# *PREDICTIVE MODEL DEVELOPMENT AND SIMULATION OF SOME PARAMETERS IN WASTE WATER A CASE STUDY OF THE SHELL PETROLEUM DEVELOPMENT COMPANY NIGERIA LIMITED, PORT HARCOURT (DIEBU CREEK FLOW STATION, BAYELSA SWAMP)*

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*MINNA, NIGER STATE*

*NOVEMBER, 2004*

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***A FINAL YEAR PROJECT SUBMITTED IN PARTIAL FULFILMENT OF THE REQUIREMENT FOR THE AWARD OF BACHELOR OF ENGINEERING (B. ENG.) TO THE DEPARTMENT OF CHEMICAL ENGINEERING, FEDERAL UNIVERSITY OF TECHNOLOGY, MINNA***

***NOVEMBER, 2004***

## *DECLARATION*

I, AJIBADE FOLASHADE MUINAT, declares that this project is my original work and has never, to my knowledge, been submitted elsewhere.

| | |
|---|---|
| AJIBADE F. MUINAT | 22/Nov/2004 DATE |

## *CERTIFICATION*

This is to certify that this research work which was duly supervised has been presented by AJIBADE FOLASHADE MUINAT (98/6846EH) in partial fulfilment of the requirement for the award of the degree of Bachelor of Engineering (B. Eng.) in Chemical Engineering.

ENGR. D. O. AGBAJELOLA
PROJECT SUPERVISOR

22-11-2004
DATE

DR. F. ABERUAGBA
HEAD OF DEPARTMENT

DATE

EXTERNAL EXAMINER

DATE

## *DEDICATION*

This project is dedicated to the glory of Almighty Allah, then to the memory of my beloved father, Late Mr. Uthman ajibade. May Almighty Allah grant him Aljannatu-l-Firdaus (Amin).

## *ACKNOWLEDGEMENT*

All praises is due to Almighty Allah (S.W.T.), The Most Gracious, The Most Merciful, for His compassion over me.

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*ABSTRACT*

The experimental data were obtained from The Shell Petroleum Development Company Nigeria Limited, Port Harcourt (Diebu Creek Flow Station, Bayelsa Swamp). The pH which was used as the optimization criteria was modelled using the empirical method of the least square. The pH is a reflection of the effects of temperature, turbidity, salinity, total dissolved solids, total suspended solids, total iron, biochemical oxygen demand, chemical oxygen demand, and zinc respectively. A modelled equation is thus obtained using MathCAD 2000 Professional and Excel software. On simulation, the modelled pHs were obtained .Comparison shows that there is good correlation between the simulated and the experimental pH. Therefore the simulated results verify the mathematical model proposed for analyzing the behaviour of the various parameters on pH as being an adequate representation and thus can serve as a tool for predicting the performance of the system. The computer simulation allows the variation of the various parameters to effect a change in the pH, therefore, enabling the use of the model developed for further analysis.

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# *CHAPTER ONE*

## *1.0 INTRODUCTION*

### *1.1 SEWAGE*

This is the wastewater released by residences, businesses and industries in a community. It is 99.94 percent water, with only 0.06 percent of the wastewater dissolved and suspended solid material. The cloudiness of sewage is caused by suspended particles that in untreated sewage ranges from 100 to 350 mg/l. A measure of the strength of the wastewater is biochemical oxygen demand, or BOD5. The BOD5 measures the amount of oxygen micro organisms require in five days to break down sewage. Untreated sewage has a BOD5 ranging from 100 mg/l to 300 mg/l. Pathogens or disease-causing organisms are present in sewage. Coli form bacteria are used as an indicator of disease-causing organisms. Sewage also contains nutrients (such as ammonia and phosphorus), minerals, and metals.

Sewage treatment is a multi-stage process to renovate wastewater before it re-enters a body of water, is applied to the land or is reused. The goal is to reduce or remove organic matter, solids, nutrients, disease-causing organisms and other pollutants from wastewater. Each receiving body of water has limits to the amount of pollutants it can receive without degradation. Therefore, each sewage treatment plant must hold a permit listing the allowable levels of BOD5, suspended solids, coliform bacteria and other pollutants. The discharge permits are called NPDES permits that stand for the National Pollutant Discharge Elimination System.

The major aim of wastewater treatment is to remove as much of the suspended solids as possible before the remaining water, called effluent, is discharged back to the environment. As solid material decays, it uses up oxygen, which is needed by the plants and animals living in the water. "Primary treatment" removes about 60 percent of suspended solids from wastewater. This treatment also involves aerating (stirring up) the wastewater, to put oxygen back in. Secondary treatment removes more than 90 percent of suspended solids.

## *1.2 MODELLING*

Modelling is nothing more than obtaining a mathematical abstraction of a real process. It is intend to enhance our ability to understand, explain, predict and possibly control the behaviour of a system (Seaborg,1989). Modelling is thus the process of establishing the interrelation between the important entities of a system. Mathematical modelling is versatile and is widely used in practice. It is a recognised and valuable adjunct, and usually a precursor of computer simulation. Models can be classified into:

a. Empirical model that is obtained from a mathematical (statistical) analysis of process operating data.
b. Theoretical model that is developed using the principles of Chemistry and Physics.
c. Semi-empirical model.

## *1.3 SIMULATION*

Simulation is the process of imitating important aspects of the behaviour of a system in real time, compressed time or expanded time by constructing and experimenting with a model of the system (Neetamkavil, 1987).

Computer simulation however means the running of a special program on a suitable type of computer which generates time responses of the model that imitate the behaviour of the process being studied.

## *1.4 AIM AND OBJECTIVES*

The aim of this project is to develop a predictive model and simulation of some parameters in wastewater. This aim can be achieved through the realization of the following objectives:

1. Collection of data.
2. Modelling.
3. Simulation of the model.

## *1.5 SCOPE OF WORK*

This work is limited to modelling and simulation of some parameters in waste water.

Case study: THE SHELL PETROLEUM DEVELOPMENT COMPANY NIGERIA LIMITED, PORT HARCOURT.

## *CHAPTER TWO*

### *2.0 LITERATURE REVIEW*

### *2.1 ANALYSIS OF WASTE WATER*

Analysis of water for is constituents provide an opportunity to apply and exploit chemical phenomena to expand our understanding of them and arrive at concrete results to evaluate the state of the water vis-à-vis its health aspects, use as a resource and role in ecosystem (Droste,1997).

Wastewater or sewage is a menace to health because it usually contains pathogens and other substances that may contaminate food and drinking water. It may also be offensive to the senses of sight and smell. There are several kinds of wastewater, among which are domestic sewage that is produced by normal activities in the home. It includes toilet drainage, ground-up garbage, and water from sinks, bath tubes, and washing machines and industrial wastewater includes liquid wastes from factories and other industrial plants.

### *2.2 CHARACTERISTICS OF WASTE WATER*

The characteristics of waste water are determined for many purposes: To obtain the physical, chemical and biological parameters; to determine the concentration of all the constituents in the waste water and to find out the best method to be used in reducing the concentration of pollutants.

#### *2.2.1 PHYSICAL CHARACTERISTICS*

The most important physical characteristics of waste water include: temperature, turbidity, total solid content, odour, colour, etc.

#### *2.2.1.1 TEMPERATURE*

The temperature of waste water is usually higher than those of water supply as a result of water being discharged from household and industrial activities. Temperature exerts an influence on the rate of oxidation of organic matter. High water temperature stress aquatic ecosystems by reducing the ability of water to hold essential dissolved gases like oxygen.

#### *2.2.1.2 TURBIDITY*

Turbidity is the measure of water clarity. The more suspended solids in the water, the murkier it becomes. Turbidity is as a result of the scattering and absorption of light by suspended solids. The size and concentration of particles influence the measurement of turbidity. A natural water or waste water will contain many different sized particles at different concentrations, the relation between suspended solids concentration and turbidity can be highly variable.

#### *2.2.1.3 TOTAL SOLIDS*

The characterization of solids is one of the most common assessments of water quality. Total solids (sometimes called total residue) is related to turbidity, except that it includes not just suspended solids, but also dissolved solids such as the mineral ions, calcium, phosphorus ions, sulphur, and bicarbonate. A certain level of these ions is essential for life.

Solids in a water fall into one of the following categories: dissolved, colloidal and suspended solids.

Dissolved solids are truly in solution and pass through a filter. The solution consisting of the dissolved components and water is homogenous, forming a single phase.

Colloidal solids are uniformly dispersed in solution but they form a solid phase that is distinct form the water phase. Colloidal solutions are termed sols.

Suspended solids are also a separate phase from the solution.

### 2.2.2 *CHEMICAL PROPERTIES OF WASTE WATER*

The chemical characteristics of waste water include its nitrogen and phosphorus contents, biochemical oxygen demand (BOD), chemical oxygen demand (COD), organic mater and so on.

#### 2.2.2.1 *PHOSPHORUS*

One of the key elements necessary for growth of plants and animals is phosphorus. It is very toxic and is subject to bioaccumulation when in its elemental form. Phosphate will stimulate the growth of aquatic animals and if an excess of it enters the water way, it enhances rapid growth of aquatic vegetation and a large amount of oxygen is being used up. Phosphate are not toxic to people or animals unless they are present in very high levels.

#### 2.2.2.2 *NITROGEN*

The major routes of entry of nitrogen into water bodies are through municipal and industrial wastewater, septic tanks discharge, animal waste addition (including birds and fish), etc. Nitrogen-containing compounds act as nutrients for bacteria in streams and rives. Nitrate reactions ($NO_3^-$) in fresh water can cause oxygen depletion. This can cause the death of organisms which depend on the supply of oxygen in the stream. Bacteria in water quickly convert nitrites ($NO_2^-$) to nitrates ($NO_3^-$).

### *2.2.2.3 BIOCHEMICAL OXYGEN DEMAND (BOD)*

Biochemical oxygen demand is an indicator for the concentration of organic-waste, bacteria, and other micro-organisms in a sample of water. Biochemical oxygen demand (BOD) is defined as the amount of oxygen required for the biological decomposition of organic matter under aerobic conditions at a standardised temperature and time of incubation. (Droste,1997). Commonly, BOD is used to test the strength of untreated and treated municipal and biodegradable industrial wastewater.

### *2.2.2.4 CHEMICAL OXYGEN DEMAND (COD)*

In environmental chemistry, the COD test is commonly used to indirectly measure the amount of organic compounds in water. Most applications of COD determines the amount of organic pollutants found in surface water (e.g. lakes and rivers), making COD a useful measure of water quality. It is expressed in mg/L which indicates the mass of oxygen demand per litre of solution.

