AN ANALYTIC STUDY OF DISSOLVED OXYGEN DEPENDENCY ON TEMPERATURE AND POLLUTANT CONCENTRATION IN A RIVER

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DECLARATION

This thesis is my original work prepared with no other than the indicated sources and support and has not been presented else where for a degree or any other award.

Signature............................ Date..

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Approval

The undersigned certify that they have read and hereby recommend for acceptance of Maasai Mara University a thesis entitled "An analytic study of dissolved oxygen dependency on temperature and pollutant concentration in a river".

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DEDICATION

This work is dedicated to my Parents. You have been a great inspiration in my life.

ACKNOWLEDGEMENTS

I take this opportunity to thank God, who has given me a chance to accomplish this work. I appreciate the careful guidance and encouragement of my supervisors Prof. Adu A.M Wasike, Dr. Muthiga and Dr. Njuguna who ably guided me throughout this work. More appreciation to the members of the faculty in the department of mathematics of Maasai Mara University for both material and moral support during my studies. Special thanks to Winfred, Favor Mwende and my brothers, Josphat Mwendwa and Bonface Mutisya and friends for their kindness and standing with me. God bless you all.

ABSTRACT

In this study, we develop a mathematical model of describing how the concentration of oxygen is affected by temperature variations and the pollutant concentration in a river. This is achieved by formulating a set of advection-diffusion reaction partial differential equations governing concentration of pollutant and the concentration of dissolved oxygen. We derive a pair of coupled advection diffusion equations that describe the dynamics of river pollution using conservation of mass laws. Analytical solutions are obtained using an asymptotic method. From the model, both concentration of dissolved oxygen and pollutant are obtained without and with the dispersion coefficient. Since temperature plays a crucial role in determining the amount of oxygen which enters in the water, its effects on the dissolved oxygen is studied. Simulation of the model is performed using Matlab. From the analysis of the model, it is observed that, when a river is highly polluted, a slight change in temperature leads to catastrophe and there is a temperature beyond which a river becomes ecologically dead. From the numerical simulations, we observe that, when there is high temperature, oxygen levels depletes rendering the river incapable of supporting aquatic life. From the analysis, setting up adaptive strategies to address extreme temperature fluctuations, their effects and reducing river pollution will help in protecting aquatic life and improving water quality.

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List of Abbreviations

BOD :-Biological Oxygen Demand

H(x) :- Heaviside function

DO:- Dissolved oxygen

PDE :- Partial differential equations

ODE :- Ordinary differential equations

CHAPTER 1

INTRODUCTION

1.1 Introduction

In this chapter, we give background information to the study. In section 1.2, we discuss the dynamics of dissolved oxygen, pollution and temperature. We give a brief introduction to pollution in section 1.3, sources of pollution in section 1.4, water quality parameters in section 1.5 and dissolved oxygen in section 1.6. In section 1.7, we describe mathematical models and Advection-Reaction Diffusion equations in section 1.8.

1.2 Background of the study

Living organisms depends on rivers and lakes for water. The amount of dissolved oxygen in water depends on the temperature of the water and pollutant concentration. An increase in its temperature leads to decrease in dissolved oxygen levels. Dissolved oxygen (DO) is one of the indicators of the biological health of a river but exhibit fluctuations depending on the season and also time of the day. Pollution of rivers has been an environmental disaster especially in the developing countries. The problem arises especially because of human activities such as agriculture. These activities significantly contributes to the contamination of water which affects living organisms because they use river waters daily. River pollution is caused by substances that enter into water, see for instance (Metcalf et al., 1991).

Temperature and oxygen are two principal water quality factors which influence the ecosystem of the river. The changes in water temperature affects biological and chemical processes. As the temperature of the water increases, it's capacity to hold dissolved oxygen decreases. This leads to lower levels of dissolved oxygen in the water. High temperature influence the toxicity of pollutants by accelerating chemical reactions which potentially transforms pollutants into a more toxic forms or maybe generate harmful products (Metcalf et al., 1991).

Global warming has resulted in steady rise of temperature which has indeed increased water temperatures. High water temperatures decreases oxygen solubility in water. In addition, temperature influences spawning periods, growth rate and mortality rate of a river aquatic inhabitants. An increase in temperature leads to reduction of DO which endangers life of aquatic animals (Chapman, 1996).

