

**KWAME NKURUMAH UNIVERSITY OF SCIENCE AND TECHNOLOGY**

**NUMERICAL DETERMINATION OF THE PORTABILITY OF TREATED  
WATER USING ORDINARY DIFFERENTIAL EQUATIONS  
A CASE STUDY IN VEA- GOWREA WATER TREATMENT PLANT**

**KNUST**

**BY**

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the degree of**

**MASTER OF SCIENCE  
INDUSTRIAL MATHEMATICS**

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**[June, 2013]**

## CERTIFICATION

I hereby declare that this submission is my own work towards the MSc and that, to the best of my knowledge. It contains no material previously published by another person or material which has been accepted for the award of any degree of the university, except where the acknowledgement has been made in the text.

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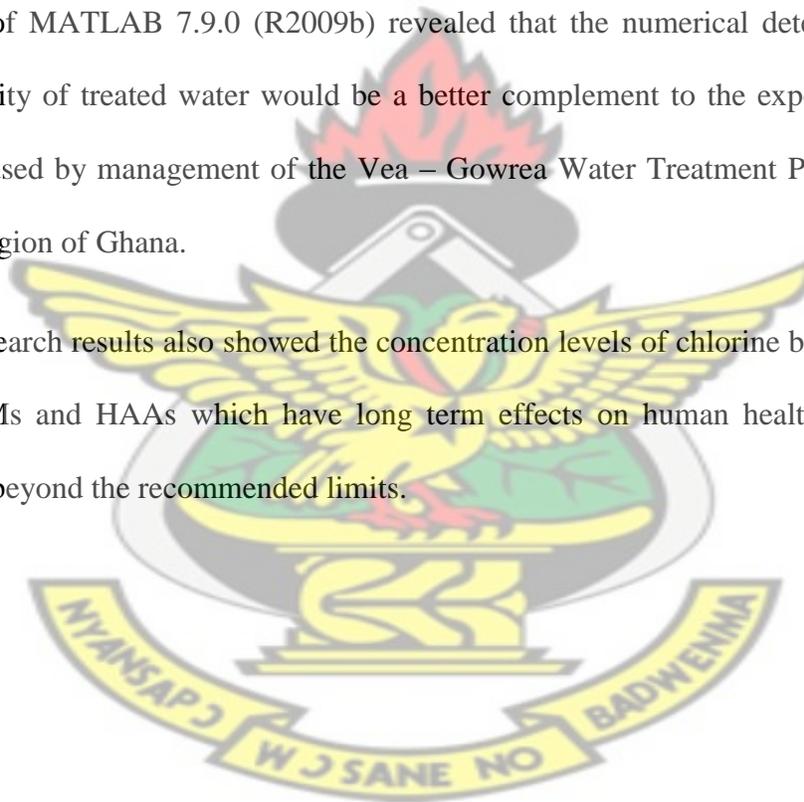
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## ABSTRACT

The problem of the Veia – Gowrea Water Treatment Plant was to develop a mathematical model of the flow of chlorine from the chlorine chamber to the clearwell, to numerically determine the concentration levels of chlorine of the treated water at any given moment so as to help minimize the number of experiments carryout every 2hours by management to ensure water portability.

Runge – Kutta second order numerical solution method to an ODE model using ode23 solver of MATLAB 7.9.0 (R2009b) revealed that the numerical determination of the portability of treated water would be a better complement to the experimental method solely used by management of the Veia – Gowrea Water Treatment Plant of the Upper East Region of Ghana.

The research results also showed the concentration levels of chlorine by – products such as THMs and HAAs which have long term effects on human health when found in excess beyond the recommended limits.



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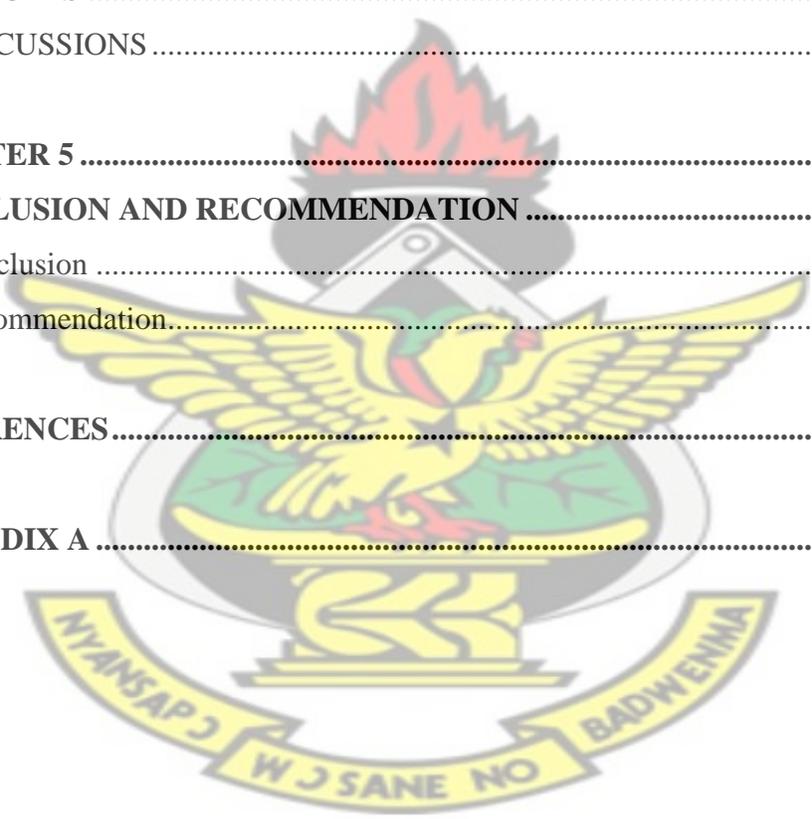
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## LIST OF ABBREVIATIONS

ODE – Ordinary Differential Equation

THMS – Trihalomethanes

HAAS – Halo – acetic acids

EPA – Environmental Impact Assessment

WHO – World Health Organization

SWDA – Safe Water Drinking Act

SDWF – Safe Drinking Water Foundation

AWWA – America Water Works Association

EPA – Environmental Impact Assessment

IARC – International Agency for Research on cancer

AWWARF – America Water Works Association Research Foundation

SWS – Sewage Water System



## DEDICATION

I dedicate this work to my parents Mr. and Mrs. Dominic Doabil, my brothers; Joseph, Padre Pio and Alphonsus for their love and support they gave me during the writing of this thesis.

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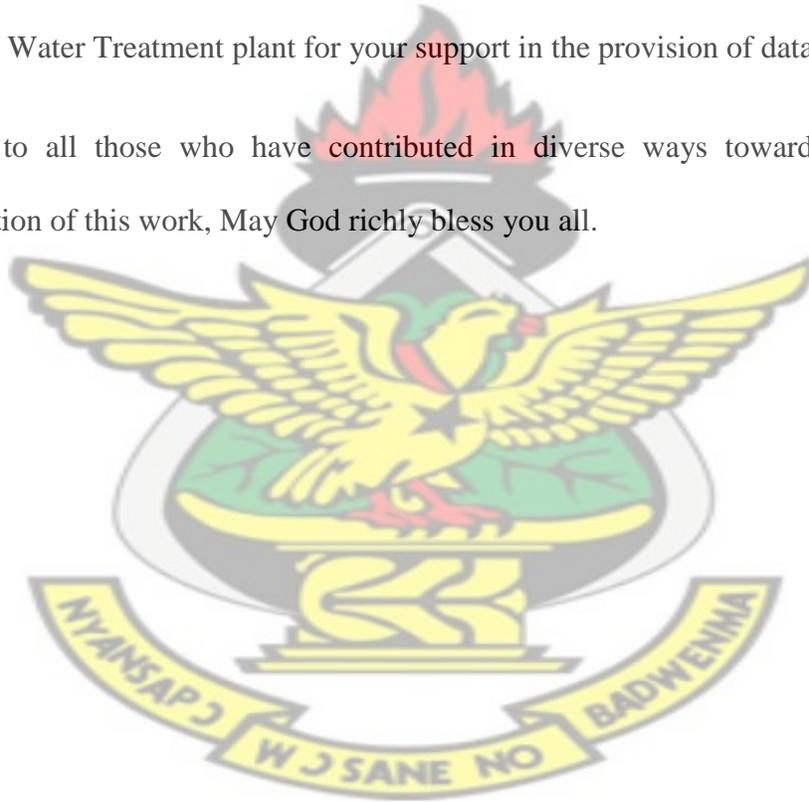
## ACKNOWLEDGEMENT

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# CHAPTER 1

## INTRODUCTION

This chapter consists of background, problem statement, objectives, methodology, justification and organization of the study.

### 1.0 Introduction

The need to provide sanitation for drinking water and hygiene remains a huge challenge today in developing countries as 1.1 billion people around the world do not have access to safe water and 2.6 billion lack access to proper sanitation. (WHO/UNICEF, 2004)

Disinfection is an important step in ensuring that water is safe to drink and Water Treatment Plants all over the globe add disinfectants in order to destroy microorganisms that can cause diseases in humans. WHO (1993) in Casey and O'Reilly (2009) states that, "Disinfection is unquestionably the most important step in the treatment of water for public supply. The destruction of microbiological pathogens is essential and almost invariably involves the use of reactive agents such as chlorine, which are not only powerful biocides but also capable of reacting with other water constituents to form new compounds with potentially long – term health effects".

A number of disinfectants are however available for water treatment plants. But according to Sarbatly and Krishnaiah (2007), the superior advantages of chlorine compared to other halogens and chemicals such as bromide and fluoride as a disinfectant, besides its side effects to human health are that, it is easy to store and

transport, competitive price, continuous prevention of microbial re-growth, and gives the most effective property to control varied pathogen spectrum.

The destruction of harmful microorganisms by chlorine is mainly related to contact time, concentration and water quality. Also, successful chlorination requires that amount of chlorine added corresponds with chlorine demand test to achieve optimal disinfection; hence a little more chlorine than required is always added to be sure that it is sufficient. However chlorine must not be added in amounts that are wasteful and create unnecessary operational costs.