Chemical oxygen demand is the amount of oxygen required to oxidize organic matter by the use of dichromate in an acid solution and to convert it to carbon dioxide and water. It is used to test the strength of waste water that is either not biodegradable or contains compounds that inhibit activities of micro organism. The value of COD is always higher than that of BOD because many organic substances can be oxidized chemically but cannot oxidize biologically.

### *2.2.3 BIOLOGICAL CHARACTERISTICS OF WASTE WATER*

Micro organisms such as bacteria are responsible for decomposition of organic waste. When organic matter such as dead plants, sewage, or even food waste is present in a water supply, the bacteria will begin the process of breaking down this waste. In this case, much of the available dissolved oxygen is consumed by anaerobic bacteria, robbing other aquatic organisms of the oxygen they need to live.

### *2.2.3.1 COLIFORM BACTERIA*

Total coliform bacteria are a collection of relatively harmless micro organisms that live in large number in the intestine of man and warm and cold blooded animals. They aid in the digestion of food. A specific subgroup of this collection is the fecal coliform bacteria, the most common member being Escherichia coli. These organisms may be separated from the total coliform group by their ability to grow at elevated temperature and are associated only with the fecal material of warm blooded animals.

Other parameters used in measuring water quality include electrical conductivity, pH, total hardness and so on.

### *2.2.3.2 ELECTRICAL CONDUCTIVITY*

This is a measure of low well a material accommodates the transport of electric charge. Conductance is an electrical phenomenon where a material contains movable particles with electric charge, which carry electricity. When a difference of electrical potential is placed across a conductor, its movable charges flow, and an electric current appears. A conductor such as a metal has high conductivity and insulation like glass or a vacuum has low conductivity.

### *2.2.3.3pH*

pH is a measure of the acidic or basic (alkaline) nature of a solution. The concentration of the hydrogen ion ($H^+$) acidity in a solution determines the pH. A pH range of 6.0 to 9.0 appears to provide protection for the life of freshwater fish and bottom dwelling invertebrates.

## 2.3 *WASTE WATER TREATMENT*

Waste water can be disposed of by discharging it into the water body or into or on land. It is usually treated before disposal. The treatment process varies with the kind and amounts of wastes in the water.

The main objectives of waste water treatment processes are reduction in biochemical oxygen demand (BOD), chemical oxygen demand (COD), suspended solids and pathogenic organisms. Also, it may be necessary to remove nutrients, toxic compounds, non-biodegradable compounds and dissolved solids.

Waste water treatment process consists of several stages:

i. Primary treatment.

ii. Secondary treatment.

iii. Tertiary treatment.

### 2.3.1 *PRIMARY TREATMENT*

Primary treatment removes most of the solids from the sewage by settling or floating. Sedimentation is usually by gravity. Chemical may be added in primary treatment to neutralise the stream or to improve the removal of small suspended particles. Primary reduction reduces subsequent biological steps and also reduces the solids loading the secondary sedimentation tank.

### 2.3.2 *SECONDARY TREATMENT*

Secondary treatment is usually a biological process which removes organic matter through biochemical oxidation. It removes bacteria and offensive smells from the sludge and water. It generally employs bacteria to consume the available nutrients and organic compounds, leaving behind inorganic salts, carbon dioxide and water.

### *2.3.3 TERTIARY TREATMENT*

Tertiary treatment removes minerals from the water to restore it to a more natural state. The most damaging remaining minerals are usually nitrates and phosphates which can cause eutrophicatin. Common techniques used in tertiary treatment include reverse osmosis, pressure membrane – purification, distillation, etc.

## *2.4 ENVIRONMENTAL IMPACT OF WASTE WATER*

Waste water can have negative effects on ecosystems, water quality, fish communities, human health and aesthetics. High level of nutrients in waste water can cause tiny floating plants to bloom which may kill fish and invertebrates. Blooms can also produce toxins which make water unsafe for swimming and sea food dangerous to eat. Too much dissolved solids in water can affect humans by inducing laxative effect and giving the water a mineral taste.

High rate of decomposition causes the decay micro organism to consume all of the available oxygen, that are required for the survival of aquatic animals.

The increased turbidity of water can reduce the diversity of life in three ways:

i. Suspended particles absorb heat from sunlight and warm the water. Warmer water holds less oxygen and organisms begin to suffer. Also, some organisms cannot live in the warmer water.

ii. Particles also block sunlight. Plants and algae grow less and release less oxygen from photosynthesis.

iii. Particles also settle on the bottom and can cover and suffocate fish eggs and insect larvae.

Exposure of individual to water that is contaminated with coliform bacteria causes water borne pathogenic diseases`which includes typhoid fever, viral and bacterial gastro enteritis.

## *2.5 MATHEMATICAL MODELLING*

Mathematical modelling is the general characterization of a process or concept in mathematical terms, thus enabling the relatively simple manipulation of variables to be accomplished in order to determine how these processes or concept would behave in different situations (Paynes, 1982). It attempts to describe the functional relationship of the variables and parameters by a set of equations and thus, showing more clearly the cause and effect relationships of the variables.

Mathematical modelling is versatile and is widely used in practice. It is a recognised and valuable adjunct and usually a precursor of computer simulation. In developing a mathematical model, you need to determine the mathematical expression that will relate what is known to what you intend to determine. In developing a mathematical system that models the system, when values are input into the model, it will act upon this input and produce an output. The major goal is to have this output be of reasonable approximation of the corresponding response or output of the actual system. Many mathematical models that are difficult or tedious to solve by normal hand calculations can be solved efficiently with the computer. However, the solution will only be as good as the mathematical model.

### *2.5.1 PRINCIPLES OF MATHEMATICAL FORMULATION*

The principles involved in the formulation of mathematical models are as stated below:

1. Basis: The basis for the mathematical models are the fundamental physical and chemical laws, such as the law of mass, energy and momentum conservation stated in their time derivative forms. Others include parameters such as mass transfer coefficient, diffusivity constant, reaction rates which are either obtained experimentally or from process operating data.
2. Assumptions: There is need to make simplifying but reasonable assumptions about the system while modelling. The outcome of the model is dependent on the assumptions as they impose limitation on the model.
3. Mathematical consistency of model: Care must be taken not to under specify or over specify the number of variables or equations describing the system because in order to obtain a solution, the numbers of variables must equal the mber of equations, that is, the degree of freedom of the system must be zero.
4. Solution of the model equation: Available solution techniques and tools must be kept in mind as the model is being developed, as a model that contains unknown and immeasurable parameters is unsolvable and amount to a waste of time and energy. In the search for a method of solution, possible approximations for the defining equations, boundary and initial conditions and acceptable final solutions are considered.
5. Verifications: The need to prove the validity of a model is an important part of mathematical modelling. Because of the complex nature of

verifying the models, it is often neglected. However, one way of achieving this objective is by comparing average experimental result for similar operating conditions to the computed results.

### *2.5.2 SIMULATION*

Martin Shubik defines simulation of a system as the operation of a model, which is a representation of the system, the model being amenable to manipulations which would be impossible, too expensive or impractical or perform on the system it portrays.

Simulation is used for two principal reasons:

i. To give greater understanding and insight into the behaviour of the physical system and the principles upon which its design is based.

ii. To provide a convenient, inexpensive and time saving means of gaining this understanding and insight under a variety of operating conditions.

### *2.5.3 COMPUTER SIMULATION*

Computer simulation however means the running of a special program on a suitable type of computer which generates time response of the model that imitates the behaviour of the process being studies. There are two types of simulation methods, namely, analogue and digital simulation. However, digital simulation is more frequently used because of the enhanced capabilities and operational speed of modern electronic computers which are used in executing computer algorithm of the models.

Modelling and simulation can be carried out with the aid of the computer using some powerful software packages like Excel, Polymath, MathCAD, Spss and so on. In this work, a mathematical modelling was performed using Excel and MathCAD.

### *2.5.4 IMPORTANCE OF MATHEMATICAL MODELLING*

It is quite often the case that we have to design the control system for a chemical process before the process is being constructed. In such as case, we cannot rely on the experimental procedures and we need a different representation of the chemical process in order to study its dynamic behaviour. This representation is usually a set of mathematical equation whose solution yields the dynamics or static behaviour of the chemical process we examine.

Mathematical modelling and simulation can result in considerable saving of both time and money. When it is impractical to experiment with the real system, mathematical modelling and simulation can be used to explore the effect of changes on a system. It can also result in an increase in the fundamental knowledge about a system since it usually involves a considerable analysis of the system.

Many chemical process developments in the recent years were undertaken through model development. A typical example of a developed model using pH as the optimization criteria was reported in the work of Adeniyi and Odigure (2002).

In their work, the pH was modelled using the empirical method of the least square method (Carnahan et al, 1969, Himmelblau, 1987) of the form

$$pH = f(\text{Temperature}, TSS, COD, \text{hardness}, Ca, Mg, Cl)$$

which becomes

$$pH = f\left(a \cdot T + b \cdot t + c \cdot C_1 + d \cdot H + e \cdot C_2 + f \cdot M + g \cdot C_3\right)$$

They represented I as the square of the error between the observed pH and a predicted value, P.

$$I = \left[P - \left(a \cdot T + b \cdot t + c \cdot C_1 + d \cdot H + e \cdot C_2 + f \cdot M + g \cdot C_3\right)\right]^2$$

For n experimental values of P and other variable,

$$nI = \sum \left(P_i - a \cdot T_i - b \cdot t_i - c \cdot C_{1i} - d \cdot H_i - e \cdot C_{2i} - f \cdot M_i - g \cdot C_{3i}\right)^2$$

They then obtained the condition for a minimum and arrived at a set of linear equations, after which basic program was used to obtain the sum from the experimental data. They used the summation to form a 7 x 7 matrix and the constant coefficients were obtained with a computer program using Gauss-Jordan elimination method.

The model equation obtained in this work was

$$P_m = \left(0.1137949399 \cdot T + 0.022099205 \cdot t + 0.0832652449 \cdot C_1 + 0.0937238337 \cdot H\right) \ldots \\ + -0.080762186 \cdot C_2 - 0.035212731 \cdot M + 0.0034813083 \cdot C_3$$

They calculated the percentage error using the modelled and experimental value.

The comparative values of their experimental results and the modelled pH values were presented in Table 1 below.