With an increase in population and social development, there is a need to address the issue of water quality and ensure water quality for biological sustainability is maintained. Due to increasing concern about water quality, mathematical models, which helps us understand how to control water pollution problem and maintain water quality even without interfering with it have been developed. The models are advantageous since they help in determining the extend in which a river is polluted, see for instance in (Pimpunchat et al., 2009).

1.3 Pollution

In this section, we briefly look at pollution. Pollution is defined as the addition of substances to water, air and land which negatively affect living organisms and also has a negative effect to the environment. Pollution of air, water and land are the three categories of pollution.

Pollution in rivers originates from various sources, each contributing different types of contaminants. The primary sources includes industrial discharge where factories and industrial plants release pollutants such as heavy metals, chemicals and toxic substances into rivers, Agricultural run off where fertilizers, pesticides and animal waste from farms are washed into rivers, sewage and wastewater where untreated or inadequately treated sewage and wastewater from residential, industrial sources add pathogens, organic matter and other pollutants to rivers.

Mining activities where mining operations discharges sediments and toxic substances like mercury into nearby water bodies and plastic waste where improper disposal of plastics break down into microplastics which end up in rivers and pose threats to aquatic life. As there are no signs of water pollution being stopped from the fact that water is being polluted day after day, there is a need to develop mathematical models in order to predict levels of pollutant in rivers, lakes and oceans.

Some of the effects of river pollution includes ecosystem damage where pollutants harm or kill aquatic organisms, disrupting food chains and reducing biodiversity, human health risks where contaminated water cause water-borne diseases and issues for communities relying on rivers for drinking water, bathing and fishing.

Eutrophication in which excessive nutrients, primarily nitrogen and phosphorus, leads to algal blooms that depletes oxygen levels in water causing dead zones and economic impacts in which pollution affects fishing, tourism and water sports industries which leads to economic loses.

1.4 Sources of pollution

In this section, we briefly look at sources of pollution. Sources of pollution are classified as point source or non-point sources, where point sources are contaminations that occurs from a single source that can easily be located while non-point source pollution is contamination derived from multiple or diffused sources where it is not easy to determine the exact origin of the pollution for instance floodwater that takes all types of waste from the land into a river.

We look at some water quality parameters in section 1.5. We shall start with temperature, followed by PH, dissolved oxygen, Biological Oxygen Demand and Chemical Oxygen Demand.

1.5 Water Quality Parameters

The healthy of a river is dependent on the quality of its water, which may be affected by presence of pollutants. Some parameters which express chemical, physical and biological composition of water are used to assess the quality of a river, see for instance (Chapman, 1996). Other parameters includes Temperature and PH.

Due to change in climate over the recent years, temperature has steadily increased, which has negatively impacted the environment especially levels of dissolved oxygen in rivers, see for instance (Chapman, 1996). High temperatures has increased rates of chemical reactions. Solubility of gases has however decreased with the temperature (Henry's law). Temperature determines the amount of oxygen that dissolves in water, when temperature increases, less oxygen dissolves in water. Warm water have low dissolved oxygen as compared to cold water. Due to climatic changes, water temperature fluctuates over the period of 24 hours in some water bodies, and also vary with the seasons, see for instance (Chapman, 1996).

Temperature governs the kind and type of aquatic life. Organisms have preferred temperature regimes that may change depending on the season. High temperatures leads to death of aquatic organisms such as fish since increase in temperature decreases dissolved oxygen levels in rivers.
Surface water temperatures range between $0°$ to $30°$ though varies depending on the season with minimum temperature occurring during cold seasons and maximum

temperature occurring during dry seasons, see for instance (Chapman, 1996).

The PH of the water is a very vital variable of water quality which influences biological processes in water bodies and shows how acidic or basic water is, see for instance (Chapman, 1996).