## 1.1 Background

### Overview

Portable water according to WIKIPEDIA (2013) is water safe enough to be consumed by humans or used with low risk of immediate or long term harm. In Ghana, portable water coverage is very low and households without access to portable water are forced to use less reliable and hygiene sources, and often pay more.

Many more industrial and municipal treatment plants have since being established and managed by government in order to salvage the water problem in the country. However, according to an inventory undertaken by the Ghana Environmental Protection Agency in 2001, less than 25% of the 46 industrial and municipal treatment plants in Ghana were functioning.

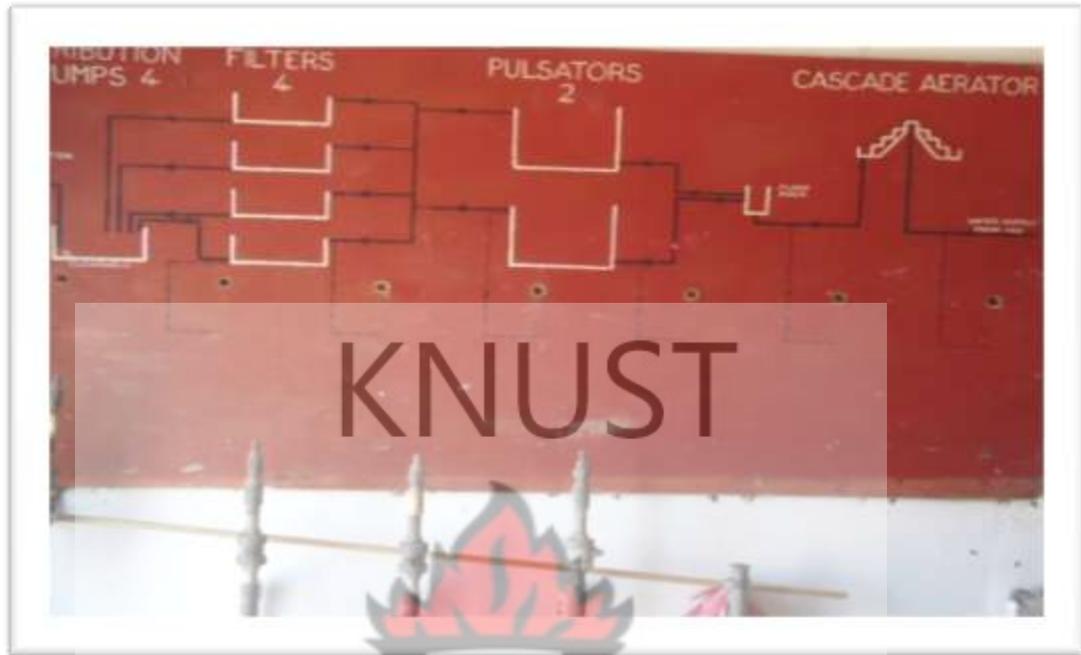
Most treatment plants in the country use chlorine as a disinfectant, and disinfection is the last barrier on the way to providing sanitary quality to drinking water. When chlorine is added to water as a disinfectant, a series of reactions occurs. The first of

these reactions occurs when organic materials and metals present in the water react with the chlorine and transform it into compounds that are unavailable for disinfection. The amount of chlorine used in these reactions is termed the chlorine demand of the water. Any chlorine concentration before the chlorine demand is met is termed as total chlorine.

Total chlorine is further divided into combined chlorine, which is the amount of chlorine that reacts with nitrates present in the water and is transformed into compounds that are much less effective disinfectants than the free or residual chlorine. Free or residual chlorine, which is the amount of chlorine available to inactivate disease – causing organisms and is thus the measure use to determine the portability of water

### **Profile of Vea – Gowrea Water Treatment Plant**

The Vea-Gowrie water treatment plant is located in Bongo district of the upper east region of Ghana. The plant which was established twenty-nine years ago draws its raw water from the Vea dam, which is also used to irrigate a number of farm lands in the district. Screened raw water from dam is drawn by propellers which move due to gravity to a Raw Water Pumping Station. The station then pumps an average of 1.2 million gallons of water daily to the treatment plant for treatment as shown in figure 1.1.below.



**Figure 1.1 A diagrammatical view of the treatment processes at the Vea - Gowrea Water Plant**

At the treatment plant as shown in figure 1.1 above, water is first of all uplifted over the Cascade Aerator where the water cascades over a series of steps. Air is naturally inducted into the water flow to accomplish iron oxidation and some reduction in dissolved gasses.

The water then flows into the Flash Mixer where coagulating chemicals such as Aluminium sulphate is quickly and evenly distributed in the water, allowing micro-flocs to form. The micro-flocs then undergo flocculation and coagulation in the Pulsators (sedimentation tanks), a process that separates solids suspended in water.

Micro-flocs then attach themselves to impurities in the water forming larger visible clusters agglomerates known as macro-flocs. These settle at the bottom and are later dislodged, allowing clear water to flow into Filters. The Filters made of layers of sand and gravel help remove even smaller and suspended difficult particles.

The filtered water then flows into the Clearwell, which is a reservoir for storage of filtered effluent. Chlorine which serves as a disinfectant then flows in to mix with filtered effluent, while the PH of the treated water is kept neutral by also the addition of hydrated lime. The 1.2 million gallons capacity clearwell of the plant pumps an average of one million gallons of water daily to consumers and to the Ghana Water Corporation storage reservoir for distribution to customers.

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## 1.2 Problem Statement

The management of Veolia – Gowree Water treatment plant in a quest to provide portable drinking water to their consumers adds chlorine to the clearwell of the plant as a disinfectant.

Chlorine is commonly used due to its ease of application and monitoring. It is also cost effective as compared to the other methods of disinfection and very effective in killing most bacteria.

However, recent findings reveal that chlorine reacts with natural occurring materials present in water to form by-products some of which include trihalomethanes and haloacetic acids which are suspected carcinogens. Chlorine is also known to produce odd taste and causes the corrosion of pipe networks if found in higher concentrations.

This has established the basis for more stringent drinking water standards including regulating the concentrations of chlorine in drinking water. The allowable chlorine level according to EPA is up to a level of 4mg/L.

Management of the Veia – Gowrea Water Treatment Plant therefore experimentally determines concentration levels of treated water every 2 hours in order to ensure its portability.

The problem of the Veia – Gowrea Water Treatment Plant is therefore to develop a mathematical model of the flow of chlorine from the chlorine chamber to the clearwell to numerically determine the concentration levels of chlorine of the treated water at any given moment so as to help minimize the number of experiments carryout every 2hours to ensure water portability.

### 1.3 Objectives

1. To model into differential equations the flow of chlorine from chlorine chamber to the clearwell of Veia – Gowrea Water Treatment Plant using rate equations.
2. To numerically determine the concentration levels of chlorine needed for portable water of the plant using Runge – Kutta second order method for ordinary differential equations.

### 1.4 Methodology

The problem of the Veia – Gowrea Water treatment plant would be to develop a differential model of the flow of chlorine from the chlorine chamber to the clearwell using rate equations, to numerically determine the chlorine concentration levels of the plant at any given moment using Runge – Kutta second order method for ordinary differential equations.

MATLAB 7.9.0 (R2009b) would be implored in the solution of the differential model, while Information and inference would be relied upon from KNUST library and the internet.

### **1.5 Justification**

- The thesis results would help management determine numerically the portability of treated water from the plant.
- It would also help minimize the number of experiments carryout to regulate chlorine concentration of the treated water.
- The cost of production of the plant would be minimized since fewer experiments would be required.

### **1.6 Organisation of the study**

The study is organized in five chapters. In chapter one, consideration is given to the introduction, background, problem, objectives, justification, methodology, and limitations of the study.

Chapter two also presents relevant and pertinent literature on the study area while the methodological elucidation of which the mathematical treatment and logical presentation of formulation, models and method of solution of the study would be presented in chapter three.

In chapter four, data collection and analysis which will include; display of data, stages in data analysis, results and discussions would be illustrated. While the research would end with conclusion and recommendation in chapter five.

## CHAPTER 2

### LITERATURE REVIEW

This chapter reviews literature on the use of chlorine as disinfectant.

#### 2.1 Introduction

Many centuries before the advent of modern science it was already known that water taken from streams could cause illness. Faust and Ally (1999) reports that disinfection can be traced back to about 2000 BC when the Sanskrit advised that water should be boiled by dipping a hot copper rod seven times into it or by exposing it to sunlight. After boiling and exposing it to the sun it should be filtered through charcoal. It was only since the 17<sup>th</sup> century that scientists could explain why certain types of water caused illness.

Meadows (1987) in Sternberg et al. (2002) said until the discovery of the microscope and the identification of bacteria in 1677 by Leeuwenhock, the field of microbiology was concerned with many practical problems such as medicine, sanitation and alcoholic fermentation. In the 1860s and 1870s Louis Pasteur and Robert Koch laid the foundation of a germ theory of disease and development of preventative vaccines. This new interest was primarily sparked by the increasing infant mortality caused by diarrhea. At about the same time an increasing number of cities developed large treatment and distribution facilities to supply the ever-increasing urban population with portable water.

AWWA (1998) describes Koch (1998a) discovery as a remarkable discovery in 1881 when he showed that chlorine could kill water borne bacteria. This probably led to the

most generally practiced measure to prevent the spreading of water borne diseases in pipe water systems.

Baker (1981) further considered Koch (1998a) discovery as the single most dramatic improvement ever made to public health. Afterwards, chlorine disinfection quickly spread across the United States, with the first continuous chlorine application occurring in 1908 at the Boonton, New Jersey drinking water facility. As the popularity of chlorine disinfection grew, so did its dosage in drinking water treatment. Gradually scientists became aware of the harmful side reactions resulting from chlorination.

Rook (1974) independently identified reactions between chlorine and dissolved organic matter that produced compounds known as trihalomethanes (THMs), which are suspected cancer-causing by-products of the disinfection process.