Table 1: Comparative pH values for experimental and developed model

| Month | Observed pH value | Model pH value | Percentage error (%) |
|---|---|---|---|
| January | 9.50 | 9.52 | 0.21 |
| February | 9.20 | 9.25 | 0.54 |
| March | 9.00 | 9.00 | 0.00 |
| April | 8.90 | 8.70 | 2.25 |
| May | 9.00 | 9.08 | 0.88 |
| June | 9.80 | 9.53 | 2.76 |
| July | 9.50 | 9.52 | 0.21 |
| August | 9.20 | 9.25 | 0.54 |
| September | 9.00 | 9.00 | 0.00 |
| October | 8.90 | 8.70 | 0.25 |
| November | 9.00 | 9.07 | 0.77 |
| December | 9.80 | 9.50 | 3.06 |

They then concluded that the developed model showed that the pH value is a reflection of the physicochemical and technological parameters. They also concluded that the parametric coefficients in the model equation obtained showed the effect of some of the measured parameters on the overall pH value (i.e. increasing acidity and alkalinity).

# *CHAPTER THREE*

## *3.0 METHODOLOGY*

The model proposed here is based on that used by Adeniyi & Odigure (2002). The model is developed using two methods:

1. Modelling with MathCAD 2000 Professional.
2. Modelling with Excel.

## *3.1 MODELLING AND SIMULATION FOR WATER QUALITY USING PH AS THE OPTIMIZATION CRITERIA*

### *3.1.1 MODELLING WITH MATHCAD 2000 PROFESSIONAL*

The pH of water is a reflection of the resultant effects of temperature, turbidity, salinity, total dissolved solids, total suspended solids, total iron, biochemical oxygen demand, chemical oxygen demand, zinc, etc.

Mathematically, based on the proposed modelling,

$$pH = f(temp, turbidity, salinity, TDS, TSS, total\_iron, COD, BOD, zinc) \qquad ---(3.1)$$

Let $Temperature = T$

$Turbidity = Tu$

$Salinity = S$

$Total\_dissolved\_solids = Td$

$Total\_suspended\_solids = Ts$

$Total\_iron = Fe$

$Biochemical\_oxygen\_demand = Bo$

$Chemical\_oxygen\_demand = Cd$

$Zinc = Zn$

Then equation (1) becomes,

$$pH = f(a \cdot T + b \cdot Tu + c \cdot S + d \cdot Td + e \cdot Ts + f \cdot Fe + g \cdot Bo + h \cdot Cd + i \cdot Zn) \qquad ---(3.2)$$

where the pH is the dependent variable in the equation; a, b, c, d, e, f, g, h and i are the

coefficients which need to be determined and T, Tu, S, Td, Ts, Fe, Bo, Cd and Zn are the

independent variables for the desired pH.
Let I represent the square of the error between the observed pH and its predicted value (P).

Using the experimentally obtained data of T, Tu, S, Td, Ts, Fe, Bo, Cd and Zn. Therefore,

$$I = [P - (a \cdot T + b \cdot Tu + c \cdot S + d \cdot Td + e \cdot Ts + f \cdot Fe + g \cdot Bo + h \cdot Cd + i \cdot Zn)]^2 \quad ---(3.3)$$

For *n* experimental values of P and T, Tu, S, Td, Ts, Fe, Bo, Cd and Zn,

$$nI = \sum (P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i)^2 \quad ---(3.4)$$

To minimize *nI* with respect to the coefficients a, b, c, d, e, f, g, h, and i using the first partial

derivatives of *nI* with respect to these constants and equating these to zero we obtain the

necessary conditions for a minimum. So from equation (4),

$$\frac{\partial}{\partial a}(nI) = -2 \cdot \sum T_i \cdot (P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i) = 0 \quad ---(3.5)$$

$$\frac{\partial}{\partial b}(nI) = -2 \cdot \sum Tu_i \cdot (P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i) = 0 \quad ---(3.6)$$

$$\frac{\partial}{\partial c}(nI) = -2 \cdot \sum S_i \cdot (P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i) = 0 \quad ---(3.7)$$

$$\frac{\partial}{\partial d}(nI) = -2 \cdot \sum Td_i \cdot (P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i) = 0 \quad ---(3.8)$$

$$\frac{\partial}{\partial e}(nI) = -2 \cdot \sum Ts_i \cdot (P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i) = 0 \quad ---(3.9)$$

$$\frac{\partial}{\partial f}(nI) = -2 \cdot \sum Fe_i \cdot (P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i) = 0 \quad ---(3.10)$$

$$\frac{\partial}{\partial g}(nI) = -2 \cdot \sum Bo_i \cdot \left(P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i\right) = 0$$

---(3.11)

$$\frac{\partial}{\partial h}(nI) = -2 \cdot \sum Cd_i \cdot \left(P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i\right) = 0$$

---(3.12)

$$\frac{\partial}{\partial i}(nI) = -2 \cdot \sum Zn_i \cdot \left(P_i - a \cdot T_i - b \cdot Tu_i - c \cdot S_i - d \cdot Td_i - e \cdot Ts_i - f \cdot Fe_i - g \cdot Bo_i - h \cdot Cd_i - i \cdot Zn_i\right) = 0$$

---(3.13)

When rearranged, these sets of linear equations become

$$\sum(T_i \cdot P_i) = a \cdot \sum(T_i)^2 + b \cdot \sum(T_i \cdot Tu_i) + c \cdot \sum(T_i \cdot S_i) + d \cdot \sum(T_i \cdot Td_i) + e \cdot \sum(T_i \cdot Ts_i) + f \cdot \sum(T_i \cdot Fe_i) + g \cdot \sum(T_i \cdot Bo_i) + h \cdot \sum(T_i \cdot Cd_i) + i \cdot \sum(T_i \cdot Zn_i) \quad ---(3.14)$$

$$\sum(Tu_i \cdot P_i) = a \cdot \sum(Tu_i \cdot T_i) + b \cdot \sum(Tu_i)^2 + c \cdot \sum(Tu_i \cdot S_i) + d \cdot \sum(Tu_i \cdot Td_i) + e \cdot \sum(Tu_i \cdot Ts_i) + f \cdot \sum(Tu_i \cdot Fe_i) + g \cdot \sum(Tu_i \cdot Bo_i) + h \cdot \sum(Tu_i \cdot Cd_i) + i \cdot \sum(Tu_i \cdot Zn_i) \quad ---(3.15)$$

$$\sum(S_i \cdot P_i) = a \cdot \sum(S_i \cdot T_i) + b \cdot \sum(S_i \cdot Tu_i) + c \cdot \sum(S_i)^2 + d \cdot \sum(S_i \cdot Td_i) + e \cdot \sum(S_i \cdot Ts_i) + f \cdot \sum(S_i \cdot Fe_i) + g \cdot \sum(S_i \cdot Bo_i) + h \cdot \sum(S_i \cdot Cd_i) + i \cdot \sum(S_i \cdot Zn_i) \quad ---(3.16)$$

$$\sum(Td_i \cdot P_i) = a \cdot \sum(Td_i \cdot T_i) + b \cdot \sum(Td_i \cdot Tu_i) + c \cdot \sum(Td_i \cdot S_i) + d \cdot \sum(Td_i)^2 + e \cdot \sum(Td_i \cdot Ts_i) + f \cdot \sum(Td_i \cdot Fe_i) + g \cdot \sum(Td_i \cdot Bo_i) + h \cdot \sum(Td_i \cdot Cd_i) + i \cdot \sum(Td_i \cdot Zn_i) \quad ---(3.17)$$

$$\sum(Ts_i \cdot P_i) = a \cdot \sum(Ts_i \cdot T_i) + b \cdot \sum(Ts_i \cdot Tu_i) + c \cdot \sum(Ts_i \cdot S_i) + d \cdot \sum(Ts_i \cdot Td_i)^2 + e \cdot \sum(Ts_i)^2 + f \cdot \sum(Ts_i \cdot Fe_i) + g \cdot \sum(Ts_i \cdot Bo_i) + h \cdot \sum(Ts_i \cdot Cd_i) + i \cdot \sum(Ts_i \cdot Zn_i) \quad ---(3.18)$$

$$\sum(Fe_i \cdot P_i) = a \cdot \sum(Fe_i \cdot T_i) + b \cdot \sum(Fe_i \cdot Tu_i) + c \cdot \sum(Fe_i \cdot S_i) + d \cdot \sum(Fe_i \cdot Td_i)^2 + e \cdot \sum(Fe_i \cdot Ts_i) + f \cdot \sum(Fe_i)^2 + g \cdot \sum(Fe_i \cdot Bo_i) + h \cdot \sum(Fe_i \cdot Cd_i) + i \cdot \sum(Fe_i \cdot Zn_i) \quad ---(3.19)$$

$$\sum(Bo_i \cdot P_i) = a \cdot \sum(Bo_i \cdot T_i) + b \cdot \sum(Bo_i \cdot Tu_i) + c \cdot \sum(Bo_i \cdot S_i) + d \cdot \sum(Bo_i \cdot Td_i)^2 + e \cdot \sum(Bo_i \cdot Ts_i) + f \cdot \sum(Bo_i \cdot Fe_i) + g \cdot \sum(Bo_i)^2 + h \cdot \sum(Bo_i \cdot Cd_i) + i \cdot \sum(Bo_i \cdot Zn_i) \quad ---(3.20)$$

$$\sum(Cd_i \cdot P_i) = a \cdot \sum(Cd_i \cdot T_i) + b \cdot \sum(Cd_i \cdot Tu_i) + c \cdot \sum(Cd_i \cdot S_i) + d \cdot \sum(Cd_i \cdot Td_i)^2 + e \cdot \sum(Cd_i \cdot Ts_i) + f \cdot \sum(Cd_i \cdot Fe_i) + g \cdot \sum(Cd_i \cdot Bo_i) + h \cdot \sum(Cd_i)^2 + i \cdot \sum(Cd_i \cdot Zn_i) \quad ---(3.21)$$

$$\sum(Zn_i \cdot P_i) = a \cdot \sum(Zn_i \cdot T_i) + b \cdot \sum(Zn_i \cdot Tu_i) + c \cdot \sum(Zn_i \cdot S_i) + d \cdot \sum(Zn_i \cdot Td_i)^2 + e \cdot \sum(Zn_i \cdot Ts_i) + f \cdot \sum(Zn_i \cdot Fe_i) + g \cdot \sum(Zn_i \cdot Bo_i) + h \cdot \sum(Zn_i \cdot Cd_i) + i \cdot \sum(Zn_i)^2 \quad ---(3.22)$$

where $\Sigma = \Sigma^{n}_{i=1}$

and n = 3 and the sums are obtained from the experimental data using mathCAD program.

