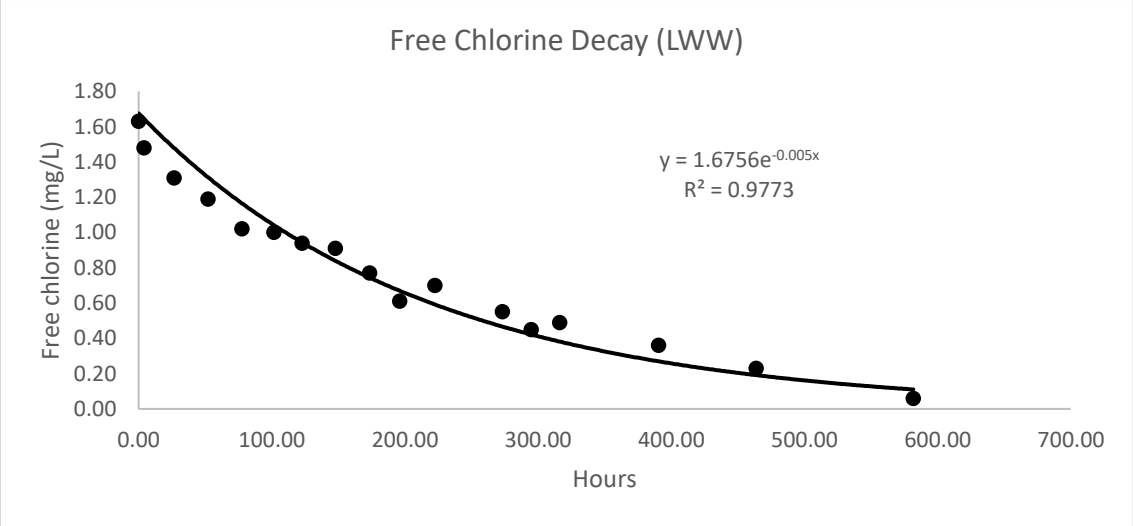

Figure 4-18: Free Chlorine Decay Result (LWW)

Using the best fit exponential decay equations for both systems (i.e., the first order decay equation: $c=c_0.e^{-kt,}$) we can solve for the value of bulk decay coefficient k_b for each system. The value of bulk decay rate for winter (i.e., February) obtained from bulk decay

experiment for the Lebanon system was equal to 0.005/hr. Similarly, the bulk decay rate for fall season (i.e., October) for Martin County System was found to be 0.012/hr. Estimates of bulk decay bulk decay rates for other seasons can be estimated using the Arrhenius equation (4-1) as shown below:

$$k_1 = k_2 * \exp((-E_a/R) * ((1/T1) - (1/T2))) \quad \text{(4-1)}$$

where k_1 = decay coefficient at temperature T1

k_2 = decay coefficient at temperature T2

E_a = activation energy = 40 kJ/mol

R = gas constant = 8.314 J/mol*K

By using the Arrhenius equation with average seasonal temperature and average activation energy of 40,000 Joule/mol (Kaczmarek et al., 2020). for chlorine decay, estimates of the bulk and wall decay rates for Lebanon (summer) and Martin County (summer) were obtained. It is observed that the bulk decay rates for Fall and Spring remain comparable due to similarity in temperatures. The final estimates for both the system and different seasons are provided in Table 4.3.

Table 4-3 The Global Bulk Decay Rates Calculated for Various Seasons

Model	Summer	Fall/Spring	Winter
Lebanon system	0.017/hr.	0.01/hr.	0.005/hr.
Martin County system	0.021/hr.	0.012/hr.	0.006/hr.

Determination of Wall Decay Rates

Once the bulk decay rate for each system was estimated, the initial wall decay coefficient of 0.01/hr. was taken from literature to analyze chlorine decay in both systems based on previous research (Hallam et al., 2002; Kowalska et al., 2006; Vasconcelos et al.,

1997). These values were entered into KYPIPE and then more accurate values of the wall decay rate for each system were determined through the process of model calibration.

To initiate the calibration process, the model was run with the initial decay coefficients. The chlorine results from the model were then compared with the measured values from the distribution system. To match the results, the bulk and wall decay coefficient which contributes to chlorine decay throughout the distribution network were readjusted with a trial-and-error approach. The predicted values of chlorine were repeatedly compared to the observed values. The wall decay rates were then repeatedly adjusted until the error between the observed and the predicted values were minimized. The final best value for the wall decay rate for the Lebanon system and Martin County system are shown in Table 4-4:

Table 4-4 The Global Wall Decay Rates Determined for Different Seasons

Model	Summer	Fall/Spring	Winter
Lebanon System	0.03/hr.	—	0.007/hr.
Martin County system	0.06/hr.	0.04/hr.	—

In calibrating the Lebanon system, observed chlorine values were obtained from 15 different monthly sampling locations that were reported to monthly MORs for the LWW. Data from approximately half of these site (i.e., 5 to 7 sites) were used to calibrate the model for two different seasons (i.e., summer and winter) while the rest of the data was used in model validation. In each case, estimates of the chlorine values at each sampling locations were average over each season. That is, the values for June, July, and August were averaged for summer calibration while the values for December, January, and February were averaged to the winter calibration.

In calibrating the Martin County system model, observed chlorine values were

obtained from five different field sampling locations. Data collected on July,2022 were used to calibrate the model for summer conditions, while data collected on October 24th,2022 were used to calibrate the model for fall conditions.

The final chlorine model calibration results for Lebanon are shown in Figure 4-15 &4-16 while the results for the Martin County system are shown in figure 4-17 and 4-18.

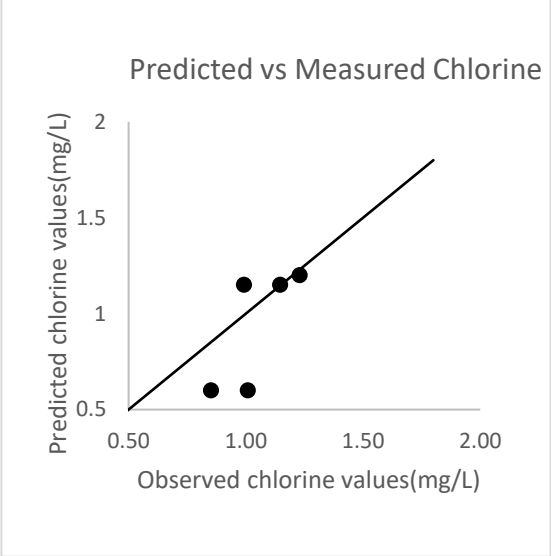

Figure 4-19 LWW Chlorine Model Calibration Result (Summer)

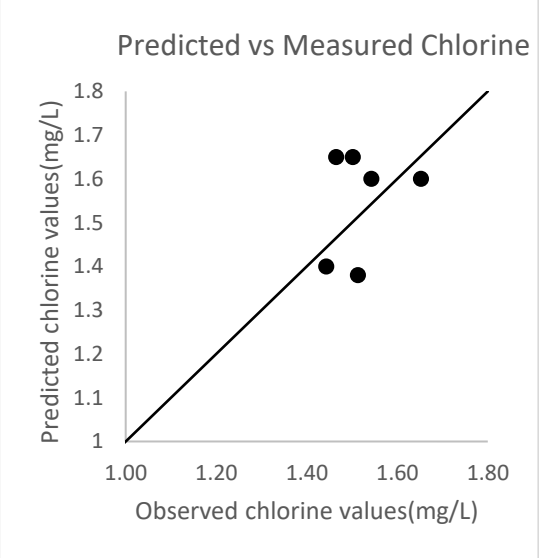

Figure 4-20 LWW Chlorine Model Calibration Results (Winter)

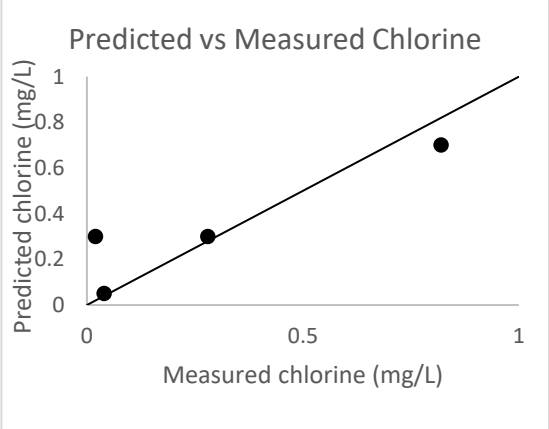

Figure 4-21 MCWD Chlorine Model Calibration Result (Summer)

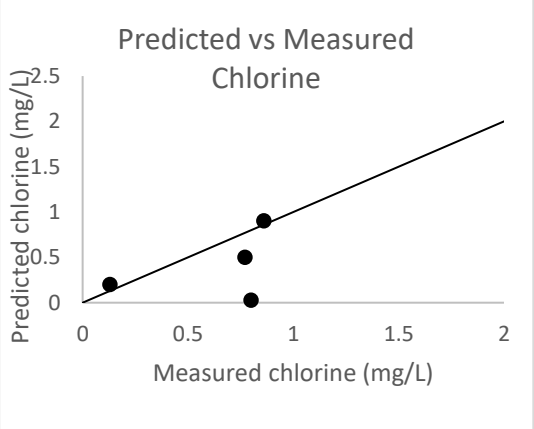

Figure 4-22 MCWD Model Calibration Result (Fall)

These graphs show that the plot between the predicted and the modeled values of the chlorine align closely with the reference line at 45°. This indicates a good correlation

between the observed and the predicted chlorine values.

4.6 Chlorine Decay Model Validation

Once the models were calibrated, the model parameters (i.e., the bulk decay rates, and the wall decay rates) for that season were fixed and the models were rerun using same parameters but with observed data from different sampling locations. For Lebanon and Martin County systems, these sampling data were obtained from monthly operating reports (MOR) for each season and each system (i.e., Lebanon -Winter and Summer; Martin county- Summer and Fall). For the Lebanon System, the summer model was validated using average chlorine values over June, July, and August, while the fall model was validated using average chlorine values over September, October, and November. For the Martin County System, the summer model was validated using chlorine values over August, while the fall model was validated using average chlorine values over October.

Several analyses were done to check the accuracy of each water quality model. Mean Absolute Error (MAE) and Root Mean Squared Error (RMSE) techniques are two major techniques used for model accuracy check. A comparison of the observed and predicted chlorine validation results for these simulations is discussed below.

Model Accuracy Validation Results for LWW Chlorine Model

The LWW model created to simulate the chlorine decay predicted the average value of chlorine for various nodes. These values were compared with the chlorine values for respective nodes from MOR reports. The differences between the observed and model predicted results for summer showed a mean absolute error of 0.19 mg/L. Also, it showed the root mean squared error of 0.24 mg/L. Similarly, the model created for prediction of winter chlorine values showed a mean absolute error of 0.18mg/L and root mean squared

error of 0.22 mg/L. A comparison of the observed and predicted results for these simulations is provided in Tables 4-5 and 4-6. As can be seen from these results, although they are not quite as good as the calibration runs, they do provide reasonable predictions and thus serve to validate the reliability of the selected parameters values of the modeled systems.

Table 4-5 Comparison of the Observed and Predicted Chlorine Results (Summer 2021)

SN	KYP Node	Jun	Jul	Aug	SD	Summer avg (mg/L)	Modeled avg (mg/L)	Absolute Error	Squared Error
1	303	1.52	0.96	1.24	0.23	1.24	1.15	0.09	0.01
2	723	1.09	1.14	0.91	0.10	1.05	1.0	0.05	0.00
3	1537	N/A	0.81	0.91	0.05	0.86	0.6	0.26	0.07
4	1641	N/A	1.01	1.37	0.18	1.19	1.2	0.01	0.00
5	1131	N/A	0.83	1.40	0.29	1.12	0.6	0.52	0.27
6	1492	N/A	0.64	1.03	0.20	0.84	0.6	0.24	0.06
7	1376	1.04	0.93	1.06	0.06	1.01	1.18	0.17	0.03
8	1701	1.10	0.79	1.18	0.17	1.02	0.8	0.22	0.05
							Absolute Error=	0.19	
								RMSE=	0.24

Table 4-6 Comparison of the Observed and Predicted Chlorine Results (Winter 2021)

SN	KYP Node	Dec	Jan	Feb	SD	Winter avg (mg/L)	Predicted avg (mg/L)	Absolute Error	Squared Error
1	303	1.60	1.67	1.87	0.11	1.71	1.6	0.11	0.01
2	723	1.57	1.73	N/A	0.08	1.65	1.6	0.05	0.00
3	1537	1.88	1.86	1.58	0.13	1.77	1.35	0.42	0.18
4	1641	1.94	1.83	1.87	0.05	1.88	1.65	0.23	0.05
5	1131	1.84	1.45	2.02	0.24	1.77	1.35	0.42	0.18
6	1492	1.64	1.71	1.49	0.09	1.61	1.4	0.21	0.05
7	1376	1.52	1.43	1.37	0.06	1.44	1.6	0.16	0.03
8	1701	1.46	1.53	1.56	0.04	1.52	1.6	0.08	0.01
							Absolute Error=	0.21	
								RMSE=	0.25

Model Accuracy Validation Results for MCWD Chlorine Model

The MCWD models were calibrated using the data from field sampling and validated using available MOR data. For model validation, these seasonal models were run to predict the average value of chlorine for the day and locations whose MOR data was available. These model-predicted values were then compared with the chlorine values for respective nodes from MOR data. The differences between the observed and predicted values for results from summer showed a mean absolute error of 0.43 mg/L along with the root mean squared error of 0.44 mg/L. Similarly, the model created for prediction of fall chlorine values showed a mean absolute error of 0.24 mg/L and root mean squared error of 0.29 mg/L when compared with MOR results from Oct-20. A comparison of the observed and predicted results for these simulations is provided in Tables 4-7 and 4-8 below. As can be seen from these results, although they are not quite as good as the calibration runs, they do provide reasonable predictions and thus serve to validate the reliability of the selected parameters values of the modeled systems.

These results indicate that these models are able to predict the chlorine values to an acceptable level.

Table 4-7 Comparison of the Observed and Predicted MCWD Chlorine Results (Summer)

SN	Nodes	Observed Cl (mg/L)	Predicted Cl (mg/L)	Absolute Error	Squared Error
1	J-255	1.08	0.6	0.48	0.23
2	J-294	0.87	1.2	0.33	0.11
3	J-37	0.75	1.2	0.45	0.20
4	J-317	0.97	0.5	0.47	0.22
			Mean Absolute Error=	0.43	
				RMSE=	0.44

Table 4-8 Comparison of the Observed and Predicted Chlorine MCWD Results (Fall)

SN	Nodes	Measured Cl (mg/L)	Predicted Cl (mg/L)	Absolute error	Squared error
1	J-255	1.17	1.65	0.48	0.23
2	J-294	1.14	1.4	0.26	0.07
3	J-317	1.17	0.8	0.37	0.14
4	J-722	1.34	1.4	0.06	0.00
			Mean Absolute Error=	0.24	
				RMSE=	0.29

4.7 Chlorine Decay Model Application and Results

Once the models were successfully calibrated and validated, an extended period water quality simulation was performed. Chlorine results were obtained using the extended period analysis throughout the system. These models were applied for each season to get corresponding chlorine results for each system.

These chlorine results clearly indicate that the chlorine concentrations near the treatment plant are relatively higher than the nodes at a farther distance. It also indicates that the chlorine values are more likely to be below regulatory limits of 0.2 mg/L if they are at distant dead ends. It is also observed that the chlorine values for winter are relatively better than the summer model for Lebanon system since chlorine decay rates tend to be correlated with the temperature. Similarly, the summer model for Martin County also seems to generate slightly lower chlorine residuals than the fall model at the extremities. This is also hypothesized to be due to higher chlorine decay rates in the summer.

The chlorine results for Martin County clearly indicate that the chlorine residuals at dead ends and at the branches far out in the system may need special attention as the chlorine values are near to the critical regulatory values. The chlorine results obtained for each seasonal model for Lebanon and Martin County System are presented in figure 4-23

through 4-26.