SDWA (1974) established the basis for more stringent drinking water standards, including regulation of the concentration of THMs.

USEPA (2006) promulgated a THM maximum contaminant level (MCL) of 0.10 mg/L. Since the discovery of THMs, chlorine use has come under scrutiny, resulting in the increased use of more expensive and complicated disinfection methods, including chloramination, ozonation, ultraviolet irradiation, and chlorine dioxide addition. Ongoing and future research aims to better determine chlorine concentration and disinfection will result in improved disinfection methods.

## 2.2 LITERATURES ON CHLORINE AS A DISINFECTANT

A large amount of research and many studies have been conducted to ensure success in treatment plants using chlorine as a disinfectant. A leading advantage of chlorine is that it has proven effective against most bacteria and viruses.

Liou and Kroon (1987) showed that when chlorine is added to water it forms hypochlorous acid or hypochlorites which have an immediate and disastrous effect on most forms of microscopic organisms.

Hau et al. (1999) also reported that chlorine is the most commonly used disinfectant due to its ease of application and monitoring, its low cost and its effectiveness in killing bacteria.

Sarbatly and Krishnaiah (2007) reported that the superior advantages of chlorine compared to other halogens chemicals such as bromide and fluoride as disinfectant, besides its side effects to human life are; it is easy to store and transport, competitive price, continuous prevention of microbial re – growth, and gives the most effective property to control varied pathogen spectrums.

SDWF (2006) described chlorine as a chemical that is used to disinfect water prior to it being discharged into the distribution system. It is used to ensure that water quality is maintained from water source to the point of consumption. When chlorine is fed into the water, it reacts with any iron, manganese, or hydrogen sulphide that may be present. If any chlorine remains (residual), it will then react with organic materials, including bacteria. Therefore, in order to ensure that water is sufficiently treated through the whole distribution system, an excess of chlorine is usually added. This amount is usually

adjusted to make sure there is always enough chlorine available to completely react with all organic present.

Sharp and Pestano (2013) reports EPA (2002) as confirming that the long term consumption of water that contains halo – acetic acids concentrations in excess than the legal limit of 60parts per billion is associated with an increased risk of cancer. It further warned that long term exposure to halo –acetic acids at or above 60parts per billion may cause injury to the brain, nerves, liver, kidneys, eyes and the reproductive system.

Vikesland et al (2001) showed that as water travels through the pipes, the disinfectants oxidize materials in both the bulk water and the pipe wall thereby reducing the amount of disinfectant available to ensure continuous disinfection.

AWWW (2007) reported that free chlorine decay kinetic and pathways are well established as a result of the long history of free chlorine usage and that chlorine modeling takes into account reacting species and their concentrations, kinetic, temperature, pipes geometry, water quality, residence time and flow hydraulic.

Kapadia (accessed on 10<sup>th</sup> April, 2013). Listed the factors that influence the changes in water quality between the treatment plant and consumer tap as; chemical and biological quality of source water, effectiveness and efficiency of treatment process, integrity of the treatment plant, storage facilities and distribution system, age, types of design and maintenance of distribution network, quality of treated water and mixing of water from different sources within a distribution network and other hydraulic conditions.

Daly et al. (2007) presented a range of mathematical approaches and prediction techniques including multivariate analysis, polynomials, exponential functions, artificial networks, linguistic equations and Langmuir Isotherms, aimed at maintaining chlorine disinfectant concentration within a reasonable operation limit that provides optimum disinfection and also limiting the concentration of disinfectants by – products.

Notter and Sleicher (1971) created empirical expression of relating the various decay constants through the use of the Sherwood number which is dimensionless. In addition to the Sherwood number which is related to mass transfer coefficient another dimensionless number exist, called Schmidt number. It is used in characterizing fluid flows in which there are simultaneous momentum and mass diffusion convection process. Schmidt number is applicable to transport phenomenon and also used in the calculation of binary mass transfer between phases. Schmidt number dependency of wall dissipation constant is crucial in most practical applications.

Koehling (1998) outlined that the amount of chlorine required for water depends upon the organic and inorganic impurities present in water after the chlorine requirement is fulfilled. Hence at this point, chlorine will appear as free chlorine residual (hypochlorite).

Ekeng (2011) on the decay of free chlorine along aged pipes and of varying diameter with pressure, showed that higher concentration of residual chlorine was observed at higher pressure in smaller age diameter pipes of longer service years than the large ones of less service years.

Chua (1996) carried out as part of research study in to THM formation, the chlorine dose applied at 12 Irish WTWs was found to vary in the range 0.7 – 3.0mg/L (average 1.55mg/L). The associated chlorine decay time was measured and the corresponding CT range was estimated to be 55 – 800mg.min/L. Hence, it was concluded that most WTWs operate a chlorination regime having CT value well in excess of the requirement for disinfection (CT 50 – 60mg, min/L).

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EPA (1998) published that water treatment invariably comprises alum coagulation followed by rapid gravity sand filtration with disinfection by gaseous chlorine, and while there is no established design norms in place for the determination of chlorine dosed. The Irish EPA has produced a comprehensive manual on disinfection which is a valuable reference for the design and operation of drinking water disinfection systems.

Double et al. (1977) on pores sizes change (“grow”) with time showed that adsorption of a substance involves the accumulation of the substance at such as a liquid and a solid (such as the reservoir wall/water interface), and that important adsorbent characteristics that affect Isotherms include surface area, pore size distribution, and surface chemistry. The maximum amount of adsorption is proportional to the amount of surface area within pores that is accessible to the adsorbent. It is therefore important to note that concrete surface change when in contact with water.

Viljoen et al (1997) also on concrete has a constant demand for chlorine experimentally showed that concrete accelerates chlorine decay in the water, via sorption processes, which include adsorption and absorption, and that sorption models that can be applied

are adsorption isotherms complex or competitive adsorption models. In pipelines this demand is of significance because of the water volume to pipe surface ratio. It further concludes that it is possible to predict the rate of chlorine loss in pipelines accurately once the decay rate for particular water composition and transport system have been assessed.

Kruger et al. (2000) posted on chlorine decay on concrete surfaces and losses to the atmosphere in water storage facilities. Different mathematical models fitted shows that chlorine concentrations decrease continuously with time in any potable water distribution system. This is due to chlorine decay and reactions with substances of both an organic and inorganic nature. In reservoirs the decay is enhanced by longer retention times. Under the conditions investigated, it was found that relatively deep penetration of water into the concrete structure tank. This result ed in a very slow “3 – dimensional” exchange of dissolved substances in the pores of the concrete.

Donald et al. (1979) posted that the effectiveness of disinfection is influenced by factors such as detention time, disinfectant dosage, pH, temperature, the presence of reducing substances and mixing intensity. They went on to conclude that the time required for the disinfection process is inversely proportional to the concentration of the disinfectant residual, and that mixing has been shown to be an important parameter in all disinfection system.

SDWF (2013) stated that the amount of chlorine that is required to disinfect water is dependent on the impurities in the water that needs to be treated. Many impurities in the water require a large amount of chlorine to react with all the impurities present. The chlorine added must first react with all the impurities in the water before chlorine residual is present. The amount of chlorine that is required to satisfy all the impurities is termed the 'chlorine demand. This can also be thought of as the amount of chlorine needed before free chlorine can be produced. Once the chlorine demand has been met, any additional chlorine added will result in a free chlorine residual proportional to the amount of chlorine added. Residual chlorine is the difference between the amount of chlorine added and that of the chlorine demand.

Yee et al. (2006) upon monitoring the evolution of chlorine demand and the trihalomethanes formation potential in water samples from Semenyih river water treatment plant isolated and fractionated using resin adsorbents into six classes, concluded that Dissolved Organic Matter(DOM) can be characterized as a function of chlorine demand. Hydrophilic neutral and hydrophobic acid fractions were found to play an important role in causing a high chlorine demand.

Rodriguez et al. (2002) presented a paper on the development of two models for simulating residual chlorine decay in raw and treated waters collected from six different utilities of Quebec city area. Both models demonstrated acceptable abilities for simulating residual chlorine decay. However, the back propagation neural network model gave significantly better results for conditions involving high chlorine dosage, high organic matter content and long reaction times during chlorination experiments.

AWWARF (1996) posted that the required chlorine dose needed to render water drinkable depends on water quality and on the operational conditions of the chlorination process and that past investigations have indicated that the operational parameters which influence chlorine demand are chlorine dose, water temperature, pH and the reaction time of chlorine.

Clark et al. (2008) based on the experimental results reported in the paper titled Controlling Disinfected Residual Losses in Drinking Water distribution systems and studies previously carried out by Digiano and Zhang (2005) and Al – Jasser (2007), that surface or pipe wall demand of chlorine varies significantly among different types of pipe material, concluded that the type of pipe material can influence the transport of free chlorine in drinking water distribution system networks. These characteristics can have regulatory implications. For instance, chlorine residuals dissipate rapidly in unlined ductile iron pipe but are maintained in PVC pipe.

Rossmann and Boulos (1996) in a comparison made between the formulation and computational performance of four numerical methods for modeling the transient behavior of water quality in drinking water distribution systems. Two were Eulerian based (the finite difference and discrete volume methods, and the other two were Lagrangian based (the time driven and event driven methods). The Eulerian approaches moved water between fixed grid points or volume segments in pipes as time was advanced in uniform increments. The Lagrangian methods updated conditions in variable sized segments of water at either uniform time increments or only at time when

a new segment reaches a downstream pipe junction. Each method was encoded into an existing distribution simulation model and ran on several pipe networks of varying sizes under equal accuracy tolerances. Results showed that the accuracies of the methods were comparable and that the Lagrangian methods were more efficient for simulating chemicals transport. Also, for modeling water age, the time driven Lagrangian method was the most efficient while the Eulerian methods were more memory efficient.