Table : Experimental water characteritics

A :=

| T | Tu | Sal | Td | Ts | Fe | Bo | Cd | Zn | pH |
|---|---|---|---|---|---|---|---|---|---|
| 27.5 | 3.5 | 240 | 580 | 7.5 | 2.66 | 12.64 | 26.38 | 0.154 | 6.56 |
| 30 | 4.8 | 14.44 | 20 | 3.52 | 4.14 | 45.6 | 20 | 0.105 | 6.9 |
| 28 | 4.8 | 14.44 | 20 | 20 | 4.21 | 3.52 | 45.6 | 0.064 | 5.6 |
| 29 | 1 | 284 | 455 | 9.36 | 2.44 | 31.62 | 20 | 0.071 | 6.8 |
| 29 | 1.25 | 416.3 | 525 | 21.63 | 3.66 | 11.3 | 30 | 0.081 | 7 |
| 30 | 3.15 | 52.6 | 330 | 32.4 | 2.88 | 4.55 | 18.36 | 0.108 | 6.9 |
| 29 | 2.2 | 84.62 | 145 | 14 | 3.3 | 12.6 | 46.4 | 0.056 | 6.9 |
| 28 | 0.65 | 125 | 210 | 20 | 2.81 | 9.26 | 39.15 | 0.053 | 7 |
| 29 | 1 | 200 | 325 | 21.8 | 2.8 | 12.6 | 29.2 | 0.1 | 7.9 |

With reference to the table above, the superscripts refers to the column

$T := A^{\langle 1 \rangle}$ $Tu := A^{\langle 2 \rangle}$ $S := A^{\langle 3 \rangle}$ $Td := A^{\langle 4 \rangle}$ $Ts := A^{\langle 5 \rangle}$

$Fe := A^{\langle 6 \rangle}$ $Bo := A^{\langle 7 \rangle}$ $Cd := A^{\langle 8 \rangle}$ $Zn := A^{\langle 9 \rangle}$ $pH := A^{\langle 10 \rangle}$

Based on the table of data, the summation shown in equations 14-22 are obtained thus:

$\sum \overrightarrow{(T)^2} = 7.4882 \times 10^3$ $\sum \overrightarrow{(T \cdot Tu)} = 645.4$ $\sum \overrightarrow{(T \cdot S)} = 4.1078 \times 10^4$

$\sum \overrightarrow{(T \cdot Td)} = 7.494 \times 10^4$ $\sum \overrightarrow{(T \cdot Ts)} = 4.3408 \times 10^3$ $\sum \overrightarrow{(T \cdot Bo)} = 4.1854 \times 10^3$

$\sum \overrightarrow{(T \cdot Fe)} = 834.11$ $\sum \overrightarrow{(T \cdot Cd)} = 7.8916 \times 10^3$ $\sum \overrightarrow{(T \cdot Zn)} = 22.833$

$\sum \overrightarrow{(Tu)^2} = 77.0775$ $\sum \overrightarrow{(Tu \cdot S)} = 2.4161 \times 10^3$ $\sum \overrightarrow{(Tu \cdot Td)} = 5.1532 \times 10^3$

$\sum \overrightarrow{(Tu \cdot Ts)} = 343.2035$ $\sum \overrightarrow{(Tu \cdot Fe)} = 77.3635$ $\sum \overrightarrow{(Tu \cdot Bo)} = 386.4325$

$\sum \overrightarrow{(Tu \cdot Cd)} = 679.2715$ $\sum \overrightarrow{(Tu \cdot Zn)} = 2.1203$ $\sum \overrightarrow{(S)^2} = 3.7753 \times 10^5$

$\sum \overrightarrow{(S \cdot Td)} = 6.0843 \times 10^5$ $\sum \overrightarrow{(S \cdot Ts)} = 2.3551 \times 10^4$ $\sum \overrightarrow{(S \cdot Fe)} = 4.3176 \times$ [illegible]

$\sum \overrightarrow{(S \cdot Bo)} = 2.241 \times 10^4$ $\sum \overrightarrow{(S \cdot Cd)} = 4.1073 \times 10^4$ $\sum \overrightarrow{(S \cdot Zn)} = 130.3292$

$\sum \overrightarrow{(Td)^2} = 1.0995 \times 10^6$ $\sum \overrightarrow{(Td \cdot Ts)} = 4.4442 \times 10^4$ $\sum \overrightarrow{(Td \cdot Fe)} = 7.6705 \times 10^3$

$\sum \overrightarrow{(Td \cdot Bo)} = 3.8001 \times 10^4$ $\sum \overrightarrow{(Td \cdot Cd)} = 7.1961 \times 10^4$ $\sum \overrightarrow{(Td \cdot Zn)} = 254.92$

$\sum \overrightarrow{(Ts)^2} = 3.1451 \times 10^3$ $\sum \overrightarrow{(Ts \cdot Fe)} = 477.479$ $\sum \overrightarrow{(Ts \cdot Bo)} = 1.6498 \times 10^3$

$\sum \overrightarrow{(Ts \cdot Cd)} = 4.6804 \times 10^3$ $\sum \overrightarrow{(Ts \cdot Zn)} = 12.7444$ $\sum \overrightarrow{(Fe)^2} = 96.209$

$\sum \overrightarrow{(Fe \cdot Bo)} = 471.721$ $\sum \overrightarrow{(Fe \cdot Cd)} = 901.3151$ $\sum \overrightarrow{(Fe \cdot Zn)} = 2.5082$

$\sum \overrightarrow{(Bo)^2} = 3.803 \times 10^3$ $\sum \overrightarrow{(Bo \cdot Cd)} = 3.776 \times 10^3$ $\sum \overrightarrow{(Bo \cdot Zn)} = 13.0679$

$\sum \overrightarrow{(Cd)^2} = 9.3507 \times 10^3$ $\sum \overrightarrow{(Cd \cdot Zn)} = 22.5071$ $\sum \overrightarrow{(Zn)^2} = 0.078$

$\sum \overrightarrow{(T \cdot pH)} = 1.7766 \times 10^3$ $\sum \overrightarrow{(Tu \cdot pH)} = 147.875$ $\sum \overrightarrow{(S \cdot pH)} = 1.0002 \times 10^4$

$\sum \overrightarrow{(Td \cdot pH)} = 1.8139 \times 10^4$ $\sum \overrightarrow{(Ts \cdot pH)} = 1.0329 \times 10^3$ $\sum \overrightarrow{(Fe \cdot pH)} = 196.2356$

$\sum \overrightarrow{(Bo \cdot pH)} = 994.0814$ $\sum \overrightarrow{(Cd \cdot pH)} = 1.864 \times 10^3$ $\sum \overrightarrow{(Zn \cdot pH)} = 5.4355$

The summations are now put in matrix form to solve for the constants. The matrix is as shown

below.

$$M := \begin{pmatrix}
\sum\overrightarrow{(\mathrm{T})^2} & \sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Tu})} & \sum\overrightarrow{(\mathrm{T}\cdot\mathrm{S})} & \sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Td})} & \sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Ts})} & \sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Zn})} \\
\sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{T})} & \sum\overrightarrow{(\mathrm{Tu})^2} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{S})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Td})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Ts})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Zn})} \\
\sum\overrightarrow{(\mathrm{T}\cdot\mathrm{S})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{S})} & \sum\overrightarrow{(\mathrm{S})^2} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Td})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Ts})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Zn})} \\
\sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Td})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Td})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Td})} & \sum\overrightarrow{(\mathrm{Td})^2} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Ts})} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Zn})} \\
\sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Ts})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Ts})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Ts})} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Ts})} & \sum\overrightarrow{(\mathrm{Ts})^2} & \sum\overrightarrow{(\mathrm{Ts}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{Ts}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{Ts}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Ts}\cdot\mathrm{Zn})} \\
\sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{Ts}\cdot\mathrm{Fe})} & \sum\overrightarrow{(\mathrm{Fe})^2} & \sum\overrightarrow{(\mathrm{Fe}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{Fe}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Fe}\cdot\mathrm{Zn})} \\
\sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{Ts}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{Fe}\cdot\mathrm{Bo})} & \sum\overrightarrow{(\mathrm{Bo})^2} & \sum\overrightarrow{(\mathrm{Bo}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Bo}\cdot\mathrm{Zn})} \\
\sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Ts}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Fe}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Bo}\cdot\mathrm{Cd})} & \sum\overrightarrow{(\mathrm{Cd})^2} & \sum\overrightarrow{(\mathrm{Cd}\cdot\mathrm{Zn})} \\
\sum\overrightarrow{(\mathrm{T}\cdot\mathrm{Zn})} & \sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{Zn})} & \sum\overrightarrow{(\mathrm{S}\cdot\mathrm{Zn})} & \sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{Zn})} & \sum\overrightarrow{(\mathrm{Ts}\cdot\mathrm{Zn})} & \sum\overrightarrow{(\mathrm{Fe}\cdot\mathrm{Zn})} & \sum\overrightarrow{(\mathrm{Bo}\cdot\mathrm{Zn})} & \sum\overrightarrow{(\mathrm{Cd}\cdot\mathrm{Zn})} & \sum\overrightarrow{(\mathrm{Zn})^2}
\end{pmatrix}
\qquad
J := \begin{pmatrix}
\sum\overrightarrow{(\mathrm{T}\cdot\mathrm{pH})} \\
\sum\overrightarrow{(\mathrm{Tu}\cdot\mathrm{pH})} \\
\sum\overrightarrow{(\mathrm{S}\cdot\mathrm{pH})} \\
\sum\overrightarrow{(\mathrm{Td}\cdot\mathrm{pH})} \\
\sum\overrightarrow{(\mathrm{Ts}\cdot\mathrm{pH})} \\
\sum\overrightarrow{(\mathrm{Fe}\cdot\mathrm{pH})} \\
\sum\overrightarrow{(\mathrm{Bo}\cdot\mathrm{pH})} \\
\sum\overrightarrow{(\mathrm{Cd}\cdot\mathrm{pH})} \\
\sum\overrightarrow{(\mathrm{Zn}\cdot\mathrm{pH})}
\end{pmatrix}$$