Results of Applied Models for LWW Chlorine Decay Analysis

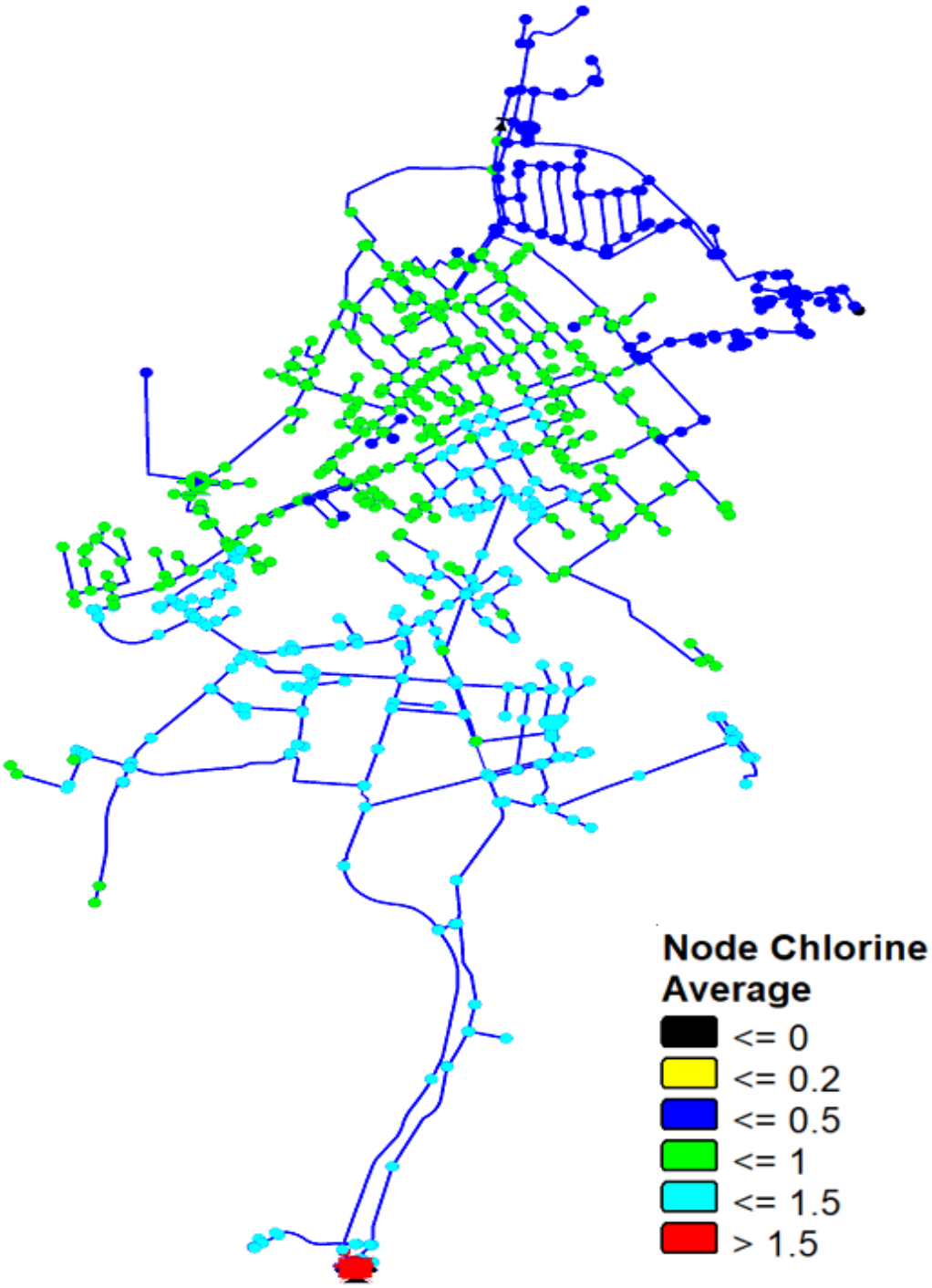

Figure 4-23 Average Chlorine Values in The LWW System Using Summer Model

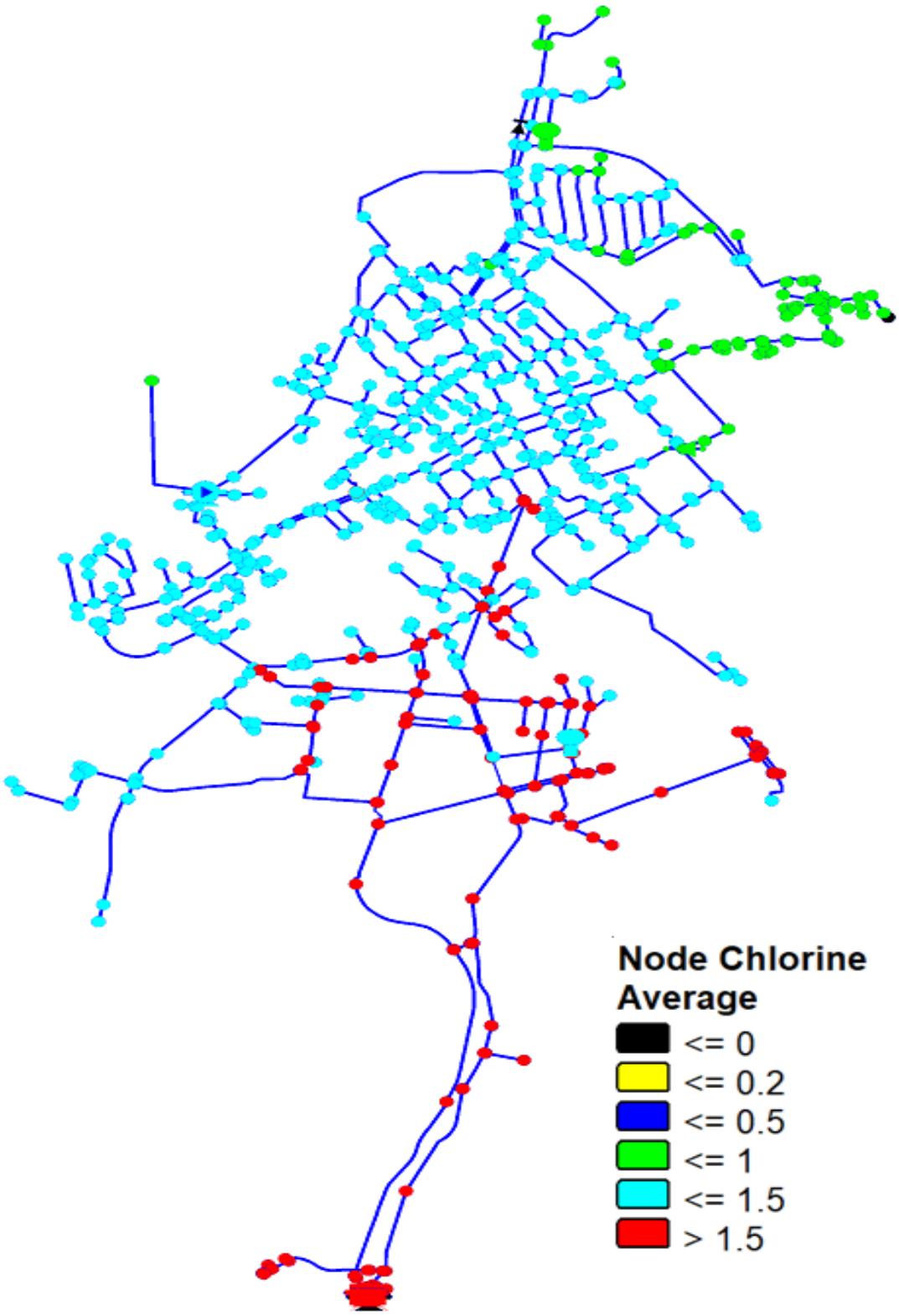

Figure 4-24 Average Chlorine Values in The LWW System Using Winter Model

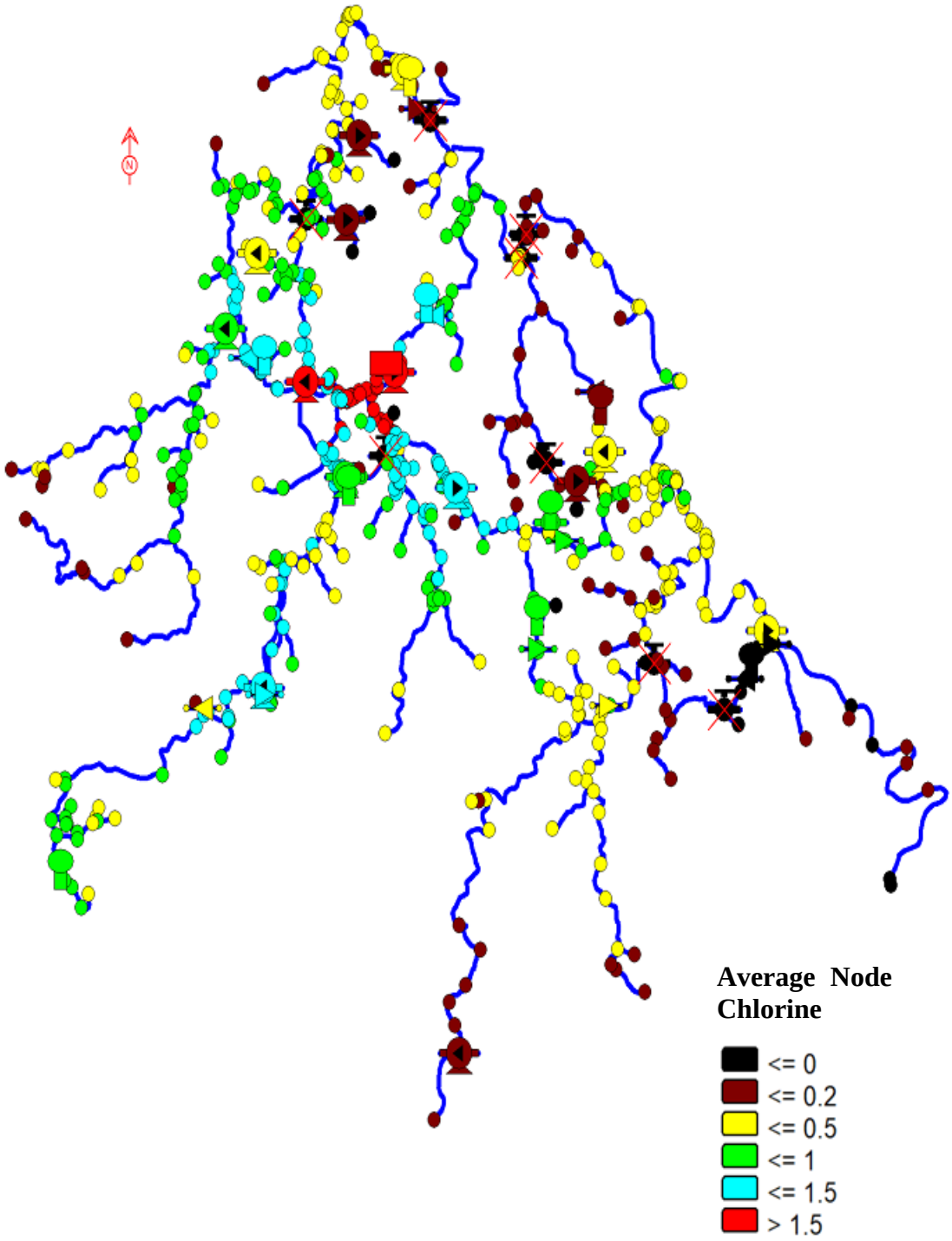

Figure 4-25 Average Chlorine Values in The MCWD System Summer Model

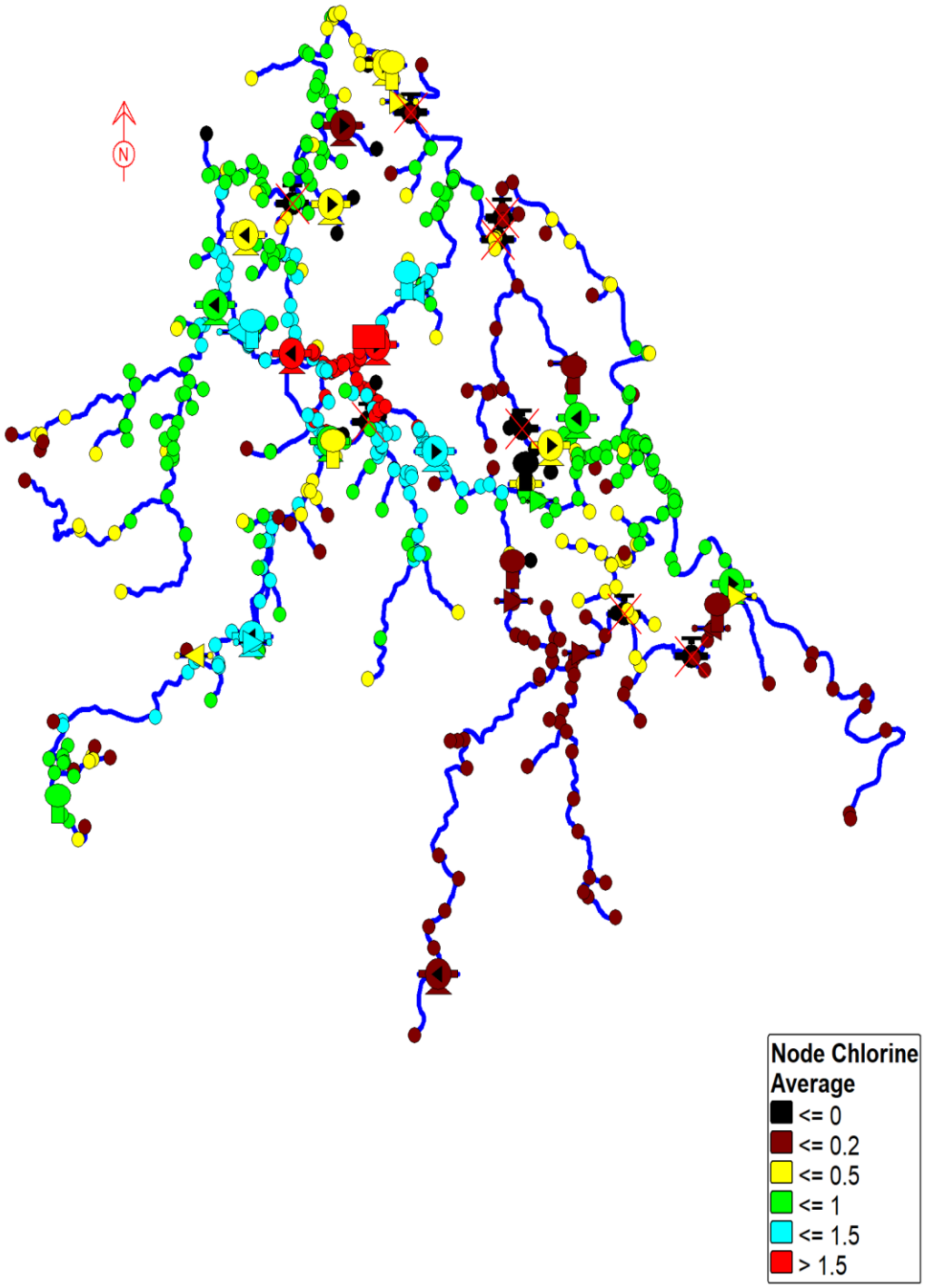

Figure 4-26 Average Chlorine Values in The MCWD System Fall Model

4.8 Relation of Water Age and Chlorine Residual

The correlation between water age and chlorine residual was studied based on model water age and chlorine results for some representative nodes in each model (see Table 4-9 and 4-10). The results were graphically represented in Figure 4-27 through 4-30. These results clearly indicate that the chlorine residuals for the nodes with higher water ages are lower than those with lower water ages.