Kastl et al. (1999) on their proposed model describe chlorine decay kinetics for various initial chlorine doses and temperatures in the water phase. The model can also describe the concentration of free and combined chlorine with time. This distinction is very important at the end of the distribution system, where free chlorine constitutes a lower percentage of total chlorine concentration, but still determines disinfection efficiency.

Rodriguez et al. (1997) implemented a single smoothing factor general regression neural network to predict the chlorine measurements. The results obtained indicate that it is quite possible to predict the chlorine consumed in a water distribution network using intelligent data driven methods such as neural networks.

Clark and Boutin (2001) reviewed several models for predicting the decay of disinfectants and the formation of disinfection by-products. These models are mostly based on first-order decay, second-order decay, power-law decay (nth order) and exponential decay assumption or reacting balance.

Robescu et al. (2008) presented a theoretical model based on dispersion equation, which was validated with experimental measurements in drinking water mains that supply

Ramni – Valcea town in Romania. The model predicts pretty well chlorine concentration in water mains.

Gibbs et al. (2003) took a drift from the traditional process – based (chlorine decay) models which depends on many factors such as temperature, initial chlorine concentration, source water quality and biofilm, when two data – driven techniques, namely linear regression model and multi - layer perceptron artificial neural networks were used to predict chlorine concentration at two key locations in the Hope valley water distribution system, which is located to the north of Adelaide, south Australia. The results obtained indicate that both techniques prove relatively successful in predicting chlorine concentration in the distribution system with the performance of the multi – layer perceptron slightly better than the regression model.

Sérodes et al. (2001) stated that, the development of statistically based models for disinfection control purposes is justifiable in cases where parameter estimation within a process – based model is imprecise or difficult to obtain. In other words, where the data required for the development of process based models are not available. This approach offers the advantage of not requiring extensive a priori knowledge of the laws of chemistry and mathematics governing the behavior of residual chlorine or the distribution system being studied. However some knowledge of the factors that will influence the chlorine decay can help identify which data are relevant for the analysis.

Le Chevalier (1991) found that monochloramine penetrates the biofilm better than free chlorine and that extent of penetration is dependent upon two competing rate processes;

diffusion and reaction. Chlorine causes oxidation, hydrolysis or deamination of virtually every component of bacterial cell. In contrast, monochloramine reacts rather specifically with nucleic acids, tryptophan and sulphur containing amino acids.

Carlson (1991) stated that, the use of chlorine as a disinfectant has played a major role in limiting potential epidemics and that most of the knowledge in the area of epidemiology was gathered from mistakes that led to epidemic outbreaks. The causes of the wide – spread of diseases from ‘contaminated’ drinking water stretch from; insufficient purification or disinfection, negligence, inadequately defined protected zones, constructional errors, cross links in the pipe system, improper disposal of waste and many more.

Pouzn (2007) put it that, chlorine taste and odour are key concerns for user acceptability in SWS programs, and that many taste and odour concerns can be addressed by using dosage regime that prevent overdosing. Also, focus groups on taste testing have found that the majority of SWS users are comfortable drinking water with a free chlorine residual of up to 2.0mg/l. however; there is significant regional variation in the acceptable maximum residual.

IARC (1991) reviewing the available data, concluded that there is inadequate evidence to determine the carcinogenicity of chlorinated drinking water to humans. Whiles action to reduce the concentration of disinfection byproducts is encouraged, disinfection itself must not be compromised; the risk posed by disinfection byproducts is considerably

smaller than the risk posed by the presence of pathogenic microorganisms in water that has not been disinfected.

Williams and Don (1959) conducted a study of sporadic water quality problems in Brantford, Ontario, water system. It was drawn into conclusion that the loss of both chlorine and chloramine residuals in the Brantford system was related to an increase in ferrous iron caused by corrosion in the distribution system pipes.

Powell and James (2000) in a comprehensive study of chlorine residual losses in drinking water distribution systems, found a very large range in wall demand for chlorine (kw). Their results suggest a relationship between kw and pipe material with cast – iron pipe rates typically 10 to 100 times higher in wall demand than PVC pipe. They also found an increase in kw with velocity which was most prominent in cast – iron.

Camper et al. (2003) studied the interactions between pipe materials, organic carbon levels and disinfectants using annular reactors with ductile – iron, PVC, epoxy and cement – lined coupons at four field sites. The investigators found that regardless of carbon levels iron had the highest numbers of bacteria.

Clark et al. (2005) conducted a study to systematically assess the effect of free chlorine loss in corroded unlined metallic pipes subject to changes in velocity. The authors conducted the study under controlled conditions in a specially constructed pipe loop located at the U.S. EPA's T and E Facility in Cincinnati, Ohio. Results from the pipe – loop study supported the concept that the rate of free chlorine residual loss is a problem

in unlined metallic pipes and a growing body of evidence that residual loss is a function of velocity; little research has been done to incorporate this knowledge into the development of chlorine residual transport models.

Digiano and Zhang (2005) developed a bench – scale reactor to test the decay rate of chlorine at the pipe wall. Two 152mm (96inc) diameter sections of old cast – iron and new cement – lined ductile iron pipe were used in their tests. They studied the effects of velocity, corrosion rate, dissolved oxygen and pH on the chlorine – wall reaction rate. They found that chlorine decay rate was described by zero – order reaction kinetics for cast – iron pipe. The zero – order rate was larger at higher velocities because of higher mass transfer to the pipe surface although a limit was reached. For the ductile – iron pipe the chlorine decay kinetics was found to be first order with respect to chlorine concentrations.

Al – Jasser (2007) attempted to assess the service age of pipes on the effective chlorine wall decay constant. Three hundred and two pipe sections of different pipe materials were collected and tested for their first – order wall constants. It was found that the effect of pipe age was not evident in cast – iron pipes whereas steel pipes were less affected.

Lee and Nam (2002) reported that a number of kinetic models have been proposed for the formulation of disinfection design criteria and that model adequacy is dependent

upon the robustness of the underlying inactivation rate law if the model accounts for the disappearance of the chemical disinfectant during the contact.

Biswas et al. (1993) stated that distribution systems are extremely complex and difficult to study in the field, and that mathematically models have proven to be an effective tool for assessing changes in water quality in drinking water distribution systems.

WHO (1993) in Casey and O'Reilly (2009) provided an appropriate context for the subject matter covered on drinking water disinfections using chlorine theory and practice. It concluded by stating that disinfection is unquestionably the most important step in the treatment of water for public supply. The destruction of microbiological pathogens is essential and almost invariably involves the use of reactive agents such as chlorine, which are not only powerful biocides but also capable of reacting with other water constituents to form new compounds with potentially long-term health effects.

Casey and O'Reilly (2009) on a book titled drinking Water Disinfection using chlorine Theory and Practice, stated that while effective disinfection is an essential treatment step in the production of most public water supplies, it does not on its own guarantee microbiologically safe water at the consumer's tap. The management, operation and integrity of the water distribution infrastructure also play an important rule.

Haas et al. (1996) argued that disinfectants such as chlorine are unstable agents taking part in chemical reactions with both organic and inorganic materials carried by the water. They might also interact with the biofilm attached to the pipe – wall. All these

interactions change the chlorine concentration in the water, which consequently may require additional disinfection.

Galal – Gorchev (1996) stated that disinfection of drinking-water is one of the main achievements of our time in the protection of public health. The use of chlorine for the destruction of microbiological pathogens is essential to protect the public from outbreaks of waterborne disease. Chlorine, as well as other disinfectants, produces a variety of chemical by-products. The risk from the presence of microbial pathogens in drinking-water is estimated to be several orders of magnitude greater than the risk from chlorination by-products. Any efforts to control these by-products must not compromise the microbiological quality of drinking-water.

Weragoda (2005) a research carried out based on three water treatment plants located in Mahasawat, pathumthani and Bangkhen, Thailand. These treatment plants were evaluated to find out the efficiency of TOC removal in the treatment process. The highest TOC removal efficiencies were achieved by the pathumthani water treatment plant as 30% and 20% in sedimentation and filtration, respectively. The main objective of the research was to correlate the results of rapid organic characterization technique with modeling of chlorine decay in each TOC fraction. Two separate empirical models were developed, using modeling software, named AQUASIM. The model on the treated water from Bangkhen water treatment plant proved that the highest chlorine demand is due to the presence of very hydrophobic acid in treated water. It could be estimated that the reduction of chlorine demand in Bangkhen treated water is 70% of its total. Besides

to that, the results of rapid organic characterization proved that the hydrophilic charge organic fraction was the most responsible for the formation of total trihalomethane. General guidelines for chlorination were developed based on the results, and the research outputs can be used to modify water treatment technology to minimize the treat of THM.

Elshorbagy et al. (200) elaborated that chlorine reacts with both natural and synthetic organic matters in the water. They observed that chlorine usually reacts with natural organic matter such as humic and fulvic acids. They further observed that the relative contribution to the formation of THMs by the humic fraction is greater than that of fulvic fraction, since humic acids reacts more readily with chlorine.

Kiene et al (1998) identified that the reactivity of the pipe wall will be a function of pipe diameter, hydrodynamic conditions, nature of the pipe material and amount and deposits of chlorine. The following results were obtained in a study aimed at modeling chlorine decay in drinking water; chlorine consumption by synthetic materials is negligible and does not appear to be an important parameter for the modeling of chlorine decay. Also In contrast, chlorine consumption of old cast iron pipes whose internal surfaces are not protected by a coating can be considered as a major parameter for chlorine decay modeling. For cast iron or steel pipes, the rate of chlorine consumption can be directly considered under the dependence of corrosion phenomena.

Ghazali (1989) identified that, when the chlorine dosage within the limit of 3 to 5 mg/l, the formation of THM is still below the 100  $\mu\text{m}/\text{L}$ , which has been recommended as the

maximum permissible limit in the USEPA. However, once the chlorine level increased beyond 7 mg/L, then the level of THM in water is increased above the permissible limit after contact time of 12 hours. It was concluded that about 50% of total THM forms within the first 3-5 hours. For the rest 50%, it takes longer time of contact. In addition to that, it was found that, THM can be reduced by boiling water. About 50-55% of THM reduction can be observed at the boiling point and further boiling for 10 min reduces about 90% of THM.