a b c d e f g h i

$$M = \begin{pmatrix} 7.4882 \times 10^{3} & 645.4 & 4.1078 \times 10^{4} & 7.494 \times 10^{4} & 4.3408 \times 10^{3} & 834.11 & 4.1854 \times 10^{3} & 7.8916 \times 10^{3} & 22.833 \\ 645.4 & 77.0775 & 2.4161 \times 10^{3} & 5.1532 \times 10^{3} & 343.2035 & 77.3635 & 386.4325 & 679.2715 & 2.1203 \\ 4.1078 \times 10^{4} & 2.4161 \times 10^{3} & 3.7753 \times 10^{5} & 6.0843 \times 10^{5} & 2.3551 \times 10^{4} & 4.3176 \times 10^{3} & 2.241 \times 10^{4} & 4.1073 \times 10^{4} & 130.3292 \\ 7.494 \times 10^{4} & 5.1532 \times 10^{3} & 6.0843 \times 10^{5} & 1.0995 \times 10^{6} & 4.4442 \times 10^{4} & 7.6705 \times 10^{3} & 3.8001 \times 10^{4} & 7.1961 \times 10^{4} & 254.92 \\ 4.3408 \times 10^{3} & 343.2035 & 2.3551 \times 10^{4} & 4.4442 \times 10^{4} & 3.1451 \times 10^{3} & 477.479 & 1.6498 \times 10^{3} & 4.6804 \times 10^{3} & 12.7444 \\ 834.11 & 77.3635 & 4.3176 \times 10^{3} & 7.6705 \times 10^{3} & 477.479 & 96.209 & 471.721 & 901.3151 & 2.5082 \\ 4.1854 \times 10^{3} & 386.4325 & 2.241 \times 10^{4} & 3.8001 \times 10^{4} & 1.6498 \times 10^{3} & 471.721 & 3.803 \times 10^{3} & 3.776 \times 10^{3} & 13.0679 \\ 7.8916 \times 10^{3} & 679.2715 & 4.1073 \times 10^{4} & 7.1961 \times 10^{4} & 4.6804 \times 10^{3} & 901.3151 & 3.776 \times 10^{3} & 9.3507 \times 10^{3} & 22.5071 \\ 22.833 & 2.1203 & 130.3292 & 254.92 & 12.7444 & 2.5082 & 13.0679 & 22.5071 & 0.078 \end{pmatrix} \begin{pmatrix} 1.7766 \times 10^{3} \\ 147.875 \\ 1.0002 \times 10^{4} \\ 1.8139 \times 10^{4} \\ 1.0329 \times 10^{3} \\ 196.2356 \\ 994.0814 \\ 1.864 \times 10^{3} \\ 5.4355 \end{pmatrix}$$

The matrix is then solved with the mathCAD 2000 Professional; the algorithm of the solution and the outputs are thus;

Muinat := lsolve(M,J)

$$\text{Muinat} = \begin{pmatrix} -1.3441 \\ 0.6020 \\ -0.0118 \\ 0.0199 \\ 0.7566 \\ -1.1306 \\ 0.6643 \\ 0.5315 \\ 49.5149 \end{pmatrix}$$

The outputs of the solution are the constants of the model equation. The constants are:

| | |
|---|---|
| $a := \text{Muinat}_1$ | $a = -1.3441$ |
| $b := \text{Muinat}_2$ | $b = 0.602$ |
| $c := \text{Muinat}_3$ | $c = -0.0118$ |
| $d := \text{Muinat}_4$ | $d = 0.0199$ |
| $e := \text{Muinat}_5$ | $e = 0.7566$ |
| $f := \text{Muinat}_6$ | $f = -1.1306$ |
| $g := \text{Muinat}_7$ | $g = 0.6643$ |
| $h := \text{Muinat}_8$ | $h = 0.5315$ |
| $i := \text{Muinat}_9$ | $i = 49.5149$ |

Having obtained the constants a, b, c, d, e, f, g, h and i, substituting the constants gives the

model pH (denoted by $pH_m$) as

$$pH_m := a \cdot T + b \cdot Tu + c \cdot S + d \cdot Td + e \cdot Ts + f \cdot Fe + g \cdot Bo + h \cdot Cd + i \cdot Zn$$

The model equation obtained which is given as

$$pH_m := a \cdot T + b \cdot Tu + c \cdot S + d \cdot Td + e \cdot Ts + f \cdot Fe + g \cdot Bo + h \cdot Cd + i \cdot Zn$$

is simulated with the software (mathCAD) and the simulated results are as given below.

$$pH_m = \begin{pmatrix} 6.55999999999972 \\ 6.90000000000002 \\ 5.5999999999992 \\ 6.79999999999961 \\ 7.00000000000036 \\ 6.90000000000043 \\ 6.90000000000186 \\ 6.99999999999845 \\ 7.90000000000023 \end{pmatrix}$$

The correctness of the model equation was verified by calculating the error and the percentage

error for each week. The error isn calculated as the difference between the experimental and the

predicted (model) pH.

$$error := pH - pH_m$$

$$error = \begin{pmatrix} 2.78 \times 10^{-13} \\ -1.8652 \times 10^{-14} \\ 8.0291 \times 10^{-13} \\ 3.9257 \times 10^{-13} \\ -3.6415 \times 10^{-13} \\ -4.3432 \times 10^{-13} \\ -1.8616 \times 10^{-12} \\ 1.5463 \times 10^{-12} \\ -2.3448 \times 10^{-13} \end{pmatrix}$$

The percentage error is given as

$$\%error := \overrightarrow{\left(\frac{error}{pH} \cdot 100\%\right)}$$

$$\%error = \begin{pmatrix} 4.2378 \times 10^{-12} \\ -2.7032 \times 10^{-13} \\ 1.4338 \times 10^{-11} \\ 5.7732 \times 10^{-12} \\ -5.2022 \times 10^{-12} \\ -6.2945 \times 10^{-12} \\ -2.698 \times 10^{-11} \\ 2.209 \times 10^{-11} \\ -2.9681 \times 10^{-12} \end{pmatrix} \%$$

The comparative results of the experimental results and the model pH values are presented in the table below.

$Table := augment(pH, pH_m, error, \%error)$

Table =

| pH | $pH_m$ | error | %error |
|---|---|---|---|
| 6.56 | 6.56 | $2.78 \cdot 10^{-13}$ | $4.2378 \cdot 10^{-12}$ |
| 6.9 | 6.9 | $1.8652 \cdot 10^{-14}$ | $2.7032 \cdot 10^{-13}$ |
| 5.6 | 5.6 | $8.0291 \cdot 10^{-13}$ | $1.4338 \cdot 10^{-11}$ |
| 6.8 | 6.8 | $3.9257 \cdot 10^{-13}$ | $5.7732 \cdot 10^{-12}$ |
| 7 | 7 | $3.6415 \cdot 10^{-13}$ | $5.2022 \cdot 10^{-12}$ |
| 6.9 | 6.9 | $4.3432 \cdot 10^{-13}$ | $6.2945 \cdot 10^{-12}$ |
| 6.9 | 6.9 | $1.8616 \cdot 10^{-12}$ | $-2.698 \cdot 10^{-11}$ |
| 7 | 7 | $1.5463 \cdot 10^{-12}$ | $2.209 \cdot 10^{-11}$ |
| 7.9 | 7.9 | $2.3448 \cdot 10^{-13}$ | $2.9681 \cdot 10^{-12}$ |

### *3.1.2 MODELLING USING MICROSOFT EXCEL*

The modelling of the pH was also carried out using the Microsoft Excel .

| | T | Tu | S | Td | Ts | Fe | Bo | Cd | Zn | P |
|---|---|---|---|---|---|---|---|---|---|---|
| Week 1 | 27.50 | 3.50 | 240.00 | 580.00 | 7.50 | 2.66 | 12.64 | 26.38 | 0.15 | 6.56 |
| Week 2 | 30.00 | 4.80 | 14.44 | 20.00 | 3.52 | 4.14 | 45.60 | 20.00 | 0.11 | 6.90 |
| Week 3 | 28.00 | 4.80 | 14.44 | 20.00 | 20.00 | 4.21 | 3.52 | 45.60 | 0.06 | 5.60 |
| Week 4 | 29.00 | 1.00 | 284.00 | 455.00 | 9.36 | 2.44 | 31.62 | 20.00 | 0.07 | 6.80 |
| Week 5 | 29.00 | 1.25 | 416.30 | 525.00 | 21.63 | 3.66 | 11.30 | 30.00 | 0.08 | 7.00 |
| Week 6 | 30.00 | 3.15 | 52.60 | 330.00 | 32.40 | 2.88 | 4.55 | 18.36 | 0.11 | 6.90 |
| Week 7 | 29.00 | 2.20 | 84.62 | 145.00 | 14.00 | 3.30 | 12.60 | 46.40 | 0.06 | 6.90 |
| Week 8 | 28.00 | 0.65 | 125.00 | 210.00 | 20.00 | 2.81 | 9.26 | 39.15 | 0.05 | 7.00 |
| Week 9 | 29.00 | 1.00 | 200.00 | 325.00 | 21.80 | 2.80 | 12.60 | 29.20 | 0.10 | 7.90 |

| | T2 | Ttu | TS | TTd | TTs | TFe | TBo | TCd | TZn | TP |
|---|---|---|---|---|---|---|---|---|---|---|
| Week 1 | 756.25 | 96.25 | 6600.00 | 15950.00 | 206.25 | 73.15 | 347.60 | 725.45 | 4.24 | 180.40 |
| Week 2 | 900.00 | 144.00 | 433.20 | 600.00 | 105.60 | 124.20 | 1368.00 | 600.00 | 3.15 | 207.00 |
| Week 3 | 784.00 | 134.40 | 404.32 | 560.00 | 560.00 | 117.88 | 98.56 | 1276.80 | 1.79 | 156.80 |
| Week 4 | 841.00 | 29.00 | 8236.00 | 13195.00 | 271.44 | 70.76 | 916.98 | 580.00 | 2.06 | 197.20 |
| Week 5 | 841.00 | 36.25 | 12072.70 | 15225.00 | 627.27 | 106.14 | 327.70 | 870.00 | 2.35 | 203.00 |
| Week 6 | 900.00 | 94.50 | 1578.00 | 9900.00 | 972.00 | 86.40 | 136.50 | 550.80 | 3.24 | 207.00 |
| Week 7 | 841.00 | 63.80 | 2453.98 | 4205.00 | 406.00 | 95.70 | 365.40 | 1345.60 | 1.62 | 200.10 |
| Week 8 | 784.00 | 18.20 | 3500.00 | 5880.00 | 560.00 | 78.68 | 259.28 | 1096.20 | 1.48 | 196.00 |
| Week 9 | 841.00 | 29.00 | 5800.00 | 9425.00 | 632.20 | 81.20 | 365.40 | 846.80 | 2.90 | 229.10 |
| row 1 | 7488.25 | 645.40 | 41078.20 | 74940.00 | 4340.76 | 834.11 | 4185.42 | 7891.65 | 22.83 | 1776.60 |