1.6 Dissolved Oxygen

Dissolved oxygen, (DO), levels are affected by water temperature, ionic strength, dissolved solids, atmospheric pressure and other parameters, see for instance (Center, 2024). Oxygen solubility decreases as these parameters increase, reducing the amount of dissolved oxygen in water. Graphically, variation of dissolved oxygen with temperature is as illustrated in Figure 1.1

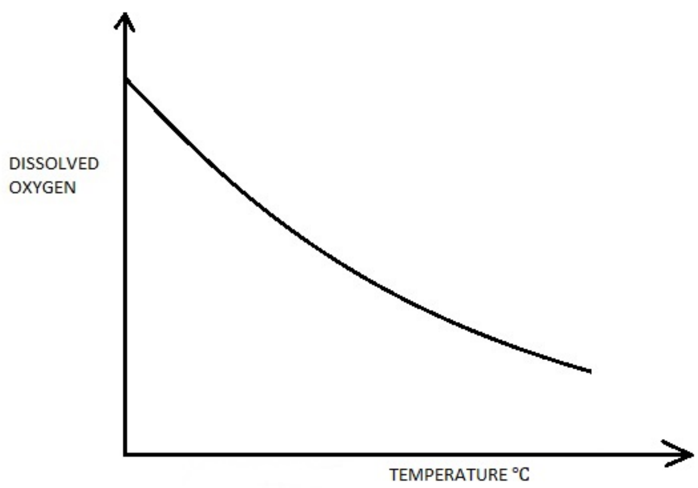

Figure 1.1: Dissolved oxygen vs temperature

The presence of organic solids, such as dead plants materials and other organic debris in rivers contribute to the consumption of dissolved oxygen, Microorganisms decompose the solids, through a process which consumes oxygen. High levels of organic solids correlate with higher biological oxygen demand(BOD), indicating an increased demand for dissolved oxygen. The graph of dissolved oxygen and solids can therefore be as shown in Figure 1.2

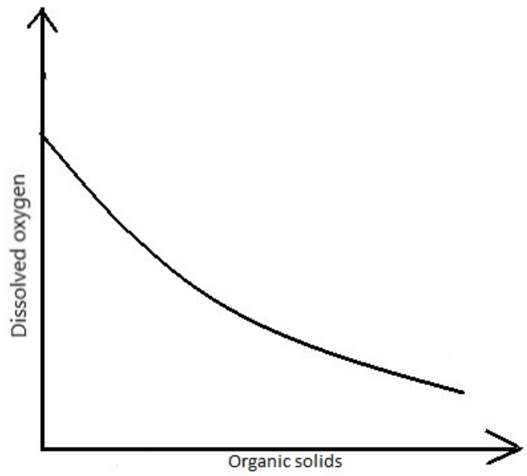

Figure 1.2: Dissolved oxygen vs solids

As suspended solids increases, dissolved oxygen levels decreases due to increased oxygen demand in decomposing organic matter, though the specific pattern depends on factors like microbial activity, temperature of the water and type of solids present.

The levels of dissolved oxygen in water is categorized into normoxia, hypoxia and anoxia; where normoxia represent the normal oxygen levels in a water body that support life functions for organisms in that water body without causing stress, hypoxia refers to levels of oxygen in a water body lower than normal levels which cause stress and harm aquatic organisms and anoxia refers to levels in a water body where there is no oxygen or extremely low levels of oxygen.

Dissolved oxygen concentration which is below 4 mg/L may adversely affect the survival of aquatic organisms. In addition, dissolved oxygen concentration below 2 mg/L may not support aquatic life and may even lead to death of aquatic organisms such as fish, see for instance (Chapman, 1996).

The reason to why we have chosen temperature to be our main parameter is due to global warming which leads to a decrease in dissolved oxygen.

It is therefore important to be able to determine the ideal levels of oxygen in water for aquatic life survival, to this end, a model is developed to help achieve this objective.

Biological Oxygen Demand (BOD) refers to the amount of oxygen which is required by microorganisms for the purpose of breaking down organic materials. The BOD determines oxygen that is consumed by microorganisms when decomposing organic matter in a river. This water quality parameter deals with the amount of oxygen consumed (mgO_2L^{-1}) by organisms in order to oxidize organic compounds. Unpolluted water have a BOD values of $2mgL^{-1}$ or less whereas water bodies receiving wastewater may have a BOD of $10mgL^{-1}$, see for instance (Chapman, 1996).