Rodriguez et al (2001) in an investigation observed that the occurrence of THMs in chlorinated water may vary significantly according to season and geographical location in the distribution system. These temporal and spatial variations are due to changes in raw and treated water quality as well as in operational parameters related to chlorination. The measurable operation parameters which influence the occurrence of trihalomethane in the distribution systems are chlorine dose, water temperature, pH and travel time of water within the system.

The researcher after reviewing the necessary literature as presented in this chapter, now presents an alternative model which applies rate equations in a mixing problems to the Veal – Gowrea water treatment plant to numerically determine the concentration of chlorine in the treated water.

## CHAPTER 3

### METHODOLOGY

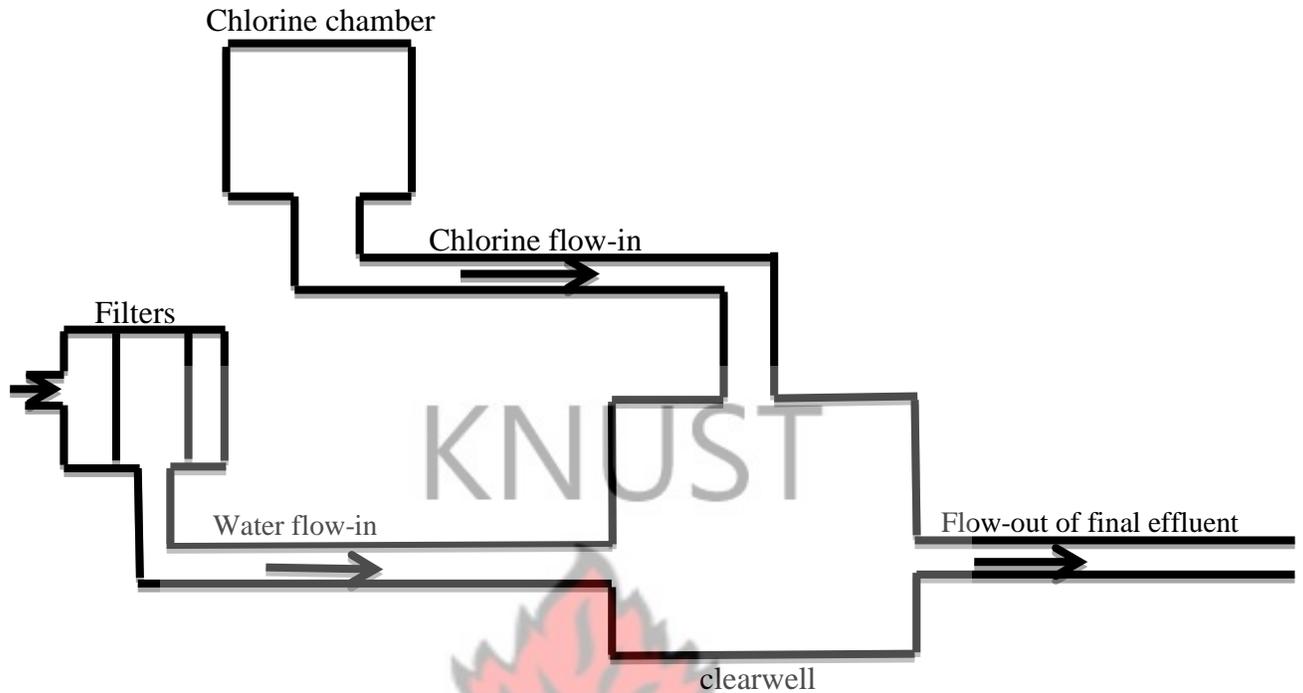
#### 3.0 INTRODUCTION

This chapter consists of the formulations and models which would be applied in determining the portability of water produced by the plant.

#### 3.1 FORMULATION

The treatment plant continuously received water from the pumping station for the treatment process. This water undergoes a series of processes which include; aeration, flocculation, sedimentation, filtration and chlorination all aimed at ensuring that the water produced is portable to consumers.

From the schematic diagram of the treatment processes of the plant as shown in figure 3.1, ambient water enters the filters after aeration, flocculation and sedimentation for filtration. The filtered water then flows in at a constant rate known as flow – in rate into a large tank (clearwell). Chlorine disinfectant from the chlorine chamber with a constant concentration is then allowed to flow in to clearwell where instantaneous mixing occurs to ensure effective disinfection. Disinfected water then flows out with a constant rate described as flow-out rate to consumers as tap water.



**Figure 3.1: A schematic diagram of the treatment process of the plant**

### 3.2 MATHEMATICAL MODEL

#### Step 1: modeling volume flow rate in clearwell

Let  $V$  = volume of water in clearwell

$\left(\frac{dV}{dt}\right)_{in}$  = flow rate of filtered water in to clearwell

$\left(\frac{dV}{dt}\right)_{out}$  = flow rate of treated water out of clearwell

$\left(\frac{dV}{dt}\right)_{net}$  = net flow rate of water in the clearwell

The volume flow rate equation is

$$\frac{d}{dt} V(t) = \left(\frac{dV}{dt}\right)_{net} = \left(\frac{dV}{dt}\right)_{in} - \left(\frac{dV}{dt}\right)_{out}$$

[3.1]

Since the plant's production of water must always exceed that of its demand.

Then,  $\left(\frac{dV}{dt}\right)_{in} > \left(\frac{dV}{dt}\right)_{out}$

This implies,  $\frac{d}{dt} V(t) = \left(\frac{dV}{dt}\right)_{net} = \left(\frac{dV}{dt}\right)_{in} - \left(\frac{dV}{dt}\right)_{out} > 0$

Assumption 1: it is assumed that the flow – in and flow – out rates are constants. This implies the net flow –rate will also be a constant represented by ‘A’.

That is  $\left(\frac{dV}{dt}\right)_{net} = A$

The volume of water in the clearwell is then given by;

$$V(t) = \int \left(\frac{dV}{dt}\right)_{net} dt = \int A dt = At + C;$$

But given that at time  $t = 0$ , the volume of water in the clearwell =  $V_0$ .

Hence  $C = V_0$

Therefore, the volume model is given as;  $V(t) = At + V_0$ . [3. 2]

### Step 2: Modeling mass of chlorine in the clearwell into an ordinary differential equation

Let  $M$  = mass of chlorine in the clearwell

$$\left(\frac{dm}{dt}\right)_{in} = \text{mass flow - in rate of chlorine into clearwell}$$

$$\left(\frac{dm}{dt}\right)_{out} = \text{mass flow – out rate of chlorine out of clearwell}$$

$$\left(\frac{dm}{dt}\right)_{net} = \text{net mass flow of chlorine in the clearwell}$$

$C_{in.}$  = concentration of chlorine from chlorine chamber to the clearwell

$C_{out}$  = concentration of chlorine out of clearwell.

The mass flow rate equation is therefore given as;

$$\frac{d}{dt} M(t) = \left(\frac{dm}{dt}\right)_{net} = \left(\frac{dm}{dt}\right)_{in} - \left(\frac{dm}{dt}\right)_{out} \quad [3. 3]$$

But,

$$\text{Concentration of chlorine in clearwell} = \frac{\text{mass of chlorine in clearwell}}{\text{volume of water in clearwell}}$$

This implies at time  $t$ , the mass of chlorine in the clearwell is given by;

$$m(t) = V(t) \cdot C(t). \quad [3.4]$$

Assumption 2: it is assumed that the concentration of chlorine is the same everywhere in the clearwell because of “instantaneous mixing”.

This means that  $C_{\text{out}} = C(t)$ .

$$\left(\frac{dm}{dt}\right)_{\text{out}} = \left(\frac{dV}{dt}\right)_{\text{out}} \cdot C_{\text{out}} = \left(\frac{dV}{dt}\right)_{\text{out}} \cdot C(t). \quad [3.4a]$$

and

$$\left(\frac{dm}{dt}\right)_{\text{in}} = \left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}} \quad [3.4b]$$

From [3.3], [3.4], [3.4a], and [3.4b], the mass flow rate equation can be written as;

$$\frac{d}{dt} m(t) = \frac{d}{dt} [V(t) \cdot C(t)] = \left[\left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}}\right] - \left[\left(\frac{dV}{dt}\right)_{\text{out}} \cdot C(t)\right] \quad [3.5]$$

From [3.2] and [3.4]

$$\frac{dm}{dt} = \left[\left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}}\right] - \left[\left(\frac{dV}{dt}\right)_{\text{out}} \cdot \frac{m(t)}{V(t)}\right] = \left[\left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}}\right] - \left[\left(\frac{dV}{dt}\right)_{\text{out}} \cdot \frac{m(t)}{V_0 + A t}\right] \quad [3.6]$$

Re-arranging [6] in to the form  $\frac{dy}{dt} + p(t)y = q(t)$ . (This is a first-order linear ordinary differential equation).

$$\text{We have the mass model as; } \frac{dm}{dt} + \left[\frac{\left(\frac{dV}{dt}\right)_{\text{out}}}{V_0 + A t}\right] m(t) = \left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}} \quad [3.7]$$

Where;

$$\frac{dy}{dt} = \frac{dm}{dt}$$

$$P(t) = \left[ \frac{\left(\frac{dV}{dt}\right)_{\text{out}}}{V_0 + A t} \right]$$

$$Y = m(t) \quad \text{and}$$

$$q(t) = \left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}}$$

### Step 3: Modeling concentration of chlorine in treated water into an ordinary differential equation

Applying product rule to the left-hand side of [3. 5] of the mass model,

We have;

$$\frac{d}{dt} [V(t) \cdot C(t)] = \frac{dV}{dt} C(t) + V(t) \frac{dC}{dt} = \left[ \left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}} \right] - \left[ \left(\frac{dV}{dt}\right)_{\text{out}} \cdot C(t) \right] \quad [3. 8]$$

$$\text{From [1], } V(t) \frac{dC}{dt} = \left[ \left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}} \right] - \left[ \left(\frac{dV}{dt}\right)_{\text{out}} \cdot C(t) \right] - [A \cdot C(t)]$$

$$\text{Hence, } V(t) \frac{dC}{dt} = \left[ \left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}} \right] - \left[ \left(\frac{dV}{dt}\right)_{\text{out}} + A \right] \cdot C(t)$$