| | TuT | Tu2 | TuS | TuTd | TuTs | TuFe | TuBo | TuCd | TuZn | TuP |
|---|---|---|---|---|---|---|---|---|---|---|
| Week 1 | 96.25 | 12.25 | 840.00 | 2030.00 | 26.25 | 9.31 | 44.24 | 92.33 | 0.54 | 22.96 |
| Week 2 | 144.00 | 23.04 | 69.31 | 96.00 | 16.90 | 19.87 | 218.88 | 96.00 | 0.50 | 33.12 |
| Week 3 | 134.40 | 23.04 | 69.31 | 96.00 | 96.00 | 20.21 | 16.90 | 218.88 | 0.31 | 26.88 |
| Week 4 | 29.00 | 1.00 | 284.00 | 455.00 | 9.36 | 2.44 | 31.62 | 20.00 | 0.07 | 6.80 |
| Week 5 | 36.25 | 1.56 | 520.38 | 656.25 | 27.04 | 4.58 | 14.13 | 37.50 | 0.10 | 8.75 |
| Week 6 | 94.50 | 9.92 | 165.69 | 1039.50 | 102.06 | 9.07 | 14.33 | 57.83 | 0.34 | 21.74 |
| Week 7 | 63.80 | 4.84 | 186.16 | 319.00 | 30.80 | 7.26 | 27.72 | 102.08 | 0.12 | 15.18 |
| Week 8 | 18.20 | 0.42 | 81.25 | 136.50 | 13.00 | 1.83 | 6.02 | 25.45 | 0.03 | 4.55 |
| Week 9 | 29.00 | 1.00 | 200.00 | 325.00 | 21.80 | 2.80 | 12.60 | 29.20 | 0.10 | 7.90 |
| row 2 | 645.40 | 77.08 | 2416.10 | 5153.25 | 343.20 | 77.36 | 386.43 | 679.27 | 2.12 | 147.88 |

| | ST | STu | S2 | STd | STs | SFe | SBo | SCd | SZn | SP |
|---|---|---|---|---|---|---|---|---|---|---|
| Week 1 | 6600.00 | 840.00 | 57600.00 | 139200.00 | 1800.00 | 638.40 | 3033.60 | 6331.20 | 36.96 | 1574.40 |
| Week 2 | 433.20 | 69.31 | 208.51 | 288.80 | 50.83 | 59.78 | 658.46 | 288.80 | 1.52 | 99.64 |
| Week 3 | 404.32 | 69.31 | 208.51 | 288.80 | 288.80 | 60.79 | 50.83 | 658.46 | 0.92 | 80.86 |
| Week 4 | 8236.00 | 284.00 | 80656.00 | 129220.00 | 2658.24 | 692.96 | 8980.08 | 5680.00 | 20.16 | 1931.20 |
| Week 5 | 12072.70 | 520.38 | 173305.69 | 218557.50 | 9004.57 | 1523.66 | 4704.19 | 12489.00 | 33.72 | 2914.10 |
| Week 6 | 1578.00 | 165.69 | 2766.76 | 17358.00 | 1704.24 | 151.49 | 239.33 | 965.74 | 5.68 | 362.94 |
| Week 7 | 2453.98 | 186.16 | 7160.54 | 12269.90 | 1184.68 | 279.25 | 1066.21 | 3926.37 | 4.74 | 583.88 |
| Week 8 | 3500.00 | 81.25 | 15625.00 | 26250.00 | 2500.00 | 351.25 | 1157.50 | 4893.75 | 6.63 | 875.00 |
| Week 9 | 5800.00 | 200.00 | 40000.00 | 65000.00 | 4360.00 | 560.00 | 2520.00 | 5840.00 | 20.00 | 1580.00 |
| row 3 | 41078.20 | 2416.10 | 377531.02 | 608433.00 | 23551.36 | 4317.58 | 22410.20 | 41073.32 | 130.33 | 10002.02 |

| | TdT | TdTu | TdS | Td2 | TdTs | TdFe | TdBo | TdCd | TdZn | TdP |
|---|---|---|---|---|---|---|---|---|---|---|
| Week 1 | 15950.00 | 2030.00 | 139200.00 | 336400.00 | 4350.00 | 1542.80 | 7331.20 | 15300.40 | 89.32 | 3804.80 |
| Week 2 | 600.00 | 96.00 | 288.80 | 400.00 | 70.40 | 82.80 | 912.00 | 400.00 | 2.10 | 138.00 |
| Week 3 | 560.00 | 96.00 | 288.80 | 400.00 | 400.00 | 84.20 | 70.40 | 912.00 | 1.28 | 112.00 |
| Week 4 | 13195.00 | 455.00 | 129220.00 | 207025.00 | 4258.80 | 1110.20 | 14387.10 | 9100.00 | 32.31 | 3094.00 |
| Week 5 | 15225.00 | 656.25 | 218557.50 | 275625.00 | 11355.75 | 1921.50 | 5932.50 | 15750.00 | 42.53 | 3675.00 |
| Week 6 | 9900.00 | 1039.50 | 17358.00 | 108900.00 | 10692.00 | 950.40 | 1501.50 | 6058.80 | 35.64 | 2277.00 |
| Week 7 | 4205.00 | 319.00 | 12269.90 | 21025.00 | 2030.00 | 478.50 | 1827.00 | 6728.00 | 8.12 | 1000.50 |
| Week 8 | 5880.00 | 136.50 | 26250.00 | 44100.00 | 4200.00 | 590.10 | 1944.60 | 8221.50 | 11.13 | 1470.00 |
| Week 9 | 9425.00 | 325.00 | 65000.00 | 105625.00 | 7085.00 | 910.00 | 4095.00 | 9490.00 | 32.50 | 2567.50 |
| row 4 | 74940.00 | 5153.25 | 608433.00 | 1099500.00 | 44441.95 | 7670.50 | 38001.30 | 71960.70 | 254.92 | 18138.80 |