Table 4-9 Average Water Age and Chlorine Residual for MCWD (Fall model)

Node	Predicted Water Age (hr.)	Observed Chlorine Values (mg/L)
J-236	53	0.86
J-790	99	0.77
J-183	171	0.13
J-260	225	0.8

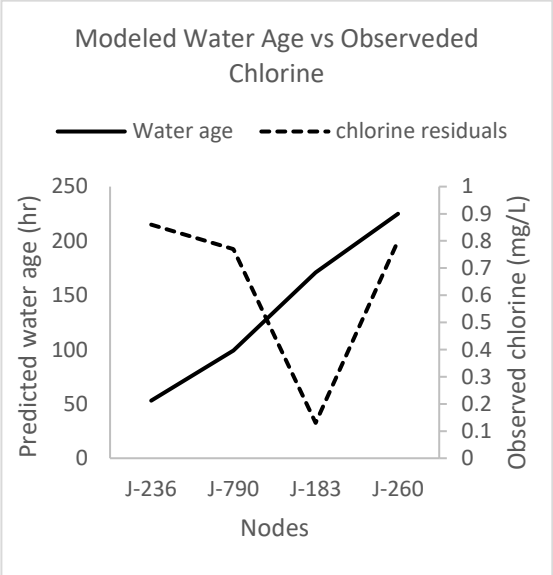

Figure 4-27 The Relation Between Modeled Water Age and Predicted Chlorine Residual (MCWD Summer)

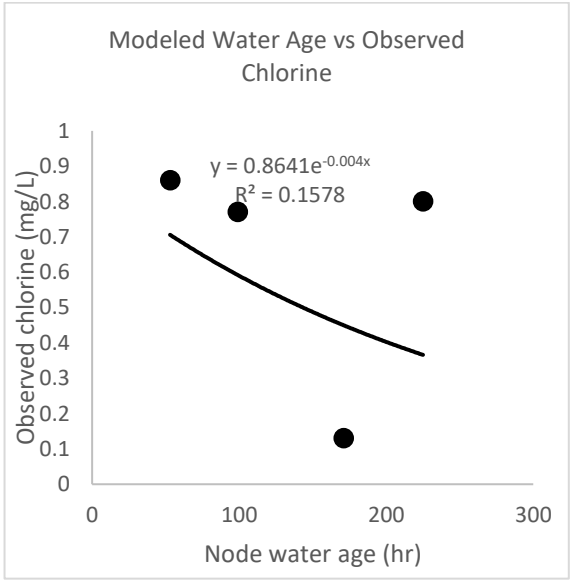

Figure 4-28 The Correlation Between Modeled Water Age and Predicted Chlorine Residual (MCWD Summer)

Table 4-10 Average Water Age and Chlorine Residual for LWW (Summer model)

LWW Node	Water Age (hr.)	Chlorine Values (mg/L)
303	81	1.15
723	106	1
1537	180	0.6
1641	74	1.2
1131	172	0.6

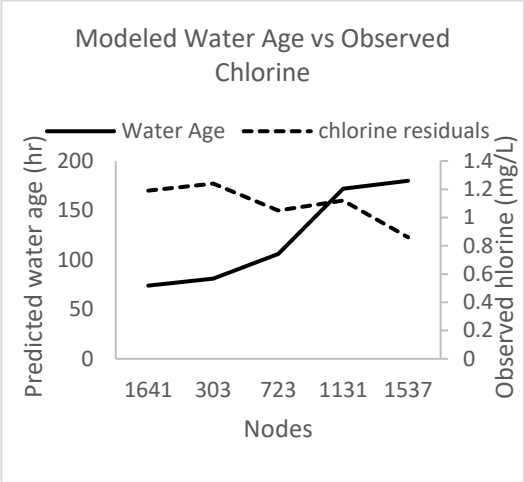

Figure 4-29 The Relation Between Modeled Water Age and Predicted Chlorine Residual (LWW)

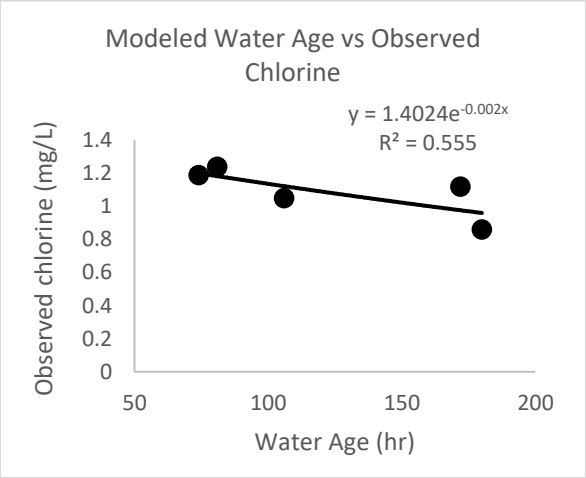

Figure 4-30 The Correlation Between Modeled Water Age and Predicted Chlorine Residual (LWW)

Preliminary functional relationship between predicted chlorine residual and water age are developed for each model based on model results for some junction nodes. These models showed a strong correlation between water age and chlorine residuals with R squared value of 0.99.

4.9 Investigation of Operational Changes for Lebanon System

The impacts of various operational changes on major water quality parameters-water age and chlorine residuals were studied using these KYPIPE models. Based on the chlorine and water age analysis, five representative sites were selected in each system for the study of the operational changes in the water quality. For this study, the chlorine and

water age at initial set hydraulic and quality conditions were noted and the simulation was done again after changing parameters of study. The differences in the results can be used for making the operational decisions.

Impacts of Changing Plant Chlorination on Chlorine Residuals in LWW

In this analysis the plant chlorine value was changed in the model and the changes in residual chlorine at representative nodes were studied. In this analysis the plant chlorine values were changed in LWW summer model from 1 to 4 mg/L and the residual chlorine at nodes were predicted before and after altering the applied chlorine.

Table 4-11 Results for LWW Summer Chlorine Values with Different Plant Chlorination

S. No.	Node	Plant chlorine of 1 mg/L	With plant Cl of 1.55 (mg/L)*	With plant chlorine of 2 mg/L	With plant chlorine of 3 mg/L	With plant chlorine of 4 mg/L
1	N-303	0.7	1.15	1.38	2.15	2.75
2	N-723	0.6	1	1.2	1.9	2.5
3	N-1537	0.35	0.6	0.65	1.2	1.5
4	N-1641	0.75	1.2	1.6	2.45	3.25
5	N-1131	0.38	0.6	0.75	1.2	1.6
6	N-1492	0.35	0.6	0.7	1.1	1.5
7	N-1376	0.75	1.18	1.5	2.38	3
8	N-1701	0.5	0.8	1	1.6	2

*Value of plant chlorination during sampling

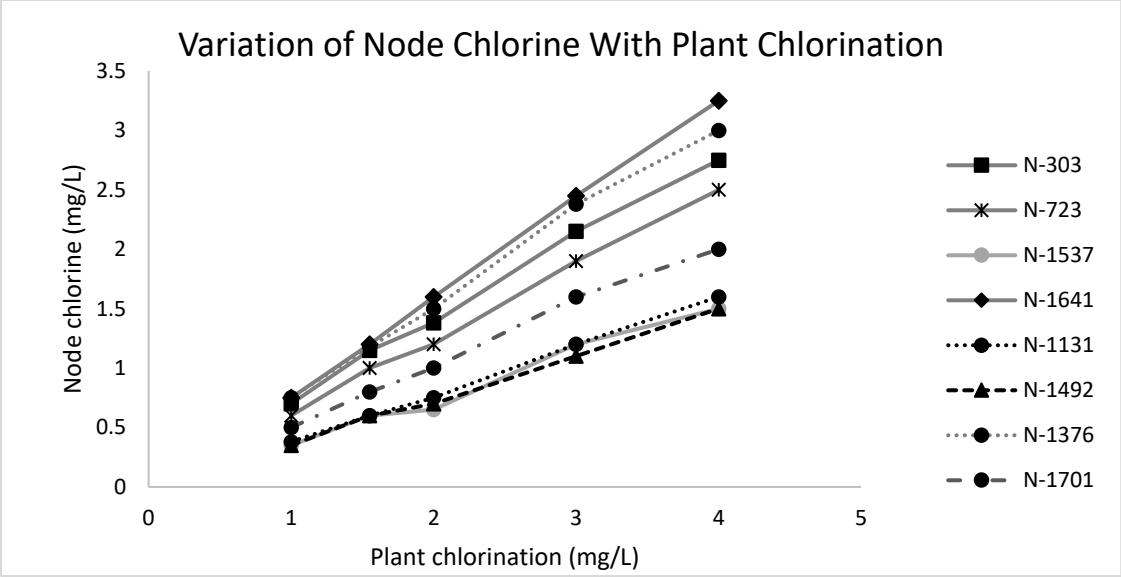

Figure 4-31 Variation of Chlorine Residuals with the Change in Plant Chlorination (LWW)

This indicates that the residual chlorine in the system can be significantly increased at most nodes by increasing the plant chlorine if other parameters favor the increment.

4.10 Investigation of Possible Operational Changes for MCWD System

Altering the Plant Chlorination on MCWD Chlorine model

Utilities are paying a high percentage of their revenue in chlorination of the treated water. They are always seeking an optimum value of chlorination that helps to make sure that the minimum value of chlorine residual is available for disinfection purposes. To investigate the impact of different levels of chlorine at the plant to residual chlorine values across the system, the plant chlorine values were varied at the plant from 1mg/L to 4 mg/L and then the results were studied at five different locations based on their distance from the treatment plant. The residuals obtained at various nodes of MCWD by applying various

plant chlorination values are tabulated below in Table 4-13. The plot of variation of the residuals with the change in plant chlorination is presented in the Figure 4-32.

Table 4-12 Results for MCWD Summer Chlorine Values with Different Plant Chlorination

Node KYPIPE	With 1mg/L plant chlorine	With 1.86 mg/L plant chlorine*	With 2mg/L plant chlorine	With 3mg/L plant chlorine	With 4mg/L plant chlorine
J-236	0.35	0.7	0.7	1.1	1.5
J-790	0.15	0.3	0.35	0.5	0.7
j-239	0.22	0.3	0.5	0.75	1
J-714	0.15	0.25	0.3	0.45	0.6
J-211	0.02	0.05	0.05	0.06	0.08

*Actual Plant chlorination value

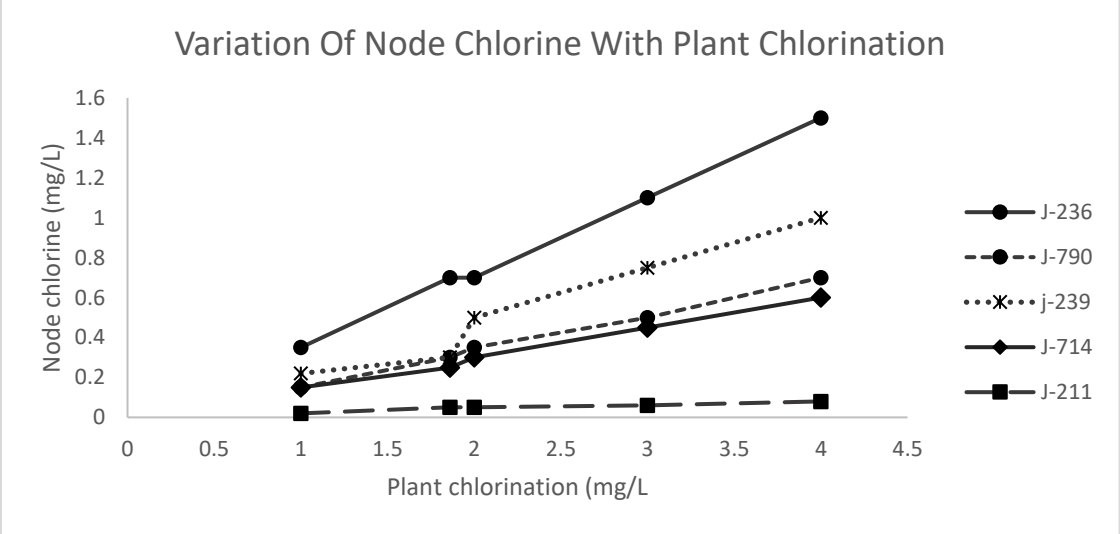

Figure 4-32 Variation of Chlorine Residuals with the Change in Plant Chlorination (MCWD)

This indicates that the residual chlorine in the system can be significantly increased at most nodes by increasing the plant chlorine if other parameters favor the increment. However, it appears that the chlorine residuals at some junction nodes (i.e., those at the extremities of system –e.g., node 211) cannot maintain an adequate chlorine residual even if the plant chlorine levels are increased up to 4 mg/L (the maximum allowable level). Conversely, it appears that junctions 714 and 790 can be raised from

below 0.2 mg/L (i.e., the regulatory standard) by increasing the chlorine levels at the plant from 1 mg/L to 2 mg/L. This illustrates the utility of the models in highlighting potential water quality issues or in guiding potential operational decisions.

Impacts of Altering the Global Demand on MCWD Chlorine model

The impact of changing water demands on the chlorine residual for the MCWD model was also investigated. These results obtained from this study are tabulated in Table 4-12 and illustrated in Figure 4-33.

Table 4-13 Chlorine Results for MCWD Model After Changing the Global Demand

Node KYPIPE	Cl With 50% Demand (mg/L)	Cl With 100% Demand(mg/L)	Cl With 150% Demand(mg/L)	Cl With 200% Demand(mg/L)
J-236	0.4	0.7	0.8	0.9
j-239	0.15	0.3	0.6	0.75
J-790	0.1	0.3	0.45	0.6
J-714	0.06	0.25	0.4	0.5
J-211	0.005	0.05	0.12	0.2

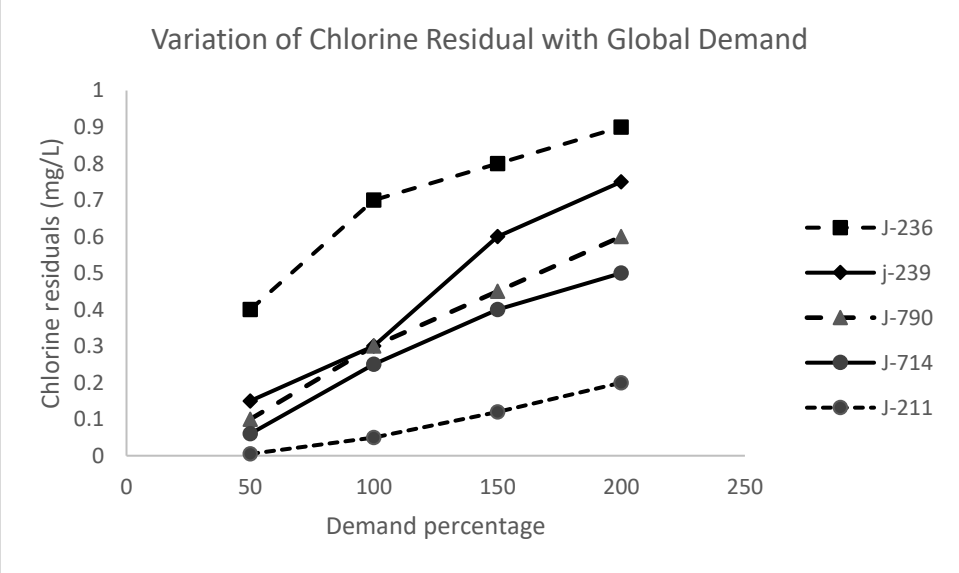

Figure 4-33: Variation of Chlorine Residual with Global Demand (MCWD)

As expected, the graph plotted by assessing the effect of changing global demand on the residual chlorine in various locations in a distribution system showed that the Cl concentration is lower with the lower demand as a result of increased travel time.

Impacts of Lowering the Water Loss in MCWD Chlorine Residuals.

The model results showed the most critical nodes in terms of chlorine residuals and in terms of water age at the peripheral areas of the system when the demand is lowest. This is because of a long travel time and more chlorine reaction in longer travel times.

This raises a particular research question regarding the MCWD system, which currently is experiencing a 70% water loss. What would be the impact on chlorine residuals if the water loss is reduced or eliminated? To investigate this question, the model was re-run with a series of additional demand reductions as shown in Table 4-14 and Figure 4-3.