[3. 8a]

$$\text{Since } \left(\frac{dV}{dt}\right)_{\text{out}} + A = \left(\frac{dV}{dt}\right)_{\text{out}} + \left(\frac{dV}{dt}\right)_{\text{net}} = \left(\frac{dV}{dt}\right)_{\text{out}} + \left[ \left(\frac{dV}{dt}\right)_{\text{in}} - \left(\frac{dV}{dt}\right)_{\text{out}} \right] = \left(\frac{dV}{dt}\right)_{\text{in}}$$

[3. 8b]

Substituting [3. 8a] into [3. 8b]

$$V(t) \frac{dC}{dt} = \left[ \left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}} \right] - \left[ \left(\frac{dV}{dt}\right)_{\text{in}} \cdot C(t) \right]$$

Dividing through by V (t), we have

$$\frac{dC}{dt} = \left[ \frac{\left(\frac{dV}{dt}\right)_{\text{in}} \cdot C_{\text{in}}}{V(t)} \right] - \left[ \frac{\left(\frac{dV}{dt}\right)_{\text{in}} \cdot C(t)}{V(t)} \right], \text{ but } V(t) = V_0 + A t$$

This implies;

$$\frac{dC}{dt} = \left[ \frac{\left(\frac{dV}{dt}\right)_{in} \cdot C_{in}}{V_0 + At} \right] - \left[ \frac{\left(\frac{dV}{dt}\right)_{in} \cdot C(t)}{V_0 + At} \right]$$

[3.9]

Re-arranging [3.9] in to the form  $\frac{dy}{dt} + p(t)y = q(t)$ . (A first – order ordinary linear differential equation).

We have the concentration model as;

$$\frac{dC}{dt} + \left[ \frac{\left(\frac{dV}{dt}\right)_{in}}{V_0 + At} \right] \cdot C(t) = \frac{\left(\frac{dV}{dt}\right)_{in} \cdot C_{in}}{V_0 + At}$$

[3.10]

Where;

$$\frac{dy}{dt} = \frac{dc}{dt}$$

$$P(t) = \left[ \frac{\left(\frac{dV}{dt}\right)_{out}}{V_0 + At} \right]$$

$$Y = C(t) \quad \text{and}$$

$$q(t) = \left(\frac{dV}{dt}\right)_{in} \cdot C_{in}$$

### 3.3 NUMERICAL METHOD OF SOLUTION

Runge – Kutta second order method is a numerical technique used to solve ordinary

differential equations of the form  $\frac{dy}{dx} = f(x, y)$ ,  $y(0) = y_0$  and only first order ordinary

differential equations can be solved by using this method.

From Euler's method given by

$$y_{i+1} = y_i + f(x_i, y_i) h, \text{ where } x_0 = 0, y_0 = y(x_0) \text{ and } h = x_{i+1} - x_i$$

The Runge – Kutta second order method is gotten from the Euler’s method being derived from Taylor’s series as follows;

$$y_{i+1} = y_i + \frac{dy}{dx} \Big|_{x_i, y_i} (x_{i+1} - x_i) + \frac{1}{2!} \frac{d^2y}{dx^2} \Big|_{x_i, y_i} (x_{i+1} - x_i)^2 + \frac{1}{3!} \frac{d^3y}{dx^3} \Big|_{x_i, y_i} (x_{i+1} - x_i)^3 + \dots$$

Writing out the first three terms of Taylor series above

$$y_{i+1} = y_i + \frac{dy}{dx} \Big|_{x_i, y_i} h + \frac{1}{2!} \frac{d^2y}{dx^2} \Big|_{x_i, y_i} h^2 + O(h^3) \quad [3.1e]$$

Where

$$h = (x_{i+1} - x_i)$$

Since;

$$\frac{dy}{dx} = f(x, y),$$

We can rewrite the Taylor series as

$$y_{i+1} = y_i + f(x_i, y_i) h + \frac{1}{2!} f'(x_i, y_i) h^2 + O(h^3) \quad [3.2e]$$

Now

$$f'(x_i, y_i) = \frac{\partial f(x, y)}{\partial x} + \frac{\partial f(x, y)}{\partial y} \frac{dy}{dx} \quad [3.3e]$$

Hence

$$\begin{aligned} y_{i+1} &= y_i + f(x_i, y_i) h + \frac{1}{2!} \left[ \frac{\partial f}{\partial x} \Big|_{x_i, y_i} + \frac{\partial f}{\partial y} \Big|_{x_i, y_i} \times \frac{dy}{dx} \Big|_{x_i, y_i} \right] h^2 + O(h^3) \\ &= y_i + f(x_i, y_i) h + \frac{1}{2} \frac{\partial y}{\partial x} \Big|_{x_i, y_i} h^2 + \frac{1}{2} \frac{\partial f}{\partial y} \Big|_{x_i, y_i} f(x_i, y_i) h^2 + O(h^3) \end{aligned} \quad [3.4e]$$

Now the term used in the Runge – Kutta second order method for  $k_2$  can be written as a Taylor series of two variables with the first three terms as

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$

$$= f(x_i, y_i) h + p_1 h \frac{1}{2} \frac{\partial f}{\partial x} |_{x_i, y_i} h^2 + q_{11} k_1 h \frac{1}{2} \frac{\partial f}{\partial y} |_{x_i, y_i} h^2 + O(h^3) \quad [3. 5e]$$

Hence

$$\begin{aligned} y_{i+1} &= y_i + (a_1 k_1 + a_2 k_2) h \\ &= y_i + \left[ a_1 f(x_i, y_i) + a_2 \left\{ f(x_i, y_i) + p_1 h \frac{\partial f}{\partial x} |_{x_i, y_i} + q_{11} k_1 h \frac{\partial f}{\partial y} |_{x_i, y_i} + O(h^2) \right\} \right] h \\ &= y_i + (a_1 + a_2) h f(x_i, y_i) + a_2 p_1 h^2 \frac{\partial f}{\partial x} |_{x_i, y_i} + a_2 q_{11} k_1 h^2 \frac{\partial f}{\partial y} |_{x_i, y_i} + O(h^3) \end{aligned}$$

[3. 6e]

Equating the terms in [3. 4e] and [3. 6e], we get

$$a_1 + a_2 = 1$$

$$a_2 p_1 = \frac{1}{2}$$

$$a_2 q_{11} = \frac{1}{2}$$

Assuming the value of one of the unknowns, the other three will then be determined from the three equations. Generally the value of  $a_2$  is chosen to evaluate the other three constants. The three values generally used for  $a_2$  are  $\frac{1}{2}$ , 1 and  $\frac{2}{3}$ , and are known as Heun's method, the midpoint method and Ralston's method, respectively.

### 3.4 MANUAL NUMERICAL ILLUSTRATION OF MODEL

Below is a numerical example with specific values for the various quantities of the models

#### Example

50mg/l of chlorine flows into a clearwell of a water plant for disinfection which initially contains 250L of filtered water in an ambient concentration of 1.5mg/l. If filtered water is being added into the clearwell of the plant at a rate of 100mg/l and disinfected water

is allowed to flow out at a rate of 60mg/l. Assuming the initial concentration of chlorine in to clearwell is 12mg/l.

We wish to find the concentration of chlorine in the clearwell at  $t = 4$  hours using Runge – Kutta second order method. Assume a step size of  $h = 2$  seconds where concentration is in mg/l and  $t =$  hours.

## SOLUTION

# KNUST

### Step 1: Definition of terms

Flow – in – rate  $\left(\frac{dV}{dt}\right)_{in} = 100\text{l/h}$

Initial volume of water  $V_0 = 250\text{L}$

Concentration of chlorine  $C_{in} = 50\text{mg/l}$

Initial concentration of chlorine  $C_0 = 12\text{mg/l}$

Flow – out rate  $\left(\frac{dV}{dt}\right)_{out} = 60\text{l/h}$

### Step 2: Volume of filtered water in the clearwell

The volume function from [2] above is given as;  $V(t) = A t + V_0$

But  $A = 100\text{l/h} - 60\text{l/h} = 40\text{l/h}$

This implies  $V(t) = 40t + 250$

### Step 3: Chlorine concentration in the treated water

The differential equation for chlorine concentration from [3. 9] above is given as;

$$\frac{dC}{dt} + \left[ \frac{\left(\frac{dV}{dt}\right)_{in}}{V_0 + At} \right] \cdot C(t) = \frac{\left(\frac{dV}{dt}\right)_{in} \cdot C_{in}}{V_0 + At}$$

Substituting in the values from step 1, we obtain;

$$\frac{dc}{dt} = \frac{100 \times 50}{V_0 + 40t} - \frac{100}{V_0 + 40t} C(t)$$

$$\text{This implies } \frac{dc}{dt} + \frac{100}{250 + 40t} C(t) = \frac{5000}{250 + 40t}$$

Applying Runge – Kutta second order method. We have

$$\frac{dc}{dt} = \frac{5000}{250 + 40t} - \frac{100}{250 + 40t} C(t)$$

$$\text{This implies; } \frac{dc}{dt} = \frac{5000 - 100 c(t)}{250 + 40t}$$

$$\text{Hence } f(t, c) = \frac{5000 - 100 c(t)}{250 + 40t}$$

Per Heun's method

$$C_{i+1} = C_i + \left( \frac{1}{2} K_1 + \frac{1}{2} K_2 \right) h$$

$$K_1 = f(t_i, C_i)$$

$$K_2 = f(t_i + h, C_i + K_1 h)$$

$$\text{For } i = 0, t_0 = 0, C_0 = C(0) = 12 \text{mg/l}$$

$$K_1 = f(t_0, C_0) = f(0, 12)$$

$$K_1 = \frac{5000 - 100(12)}{250 + 40(0)} = 15.2$$

$$K_2 = f(t_0 + h, C_0 + K_1 h)$$

$$K_2 = f(2, 42.4)$$

$$K_2 = \frac{5000 - 100(42.4)}{250 + 40(2)} = 2.3030$$

$$\text{Hence, } C_1 = C_0 + \left( \frac{1}{2} K_1 + \frac{1}{2} K_2 \right) h$$

$$C_1 = 12 + \left( \frac{1}{2}(15.2) + \frac{1}{2}(2.3030) \right) 2 = 29.503 \text{mg/l}$$