Chemical oxygen demand refers to the amount of oxygen that is needed to break down organic material via oxidation. Concentrations of the chemical oxygen demand that is observed in surface waters ranges from $20mgL^{-1}O_2$ or less in unpolluted water to $200mgL^{-1}O_2$ in waters receiving effluents, see for instance (Chapman, 1996).

In section 1.7 we shall describe the use of mathematical models.

1.7 Mathematical models

Mathematical models exist to describe how a rise in pollutant concentration and an increase in temperature affect the overall dissolved oxygen levels in a river. These models often take into account various factors such as biological oxygen demand(BOD), temperature-dependent oxygen solubility, nutrient loading and biological oxygen consumption rates.

One commonly used model is the Streeter-Phelps model, which describes the dynamics of DO in a river over time. This model considers the input of pollutants, their decay rates, and temperature dependence of oxygen solubility to predict dissolved oxygen concentrations along the length of a river (Pimpunchat et al., 2009).

Another approach is the use of mechanistic models based on mass balance equations, which incorporate the effects of temperature and pollutant concentrations on oxygen dynamics in rivers. These models can vary in complexity, from simple linear relationships to more complex differential equations(Chapra, 1996).

Overall, Mathematical models provide valuable tools for understanding and predicting how changes in pollutant concentration and temperature can impact dissolved oxygen levels in rivers, helping inform management and mitigation strategies to protect aquatic ecosystems.

An increase in temperature typically leads to a decrease in the amount of dissolved oxygen in rivers. Warmer water holds less oxygen than cooler waters because the solubility of oxygen decreases as temperature rises. This can have significant impacts on aquatic ecosystems, as many organisms rely on dissolved oxygen for survival. Decreased oxygen levels can stress or even suffocate aquatic life, leading to negative consequences for the overall health of river ecosystems.

An increase in pollutant concentration in a river can negatively affect its dissolved oxygen levels through various mechanisms. Pollutants such as organic matter or nutrients for example nitrogen and phosphorous can lead to excessive algal growth through eutrophication. When these algal die and decompose, bacteria consume oxygen during the decomposition process, leading to a decrease in dissolved oxygen levels. Overall, a rise in pollutant concentration often exacerbates the decline in dissolved oxygen levels, posing significant threats to river ecosystems.

1.8 Advection-reaction diffusion equations

Reaction-diffusion equation is a partial differential equation that describes the time evolution of the concentration of one or more chemical substances undergoing both diffusion and reaction process. The general form of one-dimensional reaction-diffusion equation is of the form

$$u_t = Du_{xx} + F(u), \tag{1.1}$$

where u is the concentration of the substance with respect to space and time t, D is the diffusion coefficient, representing the rate at which the substance diffuses through space, $F(u)$ is the reaction term, describing the changes due to chemical reactions.

Advection-reaction diffusion equations is an extension of the Reaction-diffusion equations with advection term, such types of equations are used to model the transport, diffusion and reaction of substances in medium where there is a flow or advection of the substance along with the diffusion and chemical reaction process. They are of the form;

$$u_t + vu_x = Du_{xx} + F(u), \tag{1.2}$$

where v is the advection velocity representing the speed at which the substance is transported by the flow.

Reaction -Advection-Diffusion models are effective for describing the distribution of dissolved oxygen in rivers, accounting for the effects of pollution and temperature.

1.9 Statement of the problem

Although mathematical models for determining oxygen concentration and pollutant concentration in a river exist, see for instance Pimpunchat et al. (2009), for equations governing the concentration of pollutant, the models considered pollutant addition along the river. For the equation governing concentration of oxygen, the models considered the rate of transfer of oxygen through the surface of the water from the air but did not consider the effect of temperature on such transfer.

To the best of my knowledge, none of these studies has incorporated temperature in the model. Temperature plays a big role in determining concentration of dissolved oxygen in a river. The temperature of water is a critical factor as it directly influences the amount of oxygen that enters into the water. Existing river pollution models have overlooked its importance. Given the significant role played by temperature in determining the concentration of dissolved oxygen, it is essential to incorporate temperature in the existing river pollution models.

1.10 Objectives of the study

The main objective of the study is to develop and analyse a model of temperature-dependent dissolved oxygen and pollutant concentration in a river.