Table 4-14 Chlorine Values Obtained by Reducing Present Water Loss (MCWD)

S. No.	Node	Cl with 100% Demand (mg/L) (70% water loss)	Cl with 60% Demand (mg/L) (50% water loss)	Cl with 35.3% Demand (mg/L) (15% water loss)	Cl with 30% Demand (mg/L) (0% water loss)
1	J-668	1.61	1.6	1.6	1.6
2	J-37	1.25	1.11	0.9	0.85
3	J-790	0.3	0.1	0.04	0.04
4	J-714	0.25	0.06	0.02	0.01
5	j-183	0.04	0.005	0	0
6	J-260	0.02	0.002	0	0

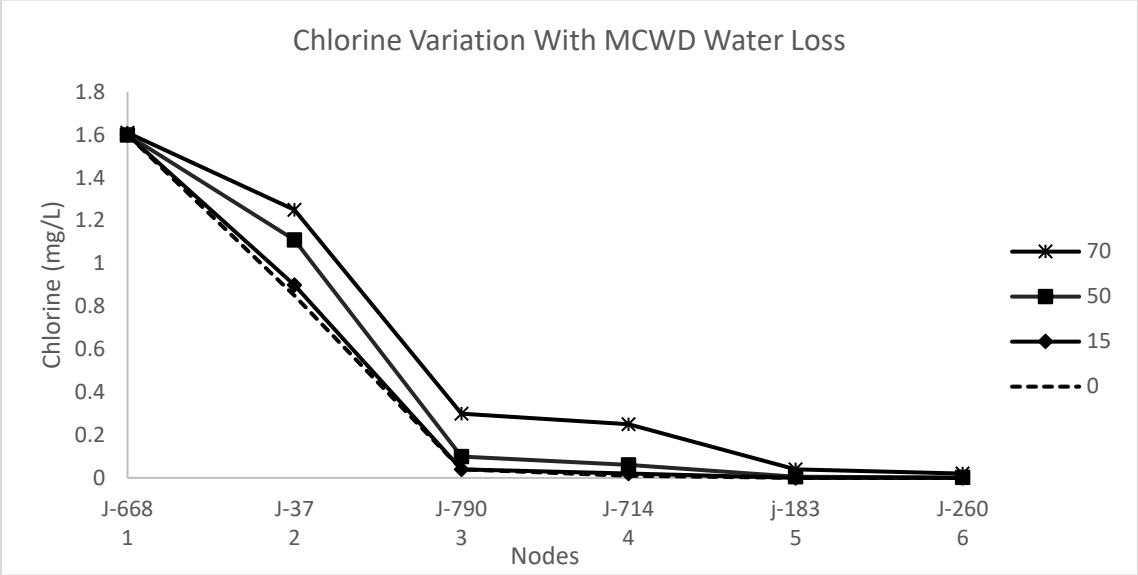

Figure 4-34: Chlorine Residual Variation While Changing the MCWD Water Loss Percentage

Figure 4-32 reveals that in addition to the fact that several nodes cannot meet the water quality standards for residual chlorine, the chlorine residuals for the peripheral nodes also tend to decrease as the total water system demand decreases, which raises significant questions about the impact of eliminating water loss for this system.

5. PREDICTION OF DISINFECTION BYPRODUCTS IN WATER DISTRIBUTION SYSTEM BY DEVELOPING TTHM REGRESSION AND COMPUTER MODELS AND STUDY OF THE IMPACTS OF OPERATIONAL CHANGES IN THEIR FORMATION

5.1 Abstract

The basic hypotheses of this chapter of proposed research are: 1) regression models can be developed that allow for the prediction of DBPs in a water distribution system as a function of either water age or chlorine demand, 2) the developed regression models can be embedded into the KYPIPE modelling environment for predicting DBP values, and 3) that the modified KYPIPE model can then be used to develop new operational strategies that will lead to a decrease in DBP concentrations throughout the actual distribution network. In this case, performance will be measured by the ability of the system to satisfy water quality regulations related to maximum DBP concentrations by changing various operational parameters. Thus, the primary goal of proposed research is to develop a model for use in predicting the concentration of DBPs in a water distribution system and evaluate whether the model could be used to improve overall operations. These basic hypotheses were tested using two different water distribution systems in Kentucky: the Lebanon, KY water distribution system and the Martin County water distribution system. These two systems were selected because they represent respectively a spectrum of systems in Kentucky: 1) a well operated system in a relatively flat terrain and 2) a poorly operated system in a relatively mountainous terrain. The physical characteristics of each system were described previously in Chapter-4.

5.2 Introduction

Conceptual modeling of disinfection by-products (DBPs) involves creating a simplified representation of several factors that can affect DBP formation in a system. Conceptual models for prediction of DBPs require the establishing of an empirical relationships of water quality and operational parameters that provides a causal link with DBPs at various times and places in the distribution system (Sadiq & Rodriguez, 2004). Major factors affecting DBP formation include pipe material and age, pipe flowrate and velocity, source water quality, treated water quality, water age, water temperature, chlorine residuals, and chlorine demand. Various researchers have proposed mathematical models (or equations) for predicting the formation of DBPs (Bellar et al., 1974; Chowdhury et al., 2009; Robert M Clark, 1998; Hua & Reckhow, 2008a). Such modelling efforts typically began after the discovery of chloroform and other organohalides in drinking water in 1974. These initial models were used to guide operational decision making associated with the water treatment process and did not consider the subsequent formation in the water distribution systems. In some cases, agencies have used these models in epidemiological studies associated with unsafe drinking water.

Unfortunately, most of the previous studies do not account for the effects of the distribution system on disinfection byproducts formation. The best way to determine the effect of the distribution system in DBP formation is through the collection of field data but this can be time consuming, tedious, and not always logistically or economically viable. Moreover, some of the parameters influencing DBPs are difficult to measure in the field and need to be transported to labs for subsequent analysis. This currently makes real time sampling of DBPs essentially impossible. This fact underscores the need for mathematical

models for predicting DBPs throughout the distribution system. The basic hypotheses related to DBP modelling were tested using the following research methodology:

- Develop two regression models of disinfection byproducts expressed as a function of chlorine demand and water age.
- Validate the developed models using DBPs concentrations collected from two actual water distribution systems along with measured chlorine values and predicted water age.
- Incorporate the DBP models into KYPIPE.
- Apply the developed models to two actual water distribution systems.
- Investigate the use of the models to develop new operational strategies that lead to a decrease in DBP formation.

Each of these steps is discussed in detail in the following sections.

5.3 Regression Modeling of Disinfection By-products

Two of the more important water quality parameters of the distribution system that affect DBP formation are chlorine demand and water age. As the chlorine decays over time, the chlorine demand rises as the water age increases in the system. As a result, chlorine demand may be considered a direct independent variable of DBP formation since it is hypothesized that some of the chlorine consumed in the decay process is being converted into DBP compounds (e.g., TTHMs or HAAs). Conversely, water age may be considered an indirect independent variable of DBP formation since time in and of itself does not cause the DBP formation. However, if water age can be shown to provide just as a reliable predictor of DBPs as chlorine demand then it may be more robust variable for modelling purpose since water age can be predicted by KYPIPE: EPANET without the need of

additional data collection (i.e., chlorine residuals) and subsequent calibration of model water quality parameters (i.e., bulk decay rate and wall decay rate). Both approaches are considered below. For the purpose of this study, the examined DBPs were limited to TTHMs.

Chlorine Demand as An Independent Variable of DBP Formation

Clark (Robert M Clark, 1998) characterized TTHM formation as a function of chlorine demand. According to this characterization, TTHM formation can be modeled as the linear function of chlorine demand as:

$$TTHM(t) = c.X(t) + Y_0 \quad \text{(5-1)}$$

where TTHM represents the TTHM concentration as function of time t, c is a coefficient, and X(t) represents the additional growth of concentration of TTHMs as a function of time t above an initial value Y_0 of TTHMs as water leaves the water treatment plant. The parameter X(t) can be shown to be a function (F_1) of the chlorine demand, CD (t), i.e., $X(t) = F_1[CD_j(t)]$, where the chlorine demand at a particular junction node j is equal to the difference between the initial concentration of Cl entering the system at a treatment plant or storage tank (i.e., $Cl_i(0)$) and the chlorine concentration observed at that same junction at time t ($Cl_j(t)$).

This can be expressed as

$$CD_j(t) = Cl_i(0) - Cl_j(t) \quad \text{(5-2)}$$

As a result, the relation of a disinfectant byproduct and chlorine demand, i.e., C_{DBP} (mg/l) at a particular junction node j can be expressed as functions F_1 as follows:

$$C_{DBPj}\,(mg/l) = F_1\,(CD_j\,(mg/l) = F_1\,(C_0 - C_0 e^{-kTj}) \quad \text{(5-3)}$$

Where, k = chlorine decay coefficient and T_j is the travel time (hours) from the treatment plant to junction j.

Water Age as An Independent Variable of DBP Formation

Alternatively, the concentration of TTHMs as a function of time X(t) can be shown to be a function (F_2) of the water age WA(t) i.e., $X(t) = F_2[WA(t)]$.

As a result, the relation of a disinfectant byproduct and water age, i.e., C_{DBP} (mg/l) at a particular junction node j and water age T can be expressed as functions F_2 as follows:

$$C_{DBPj}\,(mg/l) = F_2\,(T_j) \quad \text{(5-4)}$$

5.4 Regression Model Development for Disinfection By-products Analysis

Following the collection of chlorine residuals and water age predictions for both the Lebanon, Kentucky, and Martin County systems, four separate, regression models for DBP (i.e., TTHM) prediction were developed using simple regression (i.e., separate chlorine demand vs DBP and water age vs DBP models for both Martin County and Lebanon system). In each case the chlorine demands, and the water age used in the regression model were obtained from calibrated hydraulic/water quality models of both systems (i.e., see chapter 4). The data used in the construction of both models is provided in Table 5-1 and 5-4 and the resulting equations are shown in Figures 5.1 through 5.6.

Table 5-1 Water Age Vs Measured TTHM (LWW, 2020)

Year	Season	Node	Average Water Age	Observed (TTHM)	Plant (TTHM)	Distribution (TTHM)
2020	winter	224	153.00	0.025	0.006	0.019
2020	summer	224	240.00	0.073	0.02	0.053
2020	winter	667	46.00	0.017	0.006	0.011
2020	summer	667	64.00	0.076	0.02	0.056

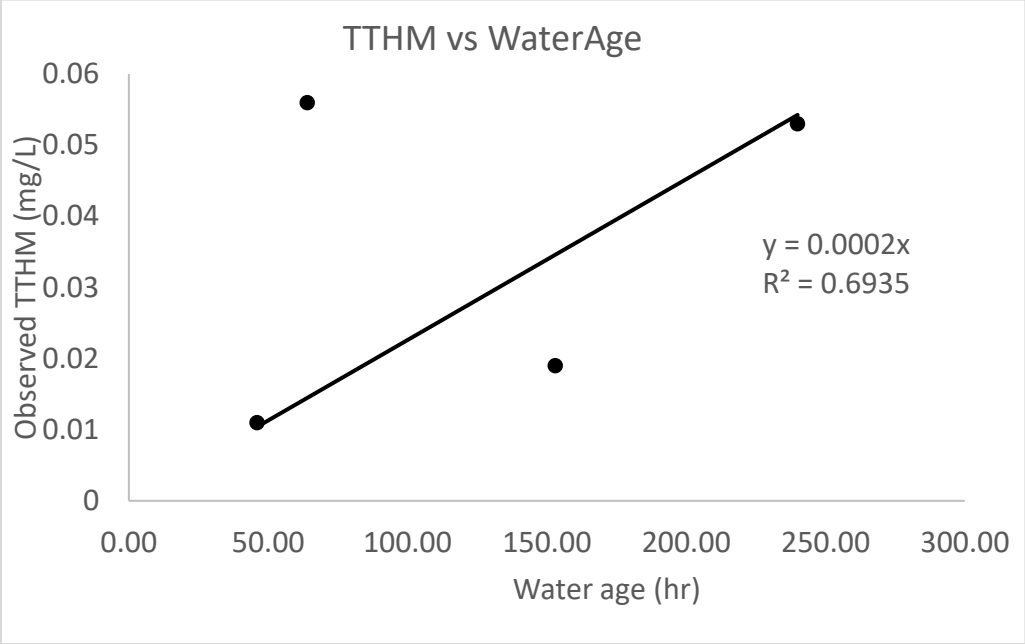

Figure 5-1 Observed TTHM vs Water Age Relation (LWW)

Table 5-2: Chlorine demand Vs Measured TTHM (LWW, 2021)

Year	Season	Node	Avg plant chlorine	Avg node chlorine	Chlorine demand (mg/L)	Observed TTHM (mg/L)	Plant TTHM (mg/L)	TTHM formed in Distribution (mg/L)
2021	winter	224	1.77	1.61	0.16	0.013	0.003	0.01
2021	spring	224	1.63	1.37	0.26	0.028	0.008	0.02
2021	summer	224	1.58	0.83	0.75	0.072	0.024	0.048
2021	fall	224	1.67	0.93	0.74	0.032	0.012	0.02
2021	winter	667	1.77	1.65	0.12	0.012	0.003	0.009
2021	spring	667	1.63	1.38	0.25	0.026	0.008	0.018
2021	summer	667	1.58	1.15	0.43	0.068	0.024	0.044
2021	fall	667	1.67	1.05	0.62	0.031	0.012	0.019

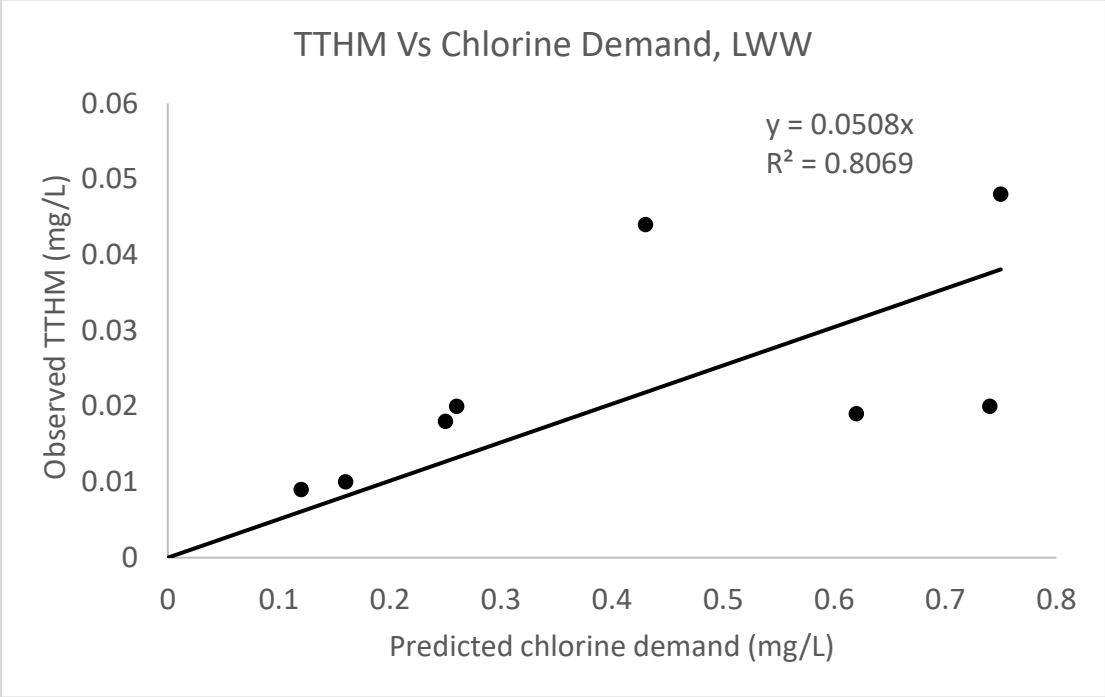

Figure 5-2: Observed TTHM Vs Chlorine Demand (LWW, 2021)

Table 5-3 TTHM concentration and Average Water age (MCWD July and Oct 2022)

Date	Node KYPIPE	Measured TTHM (mg/L)	Average KY Water age (hr.)	TTHM formed in distribution
July 2022	WTP			
July 2022	J-236	0.089	53	0.035
July 2022	J-790	0.123	99	0.069
July 2022	j-183	0.155	171	0.101
July 2022	J-260	0.157	225	0.103