For  $i = 1$ ,  $t_1 = t_0 + h = 0 + 2 = 2$ ,  $C_1 = C(1) = 29.503\text{mg/l}$

$$K_1 = f(t_1, C_1) = f(2, 29.503)$$

$$K_1 = \frac{5000 - 100(29.503)}{250 + 40(2)} = 6.2112$$

$$K_2 = f(t_1 + h, C_1 + K_1 h)$$

$$K_2 = f(24, 41.9254)$$

$$K_2 = \frac{5000 - 100(41.9254)}{250 + 40(4)} = 1.9694$$

$$\text{Hence, } C_2 = C_1 + \left(\frac{1}{2}K_1 + \frac{1}{2}K_2\right)h$$

$$C_2 = 29.503 + \left(\frac{1}{2}(6.2112) + \frac{1}{2}(1.9694)\right)2 = 37.6836\text{mg/l}$$

For  $i = 2$ ,  $2 = t_1 + h = 2 + 2 = 4$ ,  $C_2 = C(2) = 37.6836\text{mg/l}$

$$K_1 = f(t_2, C_2) = f(4, 37.6836)$$

$$K_1 = \frac{5000 - 100(37.6836)}{250 + 40(4)} = 3.004$$

$$K_2 = f(t_2 + h, C_2 + K_1 h)$$

$$K_2 = f(6, 43.6916)$$

$$K_2 = \frac{5000 - 100(43.6916)}{250 + 40(6)} = 1.2874$$

$$\text{Hence, } C_3 = C_2 + \left(\frac{1}{2}K_1 + \frac{1}{2}K_2\right)h$$

$$C_3 = 37.6836 + \left(\frac{1}{2}(3.004) + \frac{1}{2}(1.2874)\right)2 = 41.975\text{mg/l}$$

$$C_3 = C(4) = 41.975\text{mg/l}$$

## CHAPTER 4

### DATA COLLECTION, ANALYSIS AND RESULTS

#### 4.0 INTRODUCTION

This chapter consists of summary of data, formulation of model instances, computational procedure, results and discussions.

#### 4.1 SUMMARY OF DATA

Table 4.1 below shows the averages of the rates of flows, concentrations of the chlorine added for disinfection, initial concentrations of the disinfected water and that of the initial volumes of the clearwell collected for the months of February, March and April 2013 from the Ve-a- Gowrea Water Treatment Plant

**Table 4.1 Summary of data from the Ve-a- Gowrea Water Plant from January - March, 2013**

MODEL PARAMETER	JANUARY	FEBRUARY	MARCH	Averages for the three months
Flow – in – rates $\left(\frac{dV}{dt}\right)_{in}$ [l/h]	476000	492000	503000	490333
Flow – out - rates $\left(\frac{dV}{dt}\right)_{out}$ [l/h]	229000	190000	252200	223733
Concentration of chlorine added for disinfection( $C_{in.}$ ) [mg/l]	3.1	3.1	3.1	3.1
Initial concentration of chlorine in clearwell after flush out ( $C_0$ ) [mg/l]	1.2500	0.50000	1.0000	0.916667
Initial volume of water in the clearwell ( $V_{0.}$ ) [L]	200000	145000	180000	175000

Table 4.2 in page 39 contains averages of experimentally determined concentrations at an interval of every 2hours for 24hours in each day from the Vea – Gowrea Water Treatment Plant from January to March, 2013.

**Table 4.2: Average Chlorine concentrations from Vea – Gowrea Water Plant [Jan – Mar, 2013]**

Time of Reading [GMT]	Contact Time [hours]	Average Chlorine Concentration [mg/l]
6:00	0.0000	0.9167
8:00	2.0000	1.2500
10:00	4.0000	1.5833
12:00	6.0000	1.6667
14:00	8.0000	1.5000
16:00	10.0000	1.5000
18:00	12.0000	0.8333
20:00	14.0000	1.2500
22:00	16.0000	1.7500
24:00	18.0000	1.6667
2:00	20.0000	1.6667
4:00	22.0000	1.5000

#### 4.2 FORMULATION OF MODEL INSTANCES

From table 4.1 in page38, an average of 3.1mg/l of chlorine flows into the clearwell of the water plant for disinfection which initially contains 175000L of filtered water in an ambient concentration of 0.916667mg/l. The filtered water is being added into the clearwell of the plant at a rate of 490333 L/H and that of the disinfected water is allowed to flow out of the clearwell at a rate of 223733 L/H.

This implies; Flow – in rate  $\left(\frac{dV}{dt}\right)_{in} = 490333 \text{ L/H}$  and flow – out rate  $\left(\frac{dV}{dt}\right)_{out} = 2237331 \text{ L/H}$

Concentration of chlorine added for disinfection ( $C_{in.}$ ) = 3.1mg/l

But initial concentration of chlorine in clearwell after flush out ( $C_0$ ) = 0.916667mg/l

And initial volume of water in the clearwell ( $V_0$ ) = 175000L

Therefore, from page 30, [3.10] the differential equation of the concentration model is given as

$$\frac{dc}{dt} + \left[ \frac{\left(\frac{dV}{dt}\right)_{in}}{V_0 + At} \right] \cdot C(t) = \frac{\left(\frac{dV}{dt}\right)_{in} \cdot C_{in}}{V_0 + At}$$

$$\frac{dc}{dt} + \frac{490333 C(t)}{175000+266600t} = \frac{490333 \times 3.1}{175000+266600t} \quad \text{upon substituting}$$

$$\text{This implies, } \frac{dc}{dt} + \frac{490333 C(t)}{175000+266600t} = \frac{1520032.3}{175000+266600t}$$

Making  $\frac{dc}{dt}$  the subject and simplifying

$$\frac{dc}{dt} = \frac{1520032.3 - 490333 C(t)}{175000+266600t} \quad (\text{first order ordinary differential equation})$$

#### 4.4 RUNGE – KUTTA NUMERICAL SOLUTION TO MODELED DIFFERENTIAL EQUATION USING MATLAB

The Runge – Kutta Second Order Method is implemented in Matlab using Ode23solve function as shown below;

Step 1: Define the system of ODE as a function.

Function dy = system (t, y)

Step 2: Set initial conditions for ODE.

tspan = [initial, interval, final]

Step 3: Call ODE23 solver using the function handle.

$$[t, y] = \text{ode23}(@\text{system}, \text{tspan}, \text{initial})$$

Step 4: Plot results.

## 4.5 RESULTS

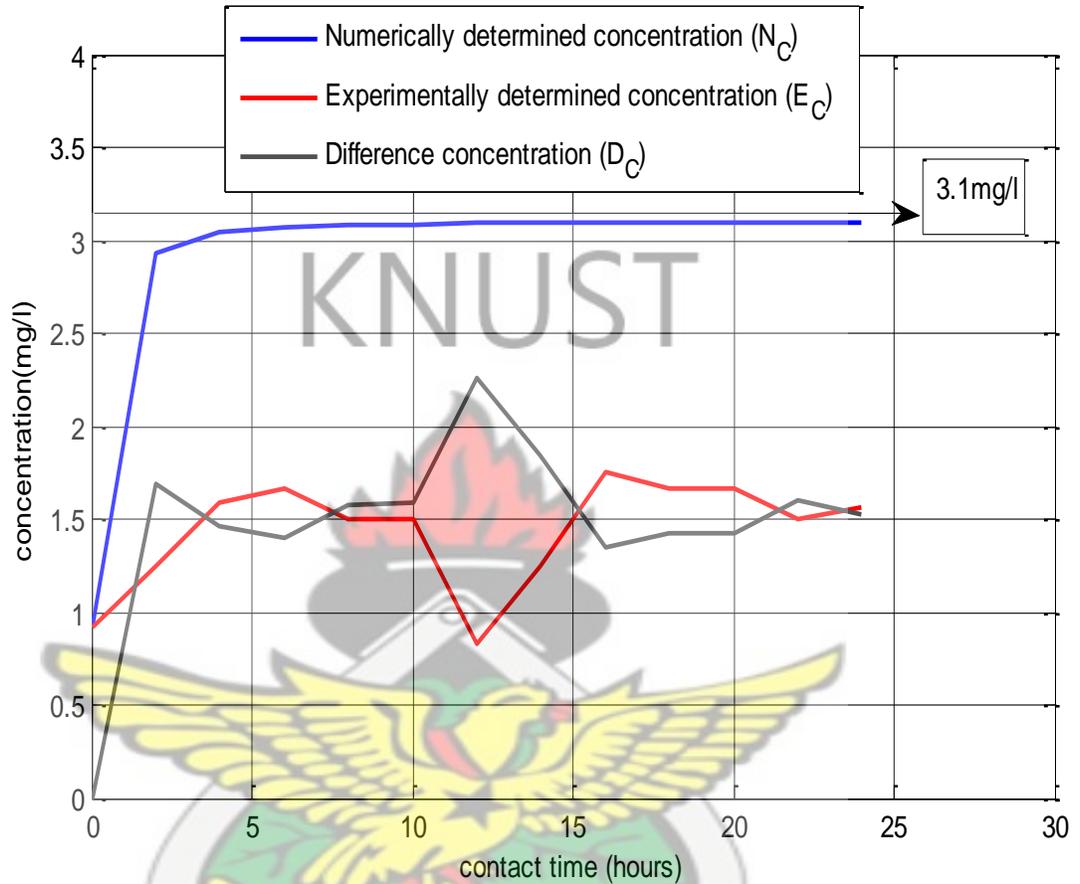
Table 4.3 in page 41 shows the numerically determined concentrations ( $N_C$ ), experimentally determined concentrations ( $E_C$ ) from plant and the difference between the two concentrations ( $D_C$ ) for an interval of every 2hours for a period of 24hours each day between January to March, 2013