| | TsT | TsTu | TsS | TsTd | Ts2 | TsFe | TsBo | TsCd | TsZn | TsP |
|---|---|---|---|---|---|---|---|---|---|---|
| Week 1 | 206.25 | 26.25 | 1800.00 | 4350.00 | 56.25 | 19.95 | 94.80 | 197.85 | 1.16 | 49.20 |
| Week 2 | 105.60 | 16.90 | 50.83 | 70.40 | 12.39 | 14.57 | 160.51 | 70.40 | 0.37 | 24.29 |
| Week 3 | 560.00 | 96.00 | 288.80 | 400.00 | 400.00 | 84.20 | 70.40 | 912.00 | 1.28 | 112.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Week 4 | 271.44 | 9.36 | 2658.24 | 4258.80 | 87.61 | 22.84 | 295.96 | [illegible] | [illegible] | [illegible] |
| Week 5 | 627.27 | 27.04 | 9004.57 | 11355.75 | 467.86 | 79.17 | 244.42 | [illegible] | [illegible] | [illegible] |
| Week 6 | 972.00 | 102.06 | 1704.24 | 10692.00 | 1049.76 | 93.31 | 147.42 | 594.86 | [illegible] | [illegible] |
| Week 7 | 406.00 | 30.80 | 1184.68 | 2030.00 | 196.00 | 46.20 | 176.40 | 649.60 | [illegible] | [illegible] |
| Week 8 | 560.00 | 13.00 | 2500.00 | 4200.00 | 400.00 | 56.20 | 185.20 | 783.00 | [illegible] | [illegible] |
| Week 9 | 632.20 | 21.80 | 4360.00 | 7085.00 | 475.24 | 61.04 | 274.68 | 636.56 | 2.18 | 172.22 |
| row 5 | 4340.76 | 343.20 | 23551.36 | 44441.95 | 3145.11 | 477.48 | 1649.79 | 4680.37 | 12.74 | 1032.93 |
| | | | | | | | | | | |
| | FeT | FeTu | FeS | FeTd | FeTs | Fe2 | FeBo | FeCd | FeZn | FeP |
| Week 1 | 73.15 | 9.31 | 638.40 | 1542.80 | 19.95 | 7.08 | 33.62 | 70.17 | 0.41 | 17.45 |
| Week 2 | 124.20 | 19.87 | 59.78 | 82.80 | 14.57 | 17.14 | 188.78 | 82.80 | 0.43 | 28.57 |
| Week 3 | 117.88 | 20.21 | 60.79 | 84.20 | 84.20 | 17.72 | 14.82 | 191.98 | 0.27 | 23.58 |
| Week 4 | 70.76 | 2.44 | 692.96 | 1110.20 | 22.84 | 5.95 | 77.15 | 48.80 | 0.17 | 16.59 |
| Week 5 | 106.14 | 4.58 | 1523.66 | 1921.50 | 79.17 | 13.40 | 41.36 | 109.80 | 0.30 | 25.62 |
| Week 6 | 86.40 | 9.07 | 151.49 | 950.40 | 93.31 | 8.29 | 13.10 | 52.88 | 0.31 | 19.87 |
| Week 7 | 95.70 | 7.26 | 279.25 | 478.50 | 46.20 | 10.89 | 41.58 | 153.12 | 0.18 | 22.77 |
| Week 8 | 78.68 | 1.83 | 351.25 | 590.10 | 56.20 | 7.90 | 26.02 | 110.01 | 0.15 | 19.67 |
| Week 9 | 81.20 | 2.80 | 560.00 | 910.00 | 61.04 | 7.84 | 35.28 | 81.76 | 0.28 | 22.12 |
| row 6 | 834.11 | 77.36 | 4317.58 | 7670.50 | 477.48 | 96.21 | 471.72 | 901.32 | 2.51 | 196.24 |
| | | | | | | | | | | |
| | BoT | BoTu | BoS | BoTd | BoTs | BoFe | Bo2 | BoCd | BoZn | BoP |
| Week 1 | 347.60 | 44.24 | 3033.60 | 7331.20 | 94.80 | 33.62 | 159.77 | 333.44 | 1.95 | 82.92 |
| Week 2 | 1368.00 | 218.88 | 658.46 | 912.00 | 160.51 | 188.78 | 2079.36 | 912.00 | 4.79 | 314.64 |
| Week 3 | 98.56 | 16.90 | 50.83 | 70.40 | 70.40 | 14.82 | 12.39 | 160.51 | 0.23 | 19.71 |
| Week 4 | 916.98 | 31.62 | 8980.08 | 14387.10 | 295.96 | 77.15 | 999.82 | 632.40 | 2.25 | 215.02 |
| Week 5 | 327.70 | 14.13 | 4704.19 | 5932.50 | 244.42 | 41.36 | 127.69 | 339.00 | 0.92 | 79.10 |
| Week 6 | 136.50 | 14.33 | 239.33 | 1501.50 | 147.42 | 13.10 | 20.70 | 83.54 | 0.49 | 31.40 |
| Week 7 | 365.40 | 27.72 | 1066.21 | 1827.00 | 176.40 | 41.58 | 158.76 | 584.64 | 0.71 | 86.94 |
| Week 8 | 259.28 | 6.02 | 1157.50 | 1944.60 | 185.20 | 26.02 | 85.75 | 362.53 | 0.49 | 64.82 |
| Week 9 | 365.40 | 12.60 | 2520.00 | 4095.00 | 274.68 | 35.28 | 158.76 | 367.92 | 1.26 | 99.54 |
| row 7 | 4185.42 | 386.43 | 22410.20 | 38001.30 | 1649.79 | 471.72 | 3803.00 | 3775.98 | 13.07 | 994.08 |
| | | | | | | | | | | |
| | CdT | CdTu | CdS | CdTd | CdTs | CdFe | CdBo | Cd2 | CdZn | CdP |
| Week 1 | 725.45 | 92.33 | 6331.20 | 15300.40 | 197.85 | 70.17 | 333.44 | 695.90 | 4.06 | 173.05 |
| Week 2 | 600.00 | 96.00 | 288.80 | 400.00 | 70.40 | 82.80 | 912.00 | 400.00 | 2.10 | 138.00 |
| Week 3 | 1276.80 | 218.88 | 658.46 | 912.00 | 912.00 | 191.98 | 160.51 | 2079.36 | 2.92 | 255.36 |
| Week 4 | 580.00 | 20.00 | 5680.00 | 9100.00 | 187.20 | 48.80 | 632.40 | 400.00 | 1.42 | 136.00 |
| Week 5 | 870.00 | 37.50 | 12489.00 | 15750.00 | 648.90 | 109.80 | 339.00 | 900.00 | 2.43 | 210.00 |
| Week 6 | 550.80 | 57.83 | 965.74 | 6058.80 | 594.86 | 52.88 | 83.54 | 337.09 | 1.98 | 126.68 |
| Week 7 | 1345.60 | 102.08 | 3926.37 | 6728.00 | 649.60 | 153.12 | 584.64 | 2152.96 | 2.60 | 320.16 |
| Week 8 | 1096.20 | 25.45 | 4893.75 | 8221.50 | 783.00 | 110.01 | 362.53 | 1532.72 | 2.07 | 274.05 |
| Week 9 | 846.80 | 29.20 | 5840.00 | 9490.00 | 636.56 | 81.76 | 367.92 | 852.64 | 2.92 | 230.68 |
| row 8 | 7891.65 | 679.27 | 41073.32 | 71960.70 | 4680.37 | 901.32 | 3775.98 | 9350.68 | 22.51 | 1863.99 |
| | | | | | | | | | | |
| | ZnT | ZnTu | ZnS | ZnTd | ZnTs | ZnFe | ZnBo | ZnCd | Zn2 | ZnP |
| Week 1 | 4.24 | 0.54 | 36.96 | 89.32 | 1.16 | 0.41 | 1.95 | 4.06 | 0.02 | 1.01 |
| Week 2 | 3.15 | 0.50 | 1.52 | 2.10 | 0.37 | 0.43 | 4.79 | 2.10 | 0.01 | 0.72 |
| Week 3 | 1.79 | 0.31 | 0.92 | 1.28 | 1.28 | 0.27 | 0.23 | 2.92 | 0.00 | 0.36 |
| Week 4 | 2.06 | 0.07 | 20.16 | 32.31 | 0.66 | 0.17 | 2.25 | 1.42 | 0.01 | 0.48 |
| Week 5 | 2.35 | 0.10 | 33.72 | 42.53 | 1.75 | 0.30 | 0.92 | 2.43 | 0.01 | 0.57 |
| Week 6 | 3.24 | 0.34 | 5.68 | 35.64 | 3.50 | 0.31 | 0.49 | 1.98 | 0.01 | 0.75 |
| Week 7 | 1.62 | 0.12 | 4.74 | 8.12 | 0.78 | 0.18 | 0.71 | 2.60 | 0.00 | 0.39 |
| Week 8 | 1.48 | 0.03 | 6.63 | 11.13 | 1.06 | 0.15 | 0.49 | 2.07 | 0.00 | 0.37 |
| Week 9 | 2.90 | 0.10 | 20.00 | 32.50 | 2.18 | 0.28 | 1.26 | 2.92 | 0.01 | 0.79 |
| row 9 | 22.83 | 2.12 | 130.33 | 254.92 | 12.74 | 2.51 | 13.07 | 22.51 | 0.08 | 5.44 |
| | | | | | | | | | | |
| | | | | | | | | | | |
| Equation | a | b | c | d | e | f | g | h | i | k |
| Equation 1 | 7488.25 | 645.40 | 41078.20 | 74940.00 | 4340.76 | 834.11 | 4185.42 | 7891.65 | 22.83 | 1776.60 |
| Equation 2 | 645.40 | 77.08 | 2416.10 | 5153.25 | 343.20 | 77.36 | 386.43 | 679.27 | 2.12 | 147.88 |
| Equation 3 | 41078.20 | 2416.10 | 377531.02 | 608433.00 | 23551.36 | 4317.58 | 22410.20 | 41073.32 | 130.33 | 10002.02 |
| Equation 4 | 74940.00 | 5153.25 | 608433.00 | 1099500.00 | 44441.95 | 7670.50 | 38001.30 | 71960.70 | 254.92 | 18138.80 |
| Equation 5 | 4340.76 | 343.20 | 23551.36 | 44441.95 | 3145.11 | 477.48 | 1649.79 | 4680.37 | 12.74 | 1032.93 |
| Equation 6 | 834.11 | 77.36 | 4317.58 | 7670.50 | 477.48 | 96.21 | 471.72 | 901.32 | 2.51 | 196.24 |
| Equation 7 | 4185.42 | 386.43 | 22410.20 | 38001.30 | 1649.79 | 471.72 | 3803.00 | 3775.98 | 13.07 | 994.08 |
| Equation 8 | 7891.65 | 679.27 | 41073.32 | 71960.70 | 4680.37 | 901.32 | 3775.98 | 9350.68 | 22.51 | 1863.99 |
| Equation 9 | 22.83 | 2.12 | 130.33 | 254.92 | 12.74 | 2.51 | 13.07 | 22.51 | 0.08 | 5.44 |
| | | | | | | | | | | |

| Solutions | |
|---|---|
| a | -1.3441 |
| b | 0.6020 |
| c | -0.0118 |
| d | 0.0199 |
| e | 0.7566 |
| f | -1.1306 |
| g | 0.6643 |
| h | 0.5315 |
| i | 49.5149 |

***SIMULATION***

| Weeks | pHm |
|---|---|
| Week 1 | 6.56 |
| Week 2 | 6.90 |
| Week 3 | 5.60 |
| Week 4 | 6.80 |
| Week 5 | 7.00 |
| Week 6 | 6.90 |
| Week 7 | 6.90 |
| Week 8 | 7.00 |
| Week 9 | 7.90 |

***COMPARISON BETWEEN EXPERIMENTAL AND MODEL RESULTS***

| | Exp. | Model | | |
|---|---|---|---|---|
| Weeks | pH | pHm | error | %error |
| Week 1 | 6.56 | 6.56 | 0.00 | 0.00 |
| Week 2 | 6.90 | 6.90 | 0.00 | 0.00 |
| Week 3 | 5.60 | 5.60 | 0.00 | 0.00 |
| Week 4 | 6.80 | 6.80 | 0.00 | 0.00 |
| Week 5 | 7.00 | 7.00 | 0.00 | 0.00 |
| Week 6 | 6.90 | 6.90 | 0.00 | 0.00 |
| Week 7 | 6.90 | 6.90 | 0.00 | 0.00 |
| Week 8 | 7.00 | 7.00 | 0.00 | 0.00 |
| Week 9 | 7.90 | 7.90 | 0.00 | 0.00 |

*CHAPTER FOUR*

# *4.0 RESULTS AND DISCUSSION OF RESULTS*

## *4.1 RESULTS*

The results obtained from the simulation of the model equation are as shown below.

Table 4.1: Results of the simulation

| Week | Experimental pH | Predicted pH | Error | Percentage error |
|---|---|---|---|---|
| Week 1 | 6.56 | 6.56 | 2.78E-13 | 4.24E-12 |
| Week 2 | 6.9 | 6.9 | -1.87E-14 | -2.70E-13 |
| Week 3 | 5.6 | 5.6 | 8.03E-13 | 1.43E-11 |
| Week 4 | 6.8 | 6.8 | 3.93E-13 | 5.77E-12 |
| Week 5 | 7 | 7 | -3.64E-13 | -5.20E-12 |
| Week 6 | 6.9 | 6.9 | -4.34E-13 | -6.29E-12 |
| Week 7 | 6.9 | 6.9 | -1.86E-12 | -2.70E-11 |
| Week 8 | 7 | 7 | 1.55E-12 | 2.21E-11 |
| Week 9 | 7.9 | 7.9 | -2.34E-13 | -2.97E-12 |

## *4.2 DISCUSSION OF RESULTS*

A model equation was developed using the experimental data. Thus, from the experimental data for week 1, when the concentration of zinc ion ($Zn^{2+}$) is increased from 0.15mg/L to 0.17mg/L, the pH also increased from 6.56 to 7.36, whereas when its value is decreased from 0.15mg/L to 0.12mg/L, the pH fall drastically from 6.56 to 4.90. This could be attributed to the fact that zinc hydrolyses in aqueous solution.

When the temperature is increased from 27.5°C to 28°C, the overall pH fall from 6.56 to 5.69 and when the temperature is reduced from 27.5 °C to 27 °C, the pH is increased from 6.56 to 7.04. Solubility of oxygen varies with temperature. Increase in temperature causes depletion in the dissolved oxygen level, and decomposition increases, thereby increasing the acidity of the water.

When the total iron concentration is increased from 2.66mg/L to 2.80mg/L, the pH decreased from 6.56 to 6.2 and when the total ion concentration is decreased from 2.66mg/L to 2.52mg/L, the pH changed from 6.56 to 6.52. This indicates that the influence of total iron concentration is not much felt on the pH. Their aqueous solution are generally acid indicating that they hydrolyse to an appreciable extent.

When the total suspended solid content is increased from 7.5mg/L to 8.0mg/L, the pH also increases from 6.56 to 6.74 and when the total suspended solid is decreased from 7.5mg/L to 7.0mg/L, the pH decreases from 6.56 to 5.99.

Also, from the experimental data for week 2, when the zinc ion concentration is increased from 0.11mg/L to 0.13mg/L, the pH increases drastically from 6.90 to 8.14, and also when the zinc ion concentration is decreased from 0.11mg/L to 0.09mg/L, the pH also reduced drastically from 6.90 to 6.16.