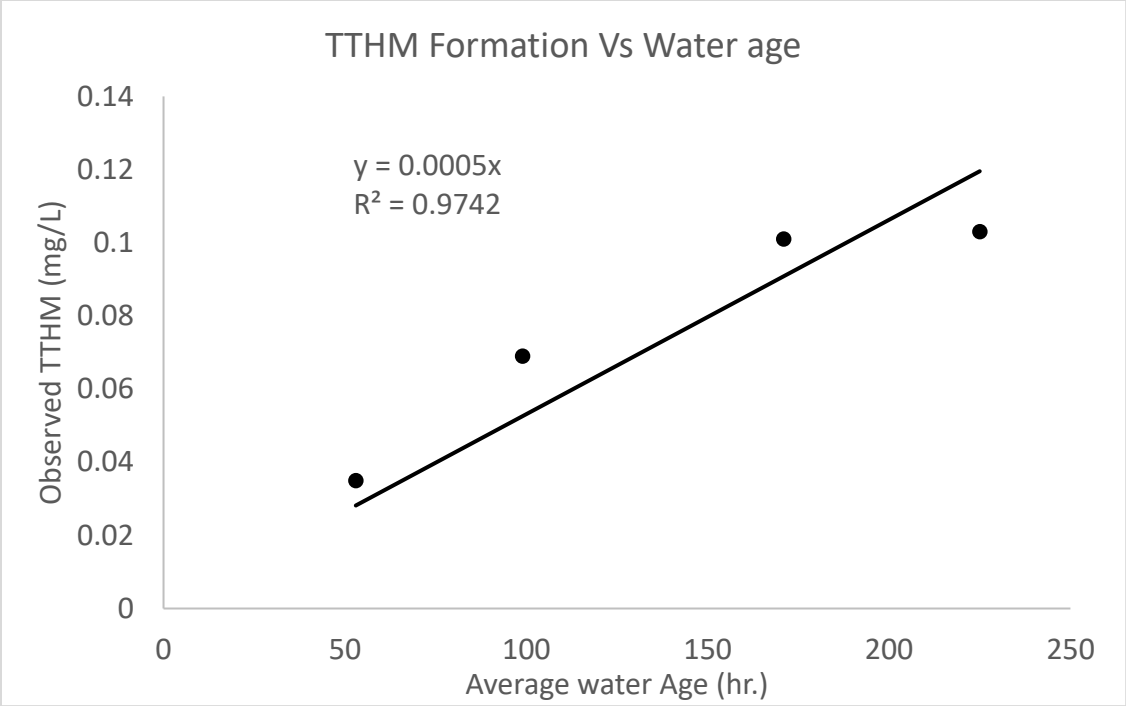

Figure 5-3 Observed TTHM and Average Water age (MCWD Oct 2022)

Table 5-4 Chlorine demand Vs Measured TTHM (MCWD, Oct 2022)

Date	KYPIPE Node	Measured Free Chlorine (mg/L)	Predicted Free Chlorine (mg/L)	Predicted Chlorine Demand (mg/L)	Observed TTHM (mg/L)	TTHM formed in distribution (mg/L)
July 2022	WTP	1.86			0.054	
July 2022	J-236	0.82	0.7	1.16	0.089	0.035
July 2022	J-790	0.28	0.3	1.56	0.123	0.069
July 2022	J-183	0.02	0.3	1.56	0.155	0.101
July 2022	J-260	0.04	0.05	1.81	0.157	0.103

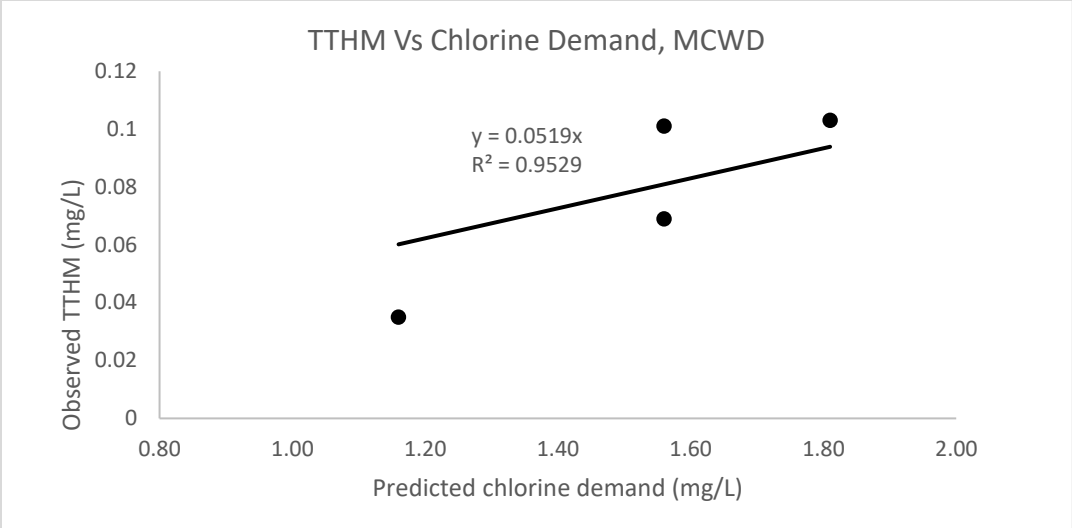

Figure 5-4: Obseved TTHM Vs Predicted Chlorine demand (MCWD 2022)

Table 5-5 Summary of Data Analysis

System	Based on	Regression Equation	R^2
Lebanon	Water age	TTHM = 0.0002* water age	0.69
Lebanon	Chlorine demand	TTHM = 0.0508* Cl demand	0.81
Martin County	Water age	TTHM = 0.0005* water age	0.97
Martin County	Chlorine demand	TTHM = 0.0519*Cl demand	0.95

As can be seen from above figures, it would appear that chlorine demand is better predictor of TTHM formation than water age, since water age may not be quite as precise since it is being predicted by a simulation model that may or may not accurately reflect the travel times in the system. However, as pointed out previously, chlorine demand requires the collection of additional field data from the system. Thus, it could be argued in some cases (like MCWD), water age might be sufficient to predict relative values of TTHM concentrations or more likely help guide in the selection of possible monitoring locations for subsequent TTHM field monitoring. However,

Based on the performance of both types of models, a decision was made to focus on the use of the TTHM formation model that uses chlorine demand as the independent variable in all subsequent model analyses.

5.5 Incorporation Of TTHM Regression Model into KYPIPE: EPANET

Following the validation of a general regression equation for use in predicting DBPs (i.e., TTHMs) as a function of chlorine demand, KYPIPE was used to allow for the parameterization of a generic regression equation for use in predicting TTHM concentration at each junction node in the water distribution system. The general form of the selected equation is as follows:

$$Y = (a_0 + a_1X^{b1} + a_2X^{b2} + a_3X^{b3} + a_4X^{b4})/ (c_0 + c_1X^{d1} + c_2X^{d2} + c_3X^{d3} + c_4X^{d4}) \quad \text{.....} \quad (5.1)$$

This format provides maximum flexibility for the user in creating their own customized function for DBP formation. For both the Lebanon and Martin County systems, the only coefficients required were a_0, a_1 and b_1 while other coefficients were kept 0 except for C_0, which was kept 1 to ensure non-zero denominator.

Once the associated parameters are specified in the model, the model performs three different sets of calculations. First, the KYPIPE model calls the EPANET and performs an extended period hydraulic simulation of the system. These results are then used to set the boundary conditions for an extended period water quality simulation of the system. These results are then passed back to the KYPIPE which determines the chlorine demand at each junction node by subtracting the chlorine values predicted at each junction node from the initial chlorine concentration at the boundary condition (e.g., water treatment plant). Once

these demands are obtained, KYPIPE uses Eq. 5-1 with appropriate coefficients to predict the TTHM values at each junction node.

5.6 Calibration and Validation of KYPIPE TTHM Model for Lebanon System

In order to achieve the project goals, the developed TTHM models should generate results that best match the water quality results from field observation. For this purpose, model calibration is necessary. As part of calibration, the models initially calibrated for chlorine decay were used to make sure the hydraulic and water quality conditions are accurately matched. The average TTHM results from this model were compared with the field TTHM values used for generating the regression equation (Table 5-6). In this case the calibration data were obtained from quarterly compliance data, while the validation data were obtained from actual field sampling. The plot of the relation between observed and model TTHM results is shown in Figure 5-5.

Table 5-6: Observed and Predicted Average TTHM Calibration Results Using LWW Model

Year	Season	Node	Avg plant chlorine	Avg node chlorine	Chlorine demand	Measured TTHM	Model TTHM
2021	winter	224	1.71	1.61	0.16	0.013	0.011
2021	summer	224	1.55	0.83	0.75	0.072	0.075
2021	winter	667	1.71	1.65	0.12	0.012	0.008
2021	summer	667	1.55	1.15	0.43	0.068	0.045

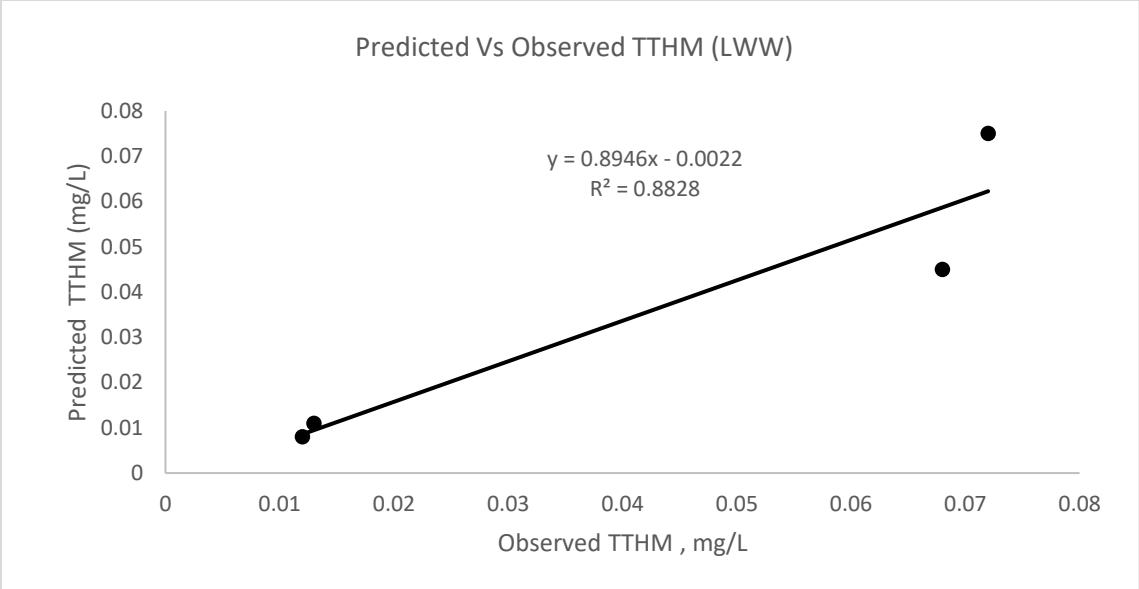

Figure 5-5: Predicted vs Observed TTHM values (LWW Model Calibration)

The calibrated DBP model was then validated using the data collected from the field sampling done on 8th February 2022. The measured plant chlorine and observed TTHM for that day was 1.63 and 0.0073 respectively. The results of the model validation exercise are shown in Table 5-7 and Figure 5-6.

Table 5-7 LWW Model Validation Using Mean Absolute and Root Mean Squared Error Method

Date	Node	Site	Measured TTHM (mg/L)	Predicted TTHM (mg/L)	Absolute Error	Squared Error
Feb-08 2023	WTP	Plant	0.0073			
Feb-08 2023	667	LEB-01	0.0077	0.0150	0.0073	0.000053
Feb-08 2023	224	LEB-02	0.0077	0.0300	0.0223	0.000497
Feb-08 2023	233	LEB-03	0.0074	0.0150	0.0076	0.000058
Feb-08 2023	1369	LEB-04	0.0077	0.0200	0.0123	0.000151
				Mean Absolute Error=	0.0124	
					Root Mean Squared Error=	0.0138

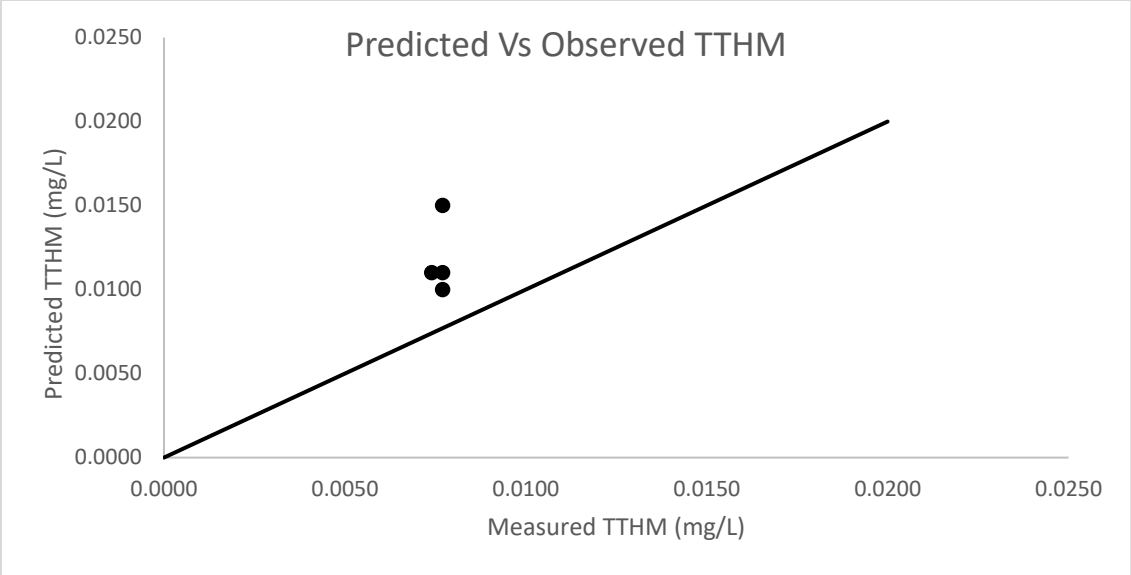

Figure 5-6 LWW TTHM Model Validation Result Using the Data Collected in Feb 2023

The validation result shows that the TTHM values predicted by the model are a little higher than the observed results. The mean absolute error and the root mean squared error values of 0.0124 and 0.0138 are obtained.

5.7 Calibration and Validation of KYPIPE TTHM Model for MCWD System

As with the Lebanon system the developed TTHM model for Martin County should also generate results that best match the quality results from field observation. This again requires model calibration. As part of the calibration, the embedded TTHM model was calibrated to ensure that the observed and predicted TTHM values matched as closely as possible. The average TTHM results predicted using the model are graphically compared with the field TTHM values used for generating the regression equation (Table 5-8). In this case the data used for calibration were obtained from field data in July 2022. A plot of the calibration results is provided in Figure 5-7. It shows that the plot between the predicted and the modeled values of the TTHM aligns with the line at 45° with R^2 value of 0.99.

Table 5-8: Observed and Predicted TTHM Calibration Results Using the MCWD Model

Date	Node KYPIPE	Predicted Free Chlorine (mg/L)	Chlorine demand from predicted Cl	Measured TTHM (mg/L)	Predicted avg TTHM
20-Jul	J-236	0.7	1.16	0.089	0.115
20-Jul	J-790	0.3	1.56	0.123	0.135
20-Jul	J-183	0.3	1.56	0.155	0.149
20-Jul	J-260	0.05	1.81	0.157	0.149

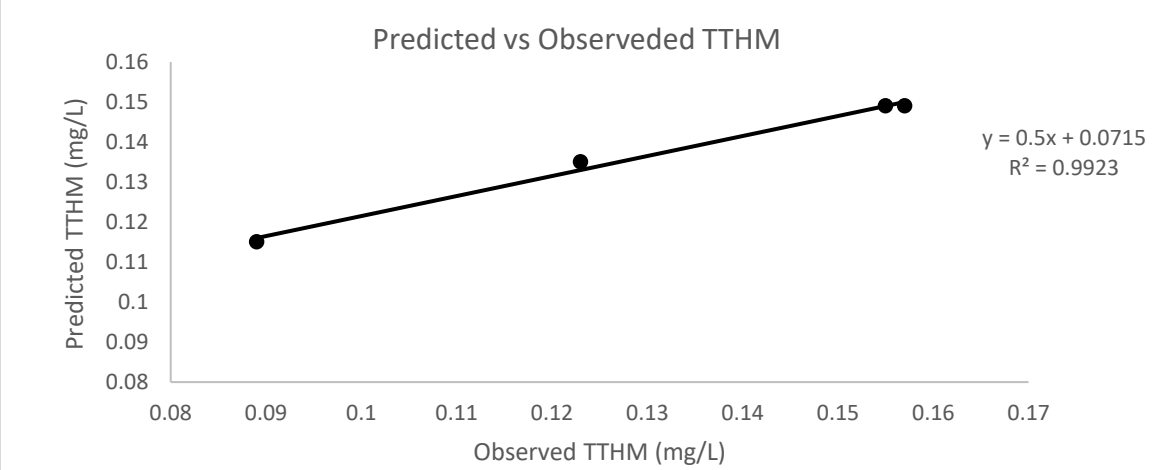

Figure 5-7 Calibration Result of MCWD TTHM Model (July 2022)

The TTHM model was validated using the field results from May. The validation results using Absolute error and root mean squared error is presented in Table 5-9. The plot of the measured and the predicted values of the TTHM are presented in Figure 5-8.