**Table 4.3 Chlorine concentrations of treated water for an interval of every 2hours for a period of 24hours between January and March, 2013**

Time [GMT]	Contact Time [hours]	Numerically determined concentration ( $N_C$ ) [mg/l]	Experimentally determined concentration from the water plant ( $E_C$ ) [mg/l]	Difference between Numerical concentrations and Experimental concentrations ( $D_C$ ) [mg/l]
6:00	0:0000	0.9167	0.9167	0.0000
8:00	2:0000	2.9340	1.2500	1.6840
10:00	4:0000	3.0415	1.5833	1.4582
12:00	6:0000	3.0700	1.6667	1.4033
14:00	8:0000	3.0817	1.5000	1.5817
16:00	10:0000	3.0876	1.5000	1.5876
18:00	12:0000	3.0910	0.8333	1.8431
20:00	14:0000	3.0931	0.1250	1.8431
22:00	16:0000	3.0946	1.7500	1.3446
24:00	18:0000	3.0956	1.6667	1.4289
1:00	20:0000	20.0000	1.6667	1.4296
2:00	22:0000	3.0969	1.5000	1.5969
4:00	24:0000	3.0974	1.5671	1.5304

Matlab plot of results in table 4.3 above yields figure 4.1 in page 43.

**Figure 4.1: MATLAB line plots of numerically determined concentrations ( $N_C$ ), experimentally determined concentrations ( $E_C$ ) and the difference concentrations ( $D_C$ ) of table 4.3**



From the results of table 4.3 and figure 4.1, it can be observed that;

1. Concentrations determined numerically ( $N_C$ ) are significantly greater than those determined experimentally ( $E_C$ ) from the plant, since the values of ( $D_C$ ) from table 4.3 are greater than 1.
2. Concentrations determined numerically ( $N_C$ ) increases and approaches a constant concentration of 3.1mg/l which is the concentration of the in – coming chlorine from the chlorine chamber.
3. Concentrations determined experimentally ( $E_C$ ) and the difference concentrations ( $D_C$ ), though increases and decreases at different time periods as

seen in figure 4.1, assumes the shape of an exponential function just like the curve of concentrations determined numerically( $N_C$ ).

#### 4.6 DISCUSSIONS

This significant difference between Concentrations determined numerically ( $N_C$ ) and that of Concentrations determined experimentally ( $E_C$ ) of the results, signifies the significant part of chlorine concentration which reacts with organic matter and metals present in the water to form chlorine by – products such as THMs and HAAs and also an insignificant portion which reacts with the walls of pipes and clearwell. Therefore higher values of  $D_C$  at any particular point of time, indicates higher concentrations of THMs and HAAs present in treated water. It will also correspond to higher concentrations of pollutant such as organic matter and metals present in the water source (dam).

Also, the increasing and decreasing curves of ( $D_C$ ) and ( $E_C$ ) of figure 4.1 signifies that the concentrations of organic matter and metals of the water is not constant and that the amount of chlorine needed for disinfection varies with time.

## CHAPTER 5

### CONCLUSION AND RECOMMENDATION

#### 5.1 Conclusion

The research results suggest successfully that the numerical determination of the portability of treated water, a case study of the Vea – Gowrea Water Treatment Plant was achieved through the numerical determined concentrations ( $N_C$ ) of treated water of the plant for an interval of 2hours for a period of 24hours each day using data collected from the plant between January and March 2013.

Also, the research was carried out based on two objectives. The first; to model into differential equations, the flow of chlorine from chlorine chamber to the clearwell of the plant using rates equations. Two models were developed, [3.2] and [3.7] known as the volume and mass models respectively. These ultimately culminated into the concentration model [3.10] using the flow rates of water and chlorine concentrations into and out of the clearwell.

Secondly, Runge – kutta second order numerical solution method to ODE using ode23 solver of MATLAB 7.9.0 (R2009b) was used to execute the differential model to numerical determine the concentration levels of chlorine of the treated water, hence its portability.

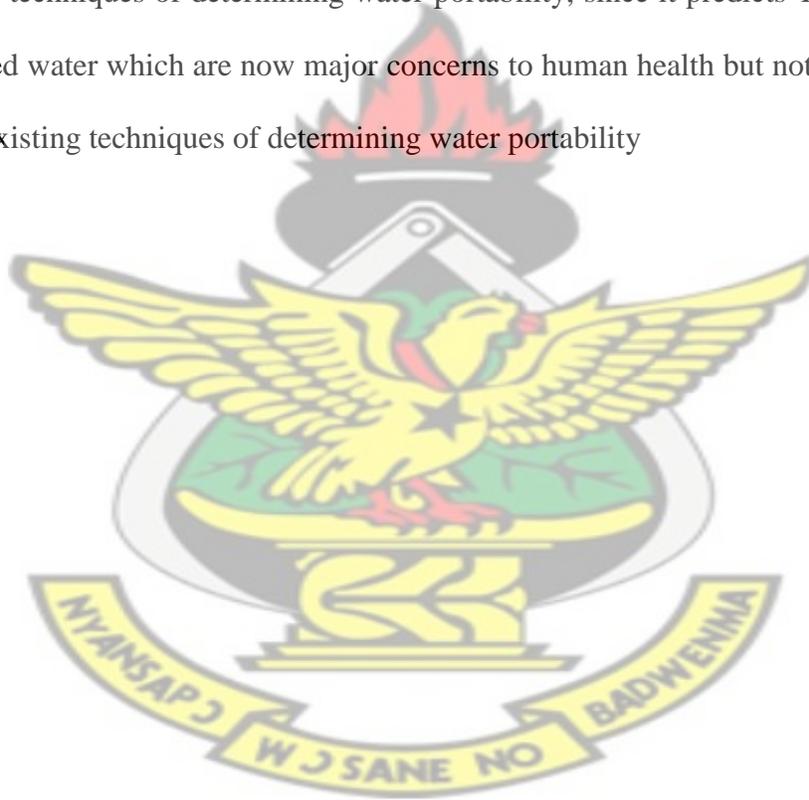
However, results of  $D_C$  of table 4.3 and figure 4.1 could further be used to predict the concentrations levels of THMs and HAAs in the treated water. It could also be a good

indicator of the level of organic matter and metals (pollutants) present in the source water (dam).

## 5.2 Recommendation

I recommend that chlorine loss due to reaction with organic matter, metals and walls of pipelines should be factored into model by any future researcher.

Also, model should be used by management of water treatment plant in conjunction with existing techniques of determining water portability, since it predicts THMS and HAAs in treated water which are now major concerns to human health but not checked in most of the existing techniques of determining water portability



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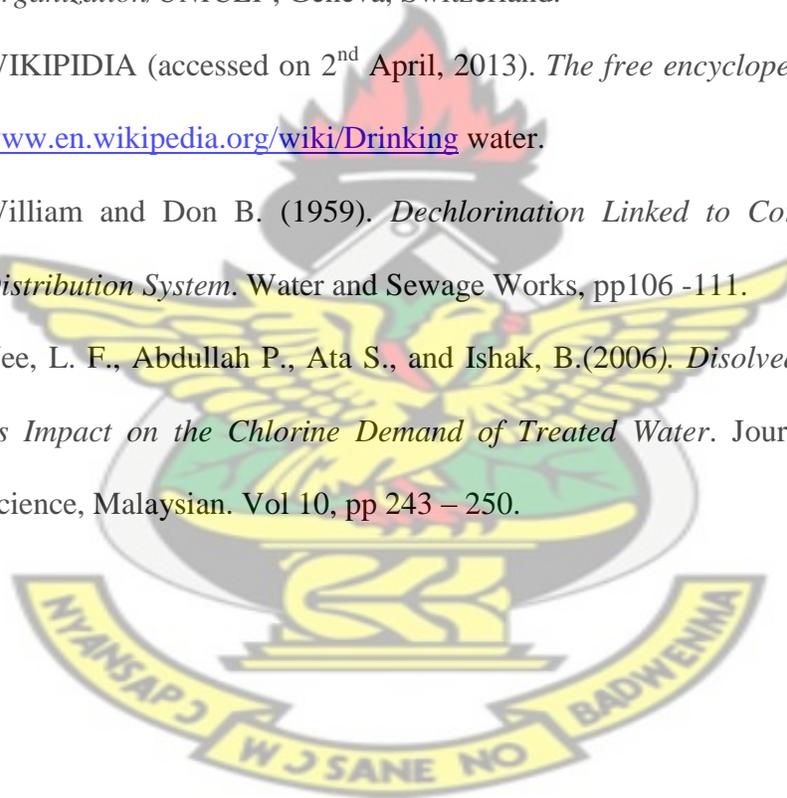
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## APPENDIX A

### MATLAB COE AND OUTPUT OF NUMERICAL SOLUTION TO RUNGU – KUTTA SECOND ORDER TO MODELED DIFFERENTIAL EQUATION USING ODE45 SOLVER OF MATLAB 7.9.0(R2009b)

```
dc=inline('(1520032.3-490333*c)/(175000+266600*t)','t','c')
```

```
dc =
```

```
Inline function:
```

```
dc(t,c) = (1520032.3-490333*c)/(175000+266600*t)
```

```
>> tspan=[0:2:24];c0=0.91667;
```

```
>> [t,c]=ode23(dc,tspan,c0);
```

```
>> [t,c]
```

```
ans =
```

0	0.9167
2.0000	2.9340
4.0000	3.0415
6.0000	3.0700
8.0000	3.0817
10.0000	3.0876
12.0000	3.0910
14.0000	3.0931
16.0000	3.0946
18.0000	3.0956
20.0000	3.0963
22.0000	3.0969
24.0000	3.0974