When the temperature is increased from 30°C to 32 °C, the pH fall from 6.90 to 4.46 and when the temperature is decreased from 30 °C to 28 °C, the pH value increases from 6.70 to 7.83. This indicates that temperature has a greater influence on the pH than total iron.

Pollutants present in water can seriously affect the resultant pH. The level of acidification or alkalization of the solution by pollutants is dependent on the chemical nature of the compound present as well as the prevailing technological conditions. From the model equation, it can be seen that some of the parameters have positive effect on the pH while some have negative effect on the pH. That is to say that when one of the parameters with positive coefficient is varied, the pH changes in direct proportion to the variation. Likewise, when one of the parameters having negative coefficient is being varies, the effect on the pH will be inversely proportional to the change.

The software package used for the modelling was MathCAD 2000 Professional and Microsoft Excel. The results obtained for the modelled pH were shown in Table 4.1. The percentage error between the experimental and modelled pH was calculated, and it was observed that the error generated is very negligible. The graph of the experimental and modelled pH against the number of weeks was plotted. This shows that the experimental and modelled is nearly overlap. This indicates that there is a good fit between the model and experimental pH. Analysis of the obtained coefficients for the various variables shows that the obtained values and signs to a great extent is a reflection of the chemical nature of the pollutants constituents. The effect of the measured parameters on the overall pH can be represented in the following order.

$$\underrightarrow{Zn > Ts > Bo > Tu > Cd > Td} \quad (pH) \quad \underleftarrow{S < Fe < T}$$

Order of increasing acidification — Order of decreasing alkalization

## *CHAPTER FIVE*

## *5.0 CONCLUSION AND RECOMMENDATION*

### *5.1 CONCLUSION*

Based on the model developed, and the results obtained, the following conclusions were reached.

The pH is a resultant effect of the prevailing physiochemical and technological parameters in waste water.

Parametric coefficients in the modelled equation obtained showed that the effect of the measure parameters on the overall pH, which is either positive or negative.

The pH is most affected by the zinc ion concentration and least by total dissolved solids.

The bar graph plotted showed that there is a good fit between the experimental pH and the model pH. Therefore, the model equation can be used as a tool in predicting the behaviour of the various parameters in different situations, thereby providing a convenient, inexpensive and time saving means of gaining this understanding.

### *5.2 RECOMMENDATION*

The following recommendations were made:

1. The model equation developed should be used as a tool for carrying out further analysis.
2. Practical computer courses should be introduced at higher level. This will improve the students' ability to carry out modelling and simulation with the aid of computer.
3. Industries should minimize their wastes via the following ways:

i) Installation of waste treatment plant and special attention paid to it.

ii) Upgrading of already existing waste treatment plants in most industries.

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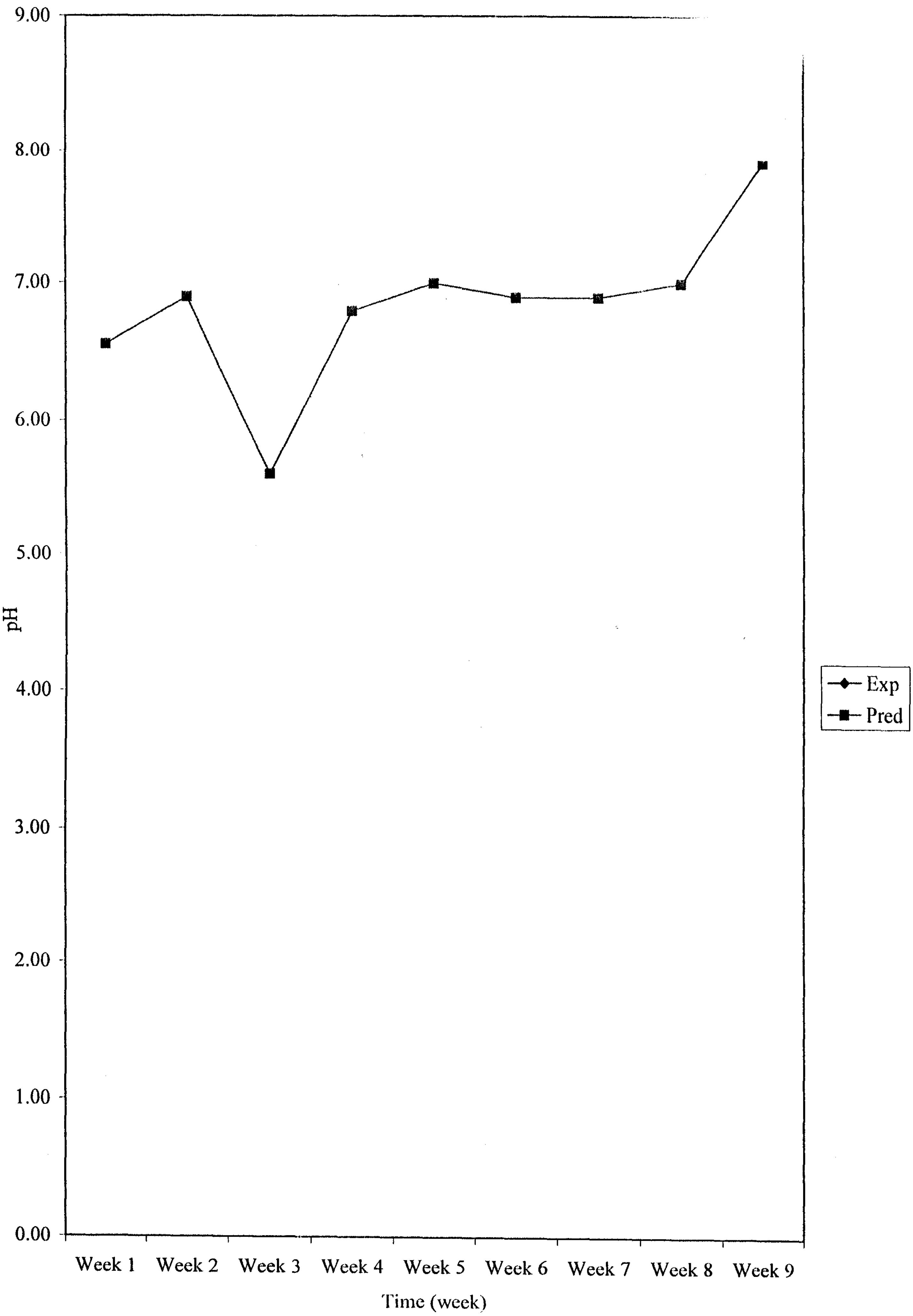


Fig. A1: Graph of experimental and predicted pH against time

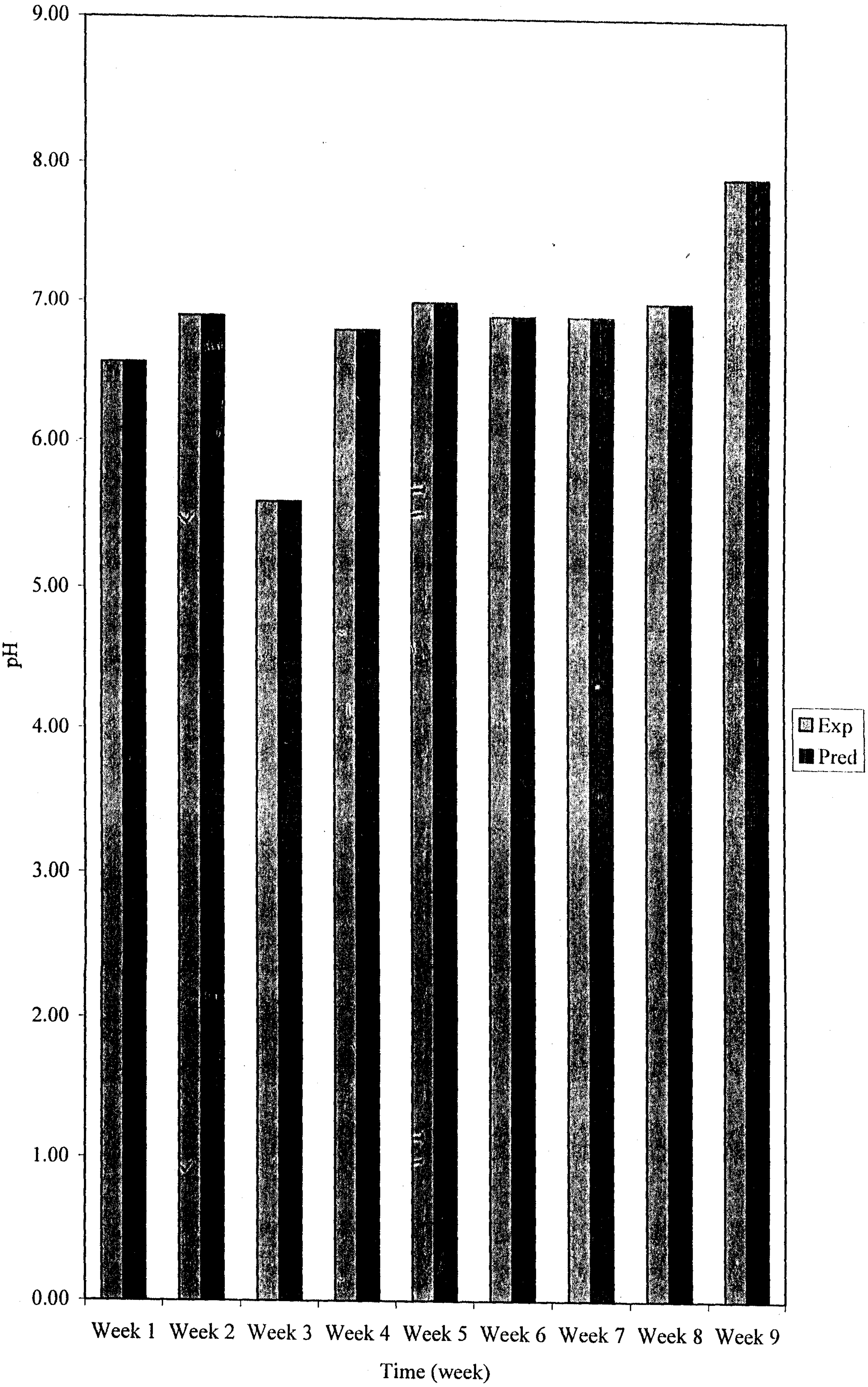


Fig. A2 :Bar chart of experimental and predicted pH against time