Table 5-9 MCWD Validation Results Using Absolute Error and Root Mean Squared Error

Node KYPIPE	Date	TTHM (mg/L)	Predicted TTHM (mg/L)	Absolute Error	Squared Error
J-236	24-May	0.0505	0.036	0.0145	0.0002
J-790	24-May	0.0506	0.054	0.0034	0.0000
j-239	26-May	0.0739	0.048	0.0259	0.0007
J-803	25-May	0.0783	0.08	0.0017	0.0000
			Mean Absolute Error=	0.0114	—
				Root Mean Squared Error=	0.015

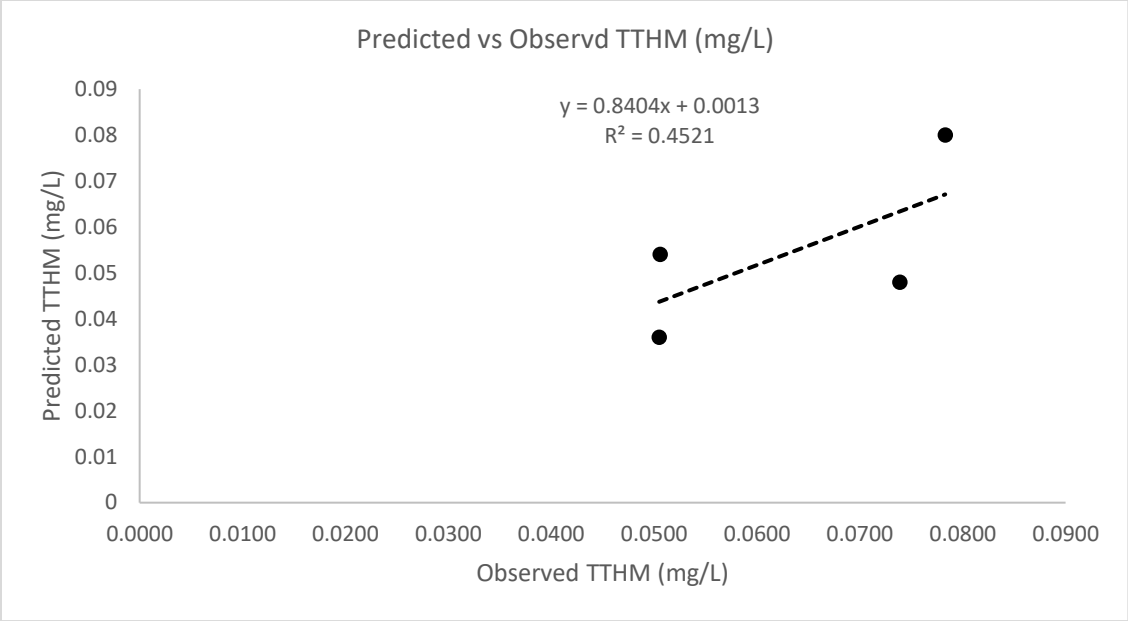

Figure 5-8 MCWD Model Validation Results Using Data from May-2022

The model validation results show that the R squared value of 0.45 for the MCWD model. Also, the mean absolute error and root mean error obtained using the available results are 0.011 and 0.015. While these results were not as good as the calibration results, they were nevertheless deemed acceptable for such a complex distribution system.

5.8 An Investigation of Possible Operational Changes for Lebanon System

Once the associated TTHM models were calibrated and then validated they were then used to examine possible strategies for use in decreasing the DBP values. The Lebanon system is known to have fluctuating demand patterns because it supplies water to other systems. As a result, the impact of demand variation and chlorination in TTHM formation were investigated.

Impact of Changing the Global Demand on LWW TTHM Model

Five representative nodes were selected from the LWW model to study the impact of change in global demand of the system on TTHM concentration. These nodes were

selected based on their varying distance from the treatment plant. In this case, demand changes of 50%, 150% and 200% were considered. The TTHM values obtained by changing the demand from half the original demand to double the original demand are shown in Table 5-10. The plot of variation of the TTHM values with the change in global demand of the system is presented in Figure 5-9.

Table 5-10: TTHM Values Obtained by Changing the LWW Global Demand

Node	TTHM with 50% Demand (mg/L)	TTHM with 100% Demand	TTHM with 150% Demand	TTHM with 200% Demand
N-224	0.0500	0.0150	0.0140	0.0140
N-233	0.0300	0.0110	0.0100	0.0110
N-1369	0.0150	0.0110	0.0110	0.011000
N-667	0.0110	0.0100	0.0100	0.0100
N-299	0.0090	0.0090	0.0080	0.0080

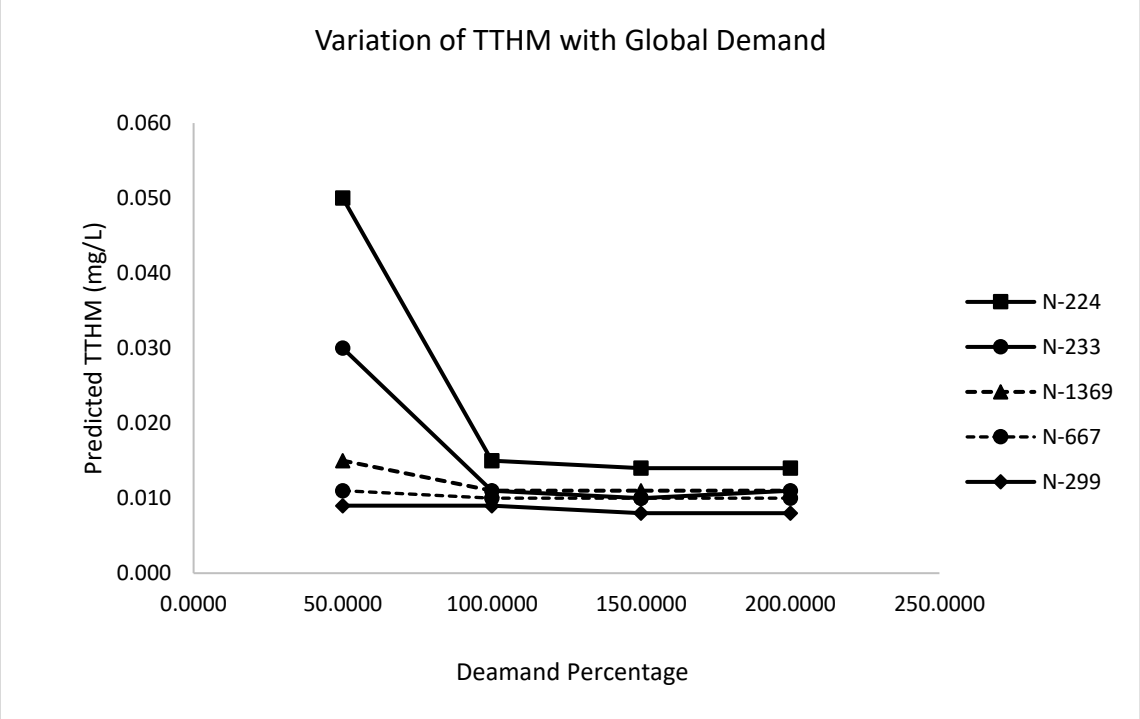

Figure 5-9 TTHM Variation While Changing the LWW Global Demand

The graph plotted by assessing the effect of changing global demand on the TTHM formation in various locations in a distribution system showed that the TTHM

concentration is higher with the lower demand because of higher associated travel times across the system. A sharp increase in TTHM values occurs in LWW model when the total system demand is reduced by 50% while the concentration in the system remains almost constant (although slight decrease) when the global demand is increased.

Impact of Changing the Plant Chlorination on LWW TTHM Model

Utilities are paying a high percentage of their revenue on chlorination of the treated water. They are always seeking an optimum value of chlorination that helps to keep the TTHM values minimum while making sure that the minimum value of chlorine residual is available for disinfection purposes. To evaluate the influence of different levels of chlorination on TTHM formation, the LWW TTHM model was run with chlorination values ranging from 1mg/L to 4 mg/L. The impacts on TTHM concentrations were then studied at five different locations based on their distance from the treatment plant. The TTHM values obtained in these locations are tabulated below in Table 5-11. A plot of variation of the TTHM values with the change in plant chlorination is presented in Figure 5-10.

Table 5-11: The TTHM Values Obtained at Various Nodes of LWW with Various Plant Chlorination

Node	TTHM With 1 (mg/L)	TTHM With 1.63 (mg/L)	TTHM With 2 (mg/L)	TTHM With 3 (mg/L)	TTHM With 4 (mg/L)
N-224	0.013	0.015	0.02	0.025	0.03
N-233	0.010	0.011	0.017	0.018	0.02
N-1369	0.008	0.012	0.012	0.018	0.02
N-667	0.009	0.010	0.011	0.012	0.017
N-299	0.008	0.008	0.009	0.009	0.010

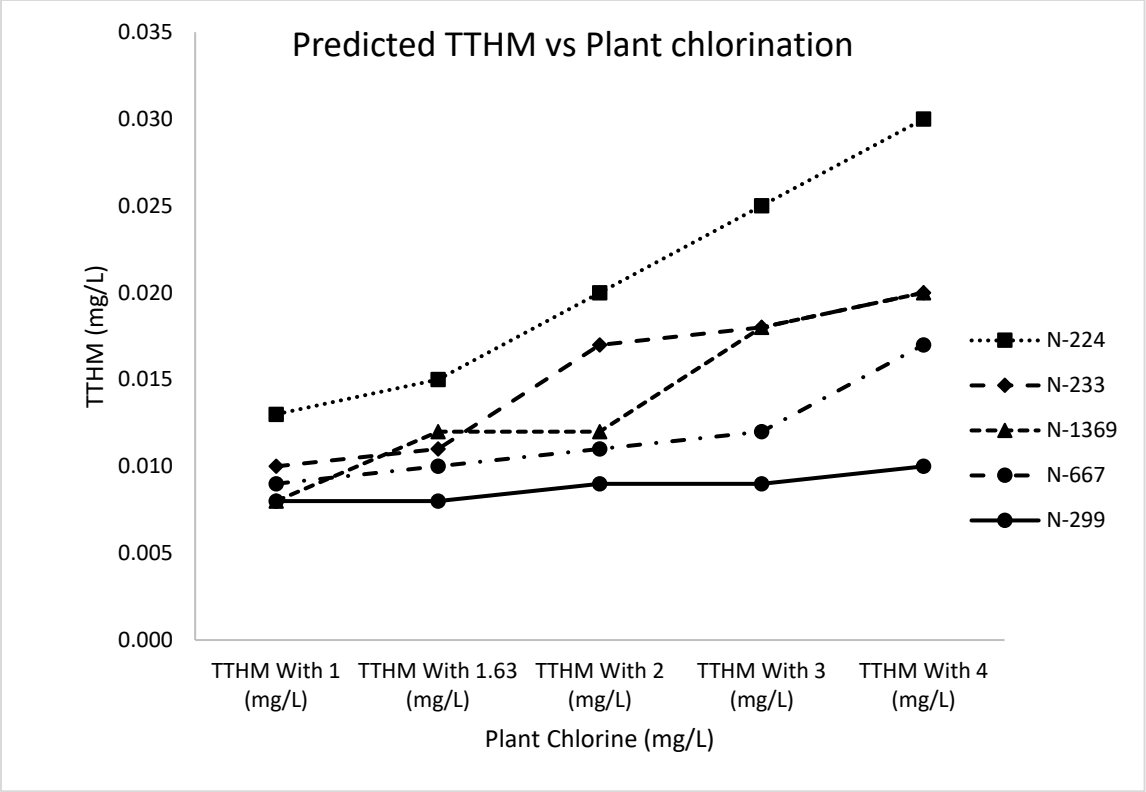

Figure 5-10 TTHM Values Obtained at Various Nodes of LWW with Various Plant Chlorination

This graph clearly indicates that the higher amount of plant chlorination increases the tendency of TTHM formation as more reactant for TTHM formation is available when more chlorine is available in the distribution system. However, as can be seen from the figure, the impact varies by individual node.

5.9 An Investigation of Possible Operational Changes for the MCWD System

As with the LWW system, the sensitivity of TTHM values in the Martin County System to changes in demand or chlorination concentration at the plant were investigated. These investigations are expected to create helpful insights into the system operation for reducing the model TTHM concentrations.

Impact of Changing the Global Demand on MCWD Model

Based on their increasing distance from the treatment plant and initial TTHM values, five representative nodes were selected to study how the TTHM concentrations varied as a function of changes in the global demand of the system. The TTHM concentrations developed in the distribution system obtained by changing the demand from half the original demand to double the original demand are shown in Table 5-12. The plot of variation of the TTHM values with the change in global demand of the system is presented in Figure 5-11.

Table 5-12: TTHM Values Obtained by Changing the Global Demand

S. No.	Node	TTHM with 50% Demand (mg/L)	TTHM with 100% Demand (mg/L)	TTHM with 150% Demand (mg/L)	TTHM with 200% Demand (mg/L)
1	J-236	0.06	0.044	0.034	0.026
2	J-239	0.07	0.055	0.04	0.026
3	J-790	0.084	0.062	0.052	0.042
4	J-714	0.082	0.07	0.058	0.045
5	J-211	0.098	0.094	0.086	0.072

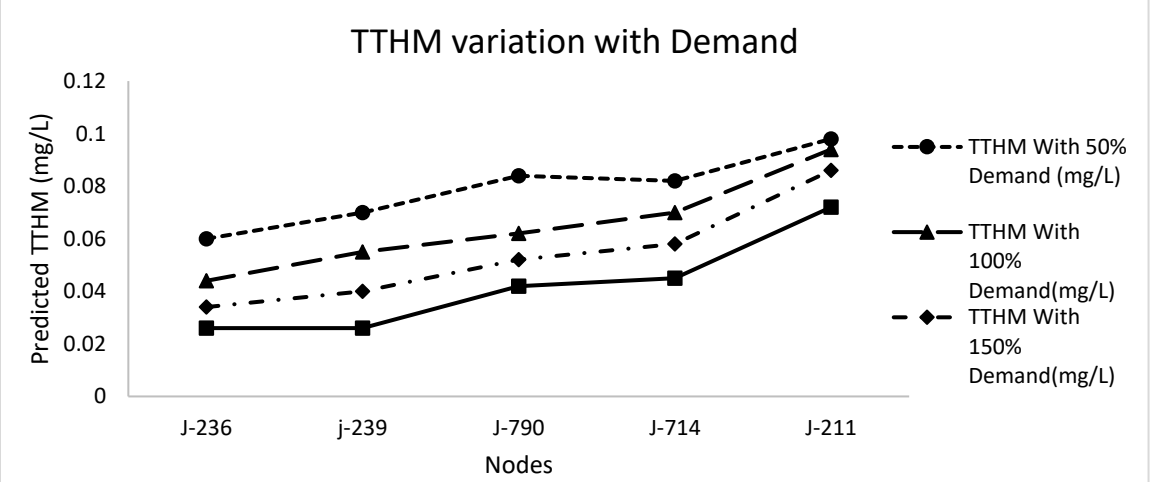

Figure 5-11 TTHM Variation While Changing the MCWD Global Demand

The graph of results showing the impact of changing global demand on the TTHM formation in various locations in a distribution system revealed that the TTHM concentrations are higher with the lower demand as a result of increased travel times. This raises a particular research question with regard to the MCWD system, which currently is experiencing a 70% water loss. What would be the impact on TTHM concentrations if the water loss is reduced or eliminated? In order to investigate this question, the model was re-run with a series of additional demand reductions as shown in Table 5-13 and Figure 5-12.

Table 5-13 TTHM Values Obtained by Changing the Global Demand

S. No.	Node	TTHM with 100% Demand (mg/L) (70% water loss)	TTHM with 60% Demand (mg/L) (50% water loss)	TTHM with 35.3% Demand (mg/L) (15% water loss)	TTHM with 30% Demand (mg/L) (0% water loss)
1	J-668	0.006	0.008	0.009	0.01
2	J-37	0.018	0.026	0.035	0.041
3	J-790	0.062	0.08	0.09	0.091
4	J-714	0.07	0.078	0.087	0.088
5	J-183	0.082	0.093	0.096	0.097
6	J-260	0.094	0.096	0.097	0.097

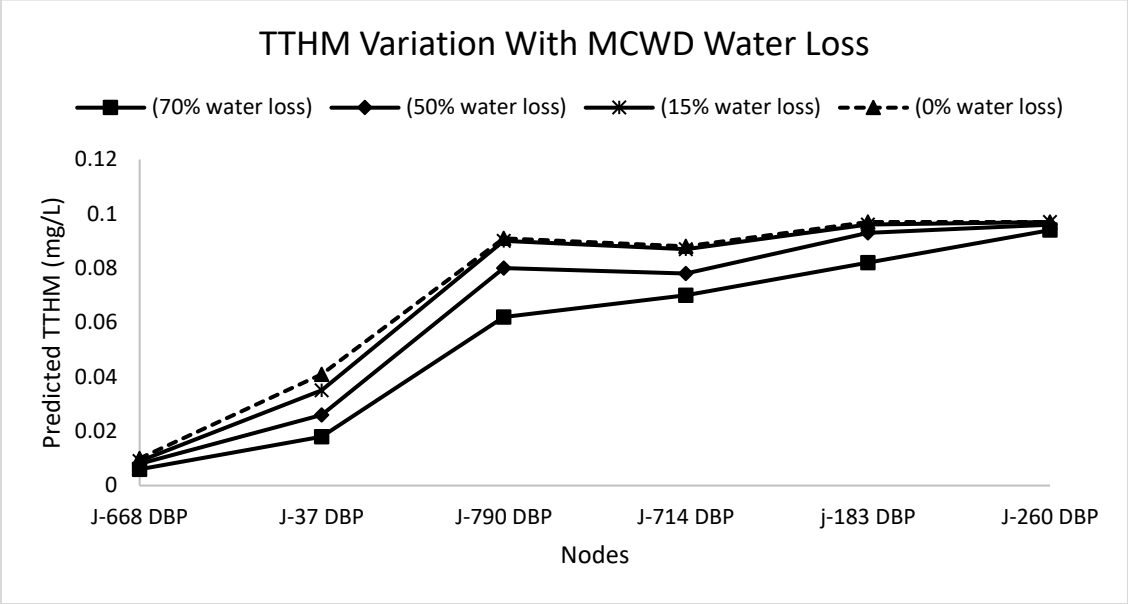

Figure 5-12 TTHM Variation While Changing the MCWD Global Demand

This graph indicates that if demand is significantly lower than the present value the TTHM formation in the distribution system gets worse even if the TTHM formation in the plant is controlled. Once again, this is associated with increased travel times in the pipe network associated with lower system demands.

Impact of Changing the Plant Chlorination on MCWD Model

The variation of TTHM values with the change in plant chlorination from 1mg/L to 4 mg/L were studied at five different locations based on their distance from the treatment plant. The TTHM values obtained at various nodes of MCWD by applying various plant chlorination values are tabulated below in Table 5-14. The plot of variation of the TTHM values with the change in plant chlorination is presented in Figure 5-13.

Table 5-14 TTHM Values Obtained at Various Nodes of MCWD With Different Plant Chlorination

S. No.	Node	TTHM with 1 mg/L	TTHM with 1.87 mg/L*	TTHM with 2 mg/L	TTHM with 3 mg/L Chlorine	TTHM with 4 mg/L chlorine
1	J-668	0.004	0.006	0.007	0.01	0.014
2	J-37	0.01	0.019	0.02	0.03	0.04
3	J-790	0.034	0.063	0.068	0.1	0.135
4	J-183	0.044	0.082	0.087	0.13	0.175
5	J-260	0.051	0.094	0.101	0.152	0.202

*Current chlorine concentration at the treatment plant

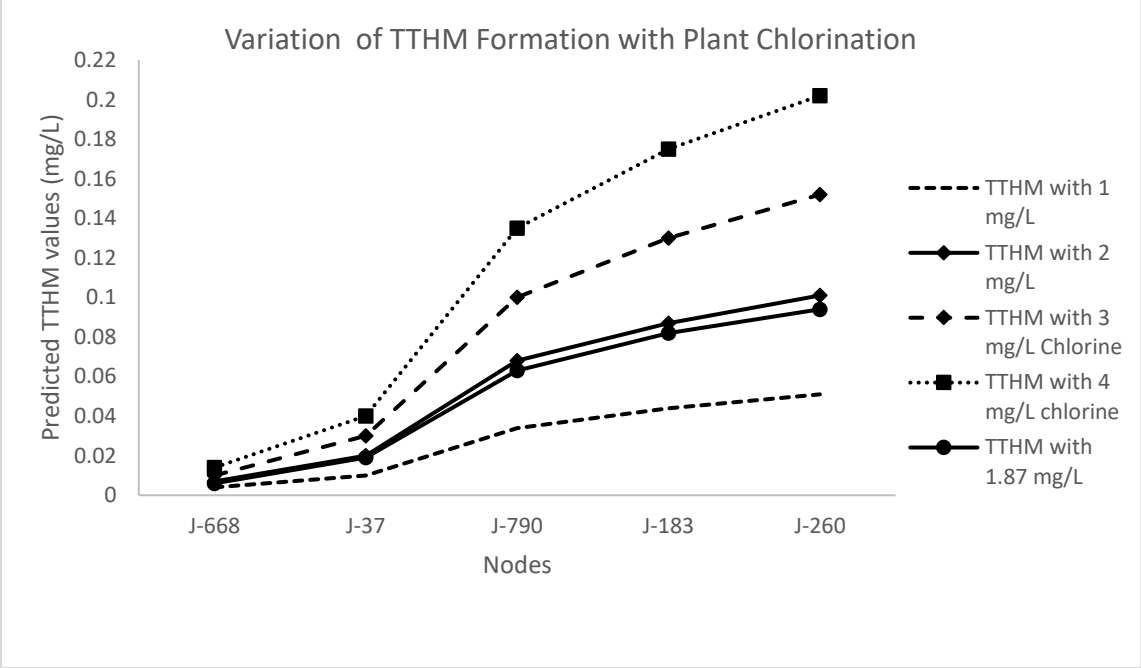

Figure 5-13 Effect of Chlorination in TTHM Formation in Various Locations of MCWD Distribution System

The graph associated with the results of these simulations showed that the TTHM concentrations increased with a higher valued of plant chlorination values. This implies that there will be a maximum plant chlorination value that should not be exceeded if the operators want to limit TTHM concentrations to be below their regulatory limit.

6. DISCUSSION AND CONCLUSIONS

The main objective of this research was to determine if the hydraulic and water quality models can be used for water quality analysis of chlorine decay and TTHM formation at various locations across a water distribution system. This is particularly important because it is not always easy or economical to take multiple field samples and analyze them in the laboratory.

Many software packages such as KYPIPE, Bentley, EPANET, Water CAD etc. are developed for hydraulic modeling of distribution system. Some of these packages can also be used for water quality modelling purposes once we have reliable hydraulic models. In this study, models of two different water distribution systems were created in KYPIPE, a commercial software package for modeling water distribution hydraulics. These models were then calibrated and successfully applied to predict observed water age, chlorine residual values, and TTHM values throughout the distribution system. The validation results for the water quality models were not as good as the calibration results but were considered acceptable for complex distribution systems with limited system operational data.

The calibrated water quality models clearly showed that the water age at the extremities of the distribution system is higher than that at the junctions closer to the treatment plant. These models also clearly indicate that the water age gets much higher in the dead ends where demand is negligible. Also, the fate of chlorine residuals is similar at the extremities as decay takes place over time while travelling from the treatment plant to the distribution node. Based on model results, a preliminary functional relationship

between chlorine residual and water age is developed for each system which can be further studied to predict the chlorine residual as a function of water age.

TTHM regression models based on water age and chlorine decay approach are able to reduce the number of parameters involved in the water quality analysis and make the prediction easier. These developed regression models for distribution system can be imbedded into KYPIPE modelling environment and used in prediction of TTHM concentration at each nook and corner of their distribution system. It can be concluded that the TTHM models which account for the distribution system as an influencing factor in TTHM formation can be useful as a decision-making tool for water quality analysis and regulatory purposes.

Both water age and chlorine demand can be useful in prediction of TTHM in water distribution systems, but their accuracy depends on available data and decency the model calibration. Based on data available for two systems, it appears that chlorine demand is better predictor of TTHM formation than water age, since water age may not be quite as precise since it is being predicted by a simulation model that may or may not accurately reflect the travel times in the system. However, chlorine demand requires the collection of additional field data from the system. In this study, the chlorine demand acted as slightly better predictor for the TTHM prediction for Lebanon system while the water age produced a higher coefficient of determination for Martin County system. Thus, it could be argued in some cases (like MCWD), water age might be sufficient to predict relative values of TTHM concentrations or more likely help guide in the selection of possible monitoring locations for subsequent TTHM field monitoring. This suggests that the choice of the appropriate independent variable (i.e., chlorine demand or water age) may be system

specific and thus may require some preliminary data analysis before one can decide on an appropriate modeling approach.

From the investigation of possible operational changes in these two systems, it can be concluded that the change in demand and plant chlorination can have significant impact in the chlorine residual and TTHM formation in the system. The reduction in system demand after controlling the water loss can cause significant decrease in the chlorine residuals in the distribution system as the flow velocity decreases and the time to reach the consumers increases allowing enough time for chlorine decay. Similarly, reduction in system demand after controlling the water loss can cause substantial increase in the TTHM formation in the distribution system as the flow velocity decreases and the time to reach the consumers increases allowing enough time for TTHM formation.

Application of higher amounts of chlorine in the plant can be another option for utilities to increase the chlorine residuals at the consumer nodes but this is not always economically feasible and is restricted to remain below the regulatory limit of 4 mg/L. Also, the study revealed that for various junctions in MCWD system, chlorine values cannot be maintained above the regulatory limits, even when the chlorine concentration at the plant is raised to maximum level. It can be concluded from these operational studies that the chlorine residuals and TTHM formation don’t merely depend on the chlorine application at the plant but also on the hydraulics and demand distribution of the system. It can also be concluded that many rural systems like the MCWD, which currently experience large percentages of water loss, may face additional water quality challenges if the water loss is significantly reduced to acceptable levels (e.g., 15%). As a result, water

quality models can be used to help managers develop potential management strategies (e.g., main flushing) in addressing such challenges.

7. RECOMMENDATIONS

7.1 Engineering Significance

The water distribution systems built since the early 1900s are mostly designed to satisfy the quantitative need of drinking water, without a strict regard to water quality degradations in the distribution system. This research aimed to look at the water quality behavior of two such systems: 1) a more urban and efficiently managed system located in a relative flat topography, and 2) a more rural and less efficiently managed system located in a mountainous topography. This research clearly indicates that if sufficient system and operational data are available, the water quality performance of such systems can be effectively modeled and used to both inform and guide managers regarding existing problems and potential future operations.

7.2 Limitations of this Approach

Although, this research has tried to cover a wide spectrum of chlorine decay and TTHM formation modelling, there remain many other unknown variables that could impact both chlorine residuals and the formation of TTHM. First, the distribution system data available in the WRIS portal is suspected to have some differences with the actual field configuration. Moreover, the connections to homes, smaller sized end distributions and some hollows are not considered for modeling. Second, this research has not been able to account for various chemical interferences in the water quality of a distribution system that affect the field data including ammonia interference with the chlorine. Also, the demand distribution is based on automatic demand distribution function of KYPIPE. The results thus generated can be suspected to have discrepancies as the field measured and model predicted results don’t perfectly match. There are various uncertainties associated with the

water distribution system. For example, the water traveling from treatment plant to the end nods of the distribution system can take several days, so the assumption that the chlorine levels leaving the plant van be used as a baseline in calculating the chlorine demand at a distinct junction node may not always be accurate.

Only two distribution systems were studied and thus, the results obtained are specific for those systems and specific operational conditions. For example, while chlorine demand was a better predictor for the LWW system, water age appears to be a better predictor for the MCWD. Secondly, while the LWW system experiences minimal water loss, the MCWD experiences greater than 70%, etc. As a result, no inference can be made about other systems and operating conditions based only on these data and results. It requires further research and adaptation to be able to match new operating conditions and systems.

7.3 Need for Future Research

There is a great need of additional research and refinement of models for predicting the water quality data more reliably. The preliminary functional relationships between chlorine residual and water age, developed based on chlorine and water age model results for each system, need further research to be able to reliably predict the chlorine residual as a function of water age. The chlorine demand and water age based approach of TTHM calculation models developed for the two systems need further study and validation to be able to predict TTHM values precisely. Moreover, there are other sets of disinfection by products that need to be studied along with TTHM to make reliable prediction of all relevant DBPs.

7.4 Recommendations

Only two utilities were studied for two seasons of the year so, this data is limited to make any critical decision regarding the harmful DBPs. It is recommended to have further study and analysis with more field data over longer periods and with more utilities. Moreover, the only DBP taken into consideration was total trihalomethanes. So, it is recommended to carry the analysis on other DBPs (e.g., HAAs) also be explored. This research has highlighted a potential problem that might be faced by those rural systems that are currently experiencing high levels of water loss. Specifically, as water loss is reduced it can be expected that chlorine residuals will decrease and TTHMs will increase. Additional research is needed to develop potential management strategies to address this issue. Finally, given the potential correlation of water age to chlorine residuals and water age, it may be possible to develop a general screening tool based purely on GIS functionality that could be applied to all water systems in Kentucky to help either identify those systems which might be susceptible to either chlorine residuals violations or TTHM violations. Alternatively, such a tool could be used to guide system managers in identifying critical sampling locations in their systems for use in monitoring compliance for both parameters.

APPENDICES

APPENDIX A. The MOR Dataset Used in The Research

Table A 1: The LWW MOR Chlorine Dataset Used in The Research

Site ID	Dec 2020	Jan 2021	Feb 2021	Jun 2021	July 2021	Aug 2021
3	1.66	1.49	1.39	0.87	1.09	0.595
4	1.66	1.43	1.24	1.17	1.15	0.706
7	1.4	1.52	1.18	1.42	0.79	0.765
53	1.575	1.48	1.34	1.1	1.75	0.84
62	1.63	1.42	1.42	—	—	—
106	1.436	1.56	1.51	1.18	—	0.44
107	1.5475	1.57	1.84	1.24	0.9	1.3
108	1.5475	1.48	1.6	1.28	1.27	1.29
111	1.6	1.67	1.87	1.52	0.955	1.24
112	1.57	1.73	—	1.09	1.135	0.91
117	1.875	1.855	1.58	—	0.81	0.905
118	1.94	1.83	1.87	—	1.01	1.365
119	1.84	1.45	2.02	—	0.83	1.4
120	1.64	1.71	1.49	—	0.64	1.03
2CH	1.524	1.43	1.37	1.035	0.93	1.06
3MR	1.456	1.53	1.56	1.1	0.785	1.18
3	1.66	1.49	1.39	0.87	1.09	0.595

Table A 2: Lebanon TTHM Compliance Data Used in LWW Model

Date	Radio Station Rd	Farmington Dr	Plant
1/24/2020	0.025	0.017	0.006
4/22/2020	0.039	0.031	0.013
7/30/2020	0.073	0.076	0.02
10/28/2020	0.047	0.037	0.013
1/21/2021	0.013	0.012	0.003
4/22/2021	0.028	0.026	0.008
7/29/2021	0.072	0.068	0.024
10/27/2021	0.032	0.031	0.012

Table A 3: The MCWD MOR Dataset Used in The Research

Date	Location	Free Chlorine
08/04/2022	Zip Zone Warfield (37.844053, -82.417514)	1.08
08/04/2022	Cardinal Country Store (37.842983, -82.543724)	0.87
08/04/2022	75 Skyline Ln Inez, Ky 41224	0.75
08/04/2022	Zip Zone Lovely	0.97
08/04/2022	AWR	0.94
10/20/2022	Zip Zone Lovely (37.829807, -82.402000)	0.96
10/20/2022	Zip Zone Warfield (37.844053, -82.417514)	1.17
10/20/2022	Zip Zone Blacklog (37.847318, -82.501761)	1.15
10/20/2022	Cardinal Country Store (37.842983, -82.543724)	1.14
10/20/2022	155 E Main St, Inez, KY 41224	1.34

APPENDIX B. Tank Level Data Used in Calibration and RMSE Calculation

TABLE B 1: Lebanon System Tank Level Record Used for Summer Model Calibration

Date	TopHour	Day	Hour	Springfield Rd Tank (Ft)	Old Calvary Rd Tank (Ft)
7/11/2021	9	1-Sun	9	22.7	52.9
7/11/2021	10	1-Sun	10	21.2	54.5
7/11/2021	11	1-Sun	11	20.5	56.1
7/11/2021	12	1-Sun	12	21.3	57.1
7/11/2021	13	1-Sun	13	21.7	56.6
7/11/2021	14	1-Sun	14	21.1	55.8
7/11/2021	15	1-Sun	15	20.4	55.2
7/11/2021	16	1-Sun	16	21	54.5
7/11/2021	17	1-Sun	17	21.4	54
7/11/2021	18	1-Sun	18	21.8	54
7/11/2021	19	1-Sun	19	21.6	54.5
7/11/2021	20	1-Sun	20	21	55.1
7/11/2021	21	1-Sun	21	20.5	55.7
7/11/2021	22	1-Sun	22	20.4	56.3
7/12/2021	7	2-Mon	31	17.2	50.5
7/12/2021	8	2-Mon	32	19.6	52.3
7/12/2021	9	2-Mon	33	19	53
7/12/2021	10	2-Mon	34	18	53.3
7/12/2021	11	2-Mon	35	17.2	53.5
7/12/2021	12	2-Mon	36	17.2	54.1
7/12/2021	13	2-Mon	37	16.7	54.5
7/12/2021	14	2-Mon	38	17.8	54.8
7/12/2021	15	2-Mon	39	18.2	55.5
7/12/2021	16	2-Mon	40	19.1	56.8
7/12/2021	17	2-Mon	41	19.4	57.9
7/12/2021	18	2-Mon	42	19.3	58.7
7/12/2021	19	2-Mon	43	18.9	58.9
7/12/2021	20	2-Mon	44	18.5	59
7/12/2021	21	2-Mon	45	19	59.2
7/12/2021	22	2-Mon	46	19.7	59.8

TABLE B 2 Lebanon System Tank Level Record Used for Winter Model Calibration

Date	TopHour	Day	Hours	Springfield Rd Tank (T-2)	Old Calvary Rd Tank (T-1)
12/21/2021	7	3-Tue	55	21.8	45.4
12/21/2021	8	3-Tue	56	21.1	49.1
12/21/2021	9	3-Tue	57	22.4	52
12/21/2021	10	3-Tue	58	22.5	54.2
12/21/2021	11	3-Tue	59	20.4	57.1
12/21/2021	12	3-Tue	60	19.5	57.9
12/21/2021	13	3-Tue	61	18.5	58.6
12/21/2021	14	3-Tue	62	17.4	59.2
12/21/2021	15	3-Tue	63	16.6	59.8
12/21/2021	16	3-Tue	64	15.6	60.7
12/21/2021	17	3-Tue	65	15.4	61
12/21/2021	18	3-Tue	66	15.5	62.2
12/21/2021	19	3-Tue	67	15.5	63.3
12/21/2021	20	3-Tue	68	16.6	65.4
12/21/2021	21	3-Tue	69	16.9	66.3
12/22/2021	7	4-Wed	79	20.8	50
12/22/2021	8	4-Wed	80	22.8	52.4
12/22/2021	9	4-Wed	81	20.3	55.6
12/22/2021	10	4-Wed	82	20	57.2
12/22/2021	11	4-Wed	83	18.9	57.7
12/22/2021	12	4-Wed	84	18.2	58.3
12/22/2021	13	4-Wed	85	17.7	58.6
12/22/2021	14	4-Wed	86	17.7	59
12/22/2021	15	4-Wed	87	18.2	60.1
12/22/2021	16	4-Wed	88	18.3	60.6
12/22/2021	17	4-Wed	89	19.3	61.4
12/22/2021	18	4-Wed	90	20.5	62.3
12/22/2021	19	4-Wed	91	21.7	63.8
12/22/2021	20	4-Wed	92	21.3	64.9
12/22/2021	21	4-Wed	93	20.9	66.2

TABLE B 3 MCWD System Tank Level Record Used for Model Calibration

Date	Time	Buck Creek T-1	Rock caste T-2	Big elk T-4	Turkey T-8
5/24/2022	0	63.8	20.70	47.50	22.90
5/24/2022	2	65.3	22.60	47.20	20.50
5/24/2022	4	67.8	24.80	46.60	25.80
5/24/2022	6	69.6	26.40	46.20	23.30
5/24/2022	8	69	25.50	45.60	20.70
5/24/2022	10	67.1	23.10	44.80	25.00
5/24/2022	12	64.4	20.40	43.90	30.20
5/24/2022	14	61.6	17.60	43.60	26.40
5/24/2022	16	63	19.00	43.60	22.60
5/24/2022	18	64.7	20.60	43.60	27.70
5/24/2022	20	65.4	21.40	43.60	29.80
5/24/2022	24	63.8	20.70	47.50	22.90
5/25/2022	0	68	24.30	43.60	20.30
5/25/2022	2	69.8	26.30	37.00	24.70
5/25/2022	4	69.4	25.60	36.70	29.70
5/25/2022	6	67.3	23.20	36.20	26.50
5/25/2022	8	64.8	21.30	39.90	20.00
5/25/2022	10	60.7	18.70	41.60	24.40
5/25/2022	12	58	18.10	41.60	28.70
5/25/2022	14	57.3	18.90	44.20	31.60
5/25/2022	16	57.7	19.90	41.80	21.10
5/25/2022	18	59.3	20.60	41.10	23.20
5/25/2022	20	62.5	22.50	38.50	31.40

APPENDIX C. Data Collected from Field Sampling for Both Systems

TABLE C 1: The TTHM Data Collected from Field Sampling for LWW System (8th Feb 2023)

Sample ID	Dibromo-chloromethane	Bromodi-chloromethane	Bromoform	Chloroform	TTHM (mg/L)
L-01	0.0000	0.0076	0.0000	0.0000	0.0076
L-01	0.0000	0.0078	0.0000	0.0000	0.0078
L-02	0.0000	0.0078	0.0000	0.0000	0.0078
L-02	0.0000	0.0077	0.0000	0.0000	0.0077
L-03	0.0000	0.0074	0.0000	0.0000	0.0074
L-04	0.0000	0.0076	0.0000	0.0000	0.0076
L-04	0.0000	0.0078	0.0000	0.0000	0.0078
PLANT 1	0.0000	0.0073	0.0000	0.0000	0.0073
PLANT 2	0.0000	0.0073	0.0000	0.0000	0.0073
BLANK	0.0000	0.0000	0.0000	0.0000	0.0000

TABLE C 2: The TTHM Data Collected from Field Sampling for MCWD System (24th Oct 2022)

Sample ID	Bromodi-chloromethane	Bromoform	Chloroform	Dibromo-chloromethane	TTHM
MC1	0.0457	0.0069	0.0689	0.0234	0.1449
MC2	0.0404	0.0066	0.0646	0.0207	0.1323
MC10	0.0389	0.0064	0.0663	0.0195	0.1312
PLANT	0.0212	0.0064	0.0263	0.0145	0.0684

TABLE C 3 The Chlorine Data Collected from Field Sampling for MCWD System (24th Oct 2022)

Site ID	Date	Time	Measured Total Chlorine (mg/L)	Measured Free Chlorine (mg/L)
WTP-treated	10/24/2022	10:56 AM	—	1.87
M01	10/24/2022	11:56 AM	0.98	0.86
M02	10/24/2022	1:45 PM	1.08	0.77
M05	10/24/2022	5:25 PM	0.38	0.13
M10	10/24/2022	4:00 PM	0.91	0.8

TABLE C 4 :Chlorine Data Collected from Field Sampling for MCWD System (20th July 2022)

Site ID	Date	Time	Total Chlorine (mg/L)	Free Chlorine (mg/L)
M01	07/20/2022	4:20 PM	0.91	0.82
M02	07/20/2022	3:40 PM	0.43	0.28
M05	07/20/2022	11:50 AM	0.08	0.02
M10	07/20/2022	12:51 PM	0.15	0.04*
WTP-treated	07/20/2022	5:00 PM	1.98	1.86

*Meat house pump not in operation.

TABLE C 5 :The TTHM Data Collected from Field Sampling for MCWD System (20th July 2022)

Sample ID	Bromodichloro-methane	Bromoform	Chloroform	Dibromo-chloromethane	TTHM (mg/L)
M-1-1	0.013	<0.001	0.076	<0.001	0.089
M-1-1	0.021	<0.001	0.113	0.001	0.135
M-2-1	0.018	<0.001	0.104	0.001	0.123
M-5-1	0.024	<0.001	0.147	0.002	0.172
M-5-2	0.019	<0.001	0.118	0.001	0.138
M-10-1	0.022	<0.001	0.134	0.001	0.157
WTP-R2W	<0.001	<0.001	<0.005	<0.001	0.000
WTP-Finished	0.010	<0.001	0.043	<0.001	0.054
Blank	<0.001	<0.001	<0.005	<0.001	0.000

TABLE C 6 :The Chlorine Data Collected from Field Sampling for MCWD System (May 2022)

Site ID	Date	Time	Temp (°C)	Conductivity (µS)	pH	Total Chlorine (mg/L)	Free Chlorine (mg/L)
M01	05/24/2022	6:30 PM	16.6	146	6.44	2.1	1.2
M02	05/24/2022	7:10 PM	16.4	138	6.44	1.5	1.2
M03	05/24/2022	3:20 PM	17.52	138	6.15	0.8	0.7
M04	05/24/2022	2:50 PM	19	137	6.08	1.2	1
M05	05/24/2022	9:00 PM	—	—	—	0.8	0.9
M06	05/24/2022	9:10 PM	19.5	555	7.96	0.4	0.4
M07	05/25/2022	9:25 AM	17.1	136	6.16	1.2	1.2
M08	05/25/2022	—	19	137	6.33	1.8	1.2
M09	05/25/2022	12:00 PM	16.94	140	6.09	1.5	1.8
M09B	05/25/2022	11:45 AM	15.42	736	7.35	0.7	
M10	05/25/2022	1:00 PM	19.65	139	6.07	1.1	0.7
M11	05/25/2022	7:40 AM	17.42	136	6.31	1.5	1.3

TABLE C 7 :The TTHM Data Collected from Field Sampling for MCWD System (May 2022)

Sample ID	Bromodichloro-methane (mg/L)	Bromoform (mg/L)	Chloroform (mg/L)	Dibromo-chloromethane (mg/L)	TTHM (mg/L)
M01-1	0.009	<0.001	0.0382	0.0033	0.0505
M02-1	0.0092	<0.001	0.0387	0.0033	0.0512
M02-2	0.0091	<0.001	0.0376	0.0033	0.05
M03-1	0.0096	<0.001	0.053	0.0034	0.066
M03-2	0.0093	<0.001	0.0504	0.0034	0.0631
M04-1	0.0095	<0.001	0.0476	0.0034	0.0605
M04-2	0.0099	<0.001	0.0511	0.0034	0.0644
M05-1	0.0104	<0.001	0.0601	0.0034	0.0739
M07-1	0.009	<0.001	0.0395	0.0033	0.0518
M07-2	0.009	<0.001	0.04	0.0033	0.0523
M08-1	0.0088	<0.001	0.0369	0.0033	0.049
M08-2	0.009	<0.001	0.0382	0.0033	0.0505
M09-1	0.0101	<0.001	0.0572	0.0034	0.0707
M09-2	0.0098	<0.001	0.0541	0.0034	0.0673
M10-1	0.0112	<0.001	0.0636	0.0035	0.0783
M11-1	0.0088	<0.001	0.0348	0.0033	0.0469

APPENDIX D. Standard Operating Procedures for Collecting the DBP Samples and Measuring Chlorine Concentrations

**SOP for Hydrant sampling and Tap Water Chlorine Residuals Measurement

Purpose: On site determination of total chlorine, and free chlorine using the Hach or Hanna pocket colorimeter.

Materials:

i. Powder free gloves
ii. HACH/ Hanna pocket colorimeter kit (pocket colorimeter, total chlorine reagent packets, free chlorine packets pillows, plastic chlorine vials)
iii. Safety glasses
iv. Timer (or smart phone)
v. Fire hydrant wrench and tools for operating fire hydrant

Safety: Wear safety glasses and gloves. Do not eat, drink, or smoke while using these chemicals. Chlorine (DPD) reagents can cause serious eye irritation so, be careful not to inhale the powder. If any chemicals get on your skin or eyes, flush with plenty of water. Be sure to remove contact lenses. If irritation occurs, seek medical attention. If chemicals contaminate the clothes, remove and wash before reuse.

Chemical Disposal- These reagents can be flushed down the sink with plenty of water in the amounts used for measurement. Return unused reagents to the lab.

Total and free Chlorine Measurement Procedure:

i. Rinse a chlorine sample cell with tap water three times and fill to the 5 mL mark and place the cap on the cell. Clean the sample cell with a kimwipe, place in the

colorimeter with the triangle pointing away from the keypad, place the cover on the colorimeter and press the zero button. The display should read 0.0.

ii. For measuring free chlorine remove the sample cell and add one free chlorine reagent. Clean the sample cell with a kimwipe and place the sample cell in the meter with the triangle pointing away from the keypad, put the cover on, and press the read button. The free chlorine concentration will be displayed within 60 seconds. Record it on the data sheet.

iii. For measuring total chlorine remove the sample cell and add one total chlorine reagent. Put the lid on the sample cell for 20 seconds to dissolve the reagent. (Note: it will not all necessarily dissolve, and this is normal and expected.) Clean the sample cell with a kimwipe. Place the sample cell in the meter with the triangle pointing away from the keypad and wait for at least three minutes to six minutes to press the read button. The total chlorine concentration will be displayed. Record it on the data sheet. Note that you will be using a total chlorine reagent packet instead of a free chlorine reagent packet.

iv. Periodically check the meters for accuracy using a total chlorine standard reference material and chlorine free water.

Total and Free Chlorine Measurement Precautions for Future:

i. Both Hanna and Hach chlorimeter were used in this research but it is better to always use same instrument for higher consistency.

ii. There can be some interfering substances such as bromine, iodine or manganese in the water that can alter the chlorine results. These interferences should be compensated to get a reliable chlorine value.

iii. The result can also be affected by acidity or alkalinity of water that does not allow full color development or color may fade instantly. Correction should be applied to get the results free from interference.

iv. Chlorine DPD method is not sufficient to get a reliable result when ammonia is present in the water.

**SOP for Tap Water Sampling for Volatile Disinfection Byproducts (TTHM)

Purpose: Collection of tap water for analysis of trihalomethanes by U.S. EPA method 551.1.

Materials:

i. Powder free gloves

ii. New, clean plastic bags

iii. 50 mL polypropylene centrifuge tubes

iv. 40 mL glass VOC sampling vials containing preservative and buffer

v. 40 mL glass VOC vials containing ultrapure water (field blank)

vi. Cooler

vii. Ice packs

viii. Safety glasses

Safety- Wear safety glasses and gloves. Do not eat, drink, or smoke while using these chemicals. If any chemicals get on your skin or eyes, flush with plenty of water. Be sure to remove contact lenses. If clothing becomes contaminated, remove and wash before reuse. If irritation occurs, seek medical attention.

DBP sample collection Procedure:

i. Be sure there are no chlorine/bleach containing cleaning products near the tap to be sampled. Make all preparations first including setting out all materials (sample containers, blanks, etc.) and getting the water flowing and flush until a stable temperature is reached.

ii. Record the temperature on the data sheet. Reduce flow to a trickle (about a pencil thickness). At this point, put on a new pair of powder free nitrile gloves and do not touch anything except the sample containers that have been set out. This includes the faucet handles, outside of plastic bags, pens, paper, etc. Also, do not touch the inside of the sample container or cap or place the cap face down on the counter.

iii. With the flow at a trickle, fill two 40 mL VOC vials, pre-preserved (containing phosphate buffer and ammonium chloride dechlorinating agent). Do not over fill the vial as the buffer and dechlorinating agent will become too dilute. If the vial spills over more than a few drops, pour the sample out and get a new vial. Fill the vial just to the top and then fill the cap with water. Add a few drops to the vial from the cap until the water mounds at the top of the vial due to surface tension. Pour the rest of the water out of the cap and place the cap on the vial carefully.

iv. Invert the vial and check for any air bubbles. If any bubbles are present, open the vial and add a few more drops of water using the cap until no more air bubbles are present.

v. Once every five sample collections, carefully open the cap to the 40 mL field blank VOC vial containing ultrapure water. Leave the cap off for 30-60

seconds and replace the cap. Check for air bubbles.

vi. Samples should be labelled, placed in a clean plastic bag, and either put directly into a refrigerator or kept on ice or ice packs in a cooler for transport. Return sample to the lab within 14 days of collection

TTHM Sampling Precautions for Future:

i. Duplicates should also be collected for each site. This will ensure more reliability of the result obtained.

ii. The pH value of the collected sample should lie in the range of 4.5 and 5.5.

*** SOP for measuring free and total chlorine and the TTHM were obtained from Dr. Jason Unrine, Director at Kentucky Water Resources Research Institute.*

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