1.10.1 Specific objectives

(i) Formulate a model of temperature-dependent dissolved oxygen and pollutant concentration in a river;

(ii) Determine the steady states of oxygen and pollutant concentration from the model formulated in (i);

(iii) Simulate the model to illustrate the results in (ii).

1.11 Methods of the study

We shall use the following methods:

(i) Formulate a model using a system of advection-diffusion reaction partial differential equations (PDE);

(ii) Analytically determine the steady state of the model in (i);

(iii) Use Matlab software to generate numerical simulations for the model.

1.12 Justification of the study

This study helps in predicting the level of pollutant and oxygen concentrations in a river. It contributes to a timely and cost effective method in determining the levels of pollution in a river. Furthermore, incorporating temperature in the models of water pollution will help in identifying potential problems of the state of rivers and on water bodies before they become more severe and facilitate the development of effective strategies to address the water pollution and protect aquatic ecosystems.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

In this chapter, we discuss the literature on the use of partial differential equations. The main idea is to review the literature on models for oxygen and pollutant concentration and give their limiting gaps.

2.2 Oxygen and Pollutant Concentration Models

Oxygen concentration models refer to mathematical representations that describe and predict the distribution of oxygen in a specific environment such as rivers. These models are used to understand how oxygen levels change, interact with other substances and how it responds to other factors. Pollutant concentration models are models used to predict and assess the distribution of the levels of pollutants in various environmental media such as rivers. They help in understanding and managing environmental pollution (Pimpunchat et al., 2009).

Mathematical models, see for instance (Pimpunchat et al., 2009), have been developed and help in predicting the levels of pollution in rivers. Streeter-Phelp's model, see for instance (Streeter, 1925), originated in 1920's and described the balance of dissolved oxygen in rivers. The model was based on the assumptions that a single biological oxygen demand input is distributed evenly at a cross section of the river. They used partial differential equations to estimate the total oxygen deficit in a river. It reads as:

$$\frac{\partial D}{\partial t} = n_1 L_b - n_2 D, \tag{2.1}$$

where $D := D(x,t)$ is the saturation deficit, given by dissolved oxygen concentration at saturation minus the actual dissolved oxygen concentration, n_1 is the deoxygenation rate, n_2 is the reaeration rate and L_b is the oxygen demand at time t. They solved Equation (2.1) analytically and represented it in the form of dissolved oxygen sag curve. This model is very useful since it describes how dissolved oxygen decreases in a river due to degradation of biological oxygen demand. The Streeter-Phelps model provide a foundation to understanding how oxygen levels change in rivers over time.

Amin (2014) considered the scalar model

$$\begin{aligned} \frac{\partial C}{\partial t} &= \alpha\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - kC, x > 0, t > 0 \\ u(0,t) &= \beta, t > 0 \\ u(x,0) &= 0, x > 0 \\ u(x,t) &\to 0, as\ \ x \to \infty \end{aligned} \tag{2.2}$$

where $C := C(x,t)$ is the concentration of a substance at distance x downstream, α is the diffusion coefficient, $v > 0$ is the velocity of the water in a river, $\beta > 0$ is the rate of discharge, kC is source and $v\frac{\partial C}{\partial x}$ represent convection of the substance. It is assumed that the concentration of a substance is being poured at a constant rate into a straight, narrow river which flows with constant velocity. They used the Laplace transform method in determining the analytical solutions of the equation. They investigated when the river is flowing with low velocity and when the river is flowing with high velocity, where they found that at a very low velocity, the concentration of the substance reach zero at a shorter distance and with the increasing velocity of the river flow, the concentration distribute at a further distance which also depends on the increasing of the coefficient α. In Amin (2014), the effect of temperature has not been considered.

Jain *et al.* (2021) considered the scalar model

$$\frac{\partial(AC)}{\partial t} = \beta\frac{\partial^2(AC)}{\partial x^2} - \frac{\partial(vAC)}{\partial x} + \sigma(S - C) - z; 0 \leq x < L, t > 0 \quad (2.3)$$

where L (m) is the length of the polluted part of the river, $A := A(x,t)$ refers to the cross-sectional area of the river (m^2), β refers to the diffusion coefficient of dissolved oxygen along the river ($m^2 day^{-1}$), v represent velocity of the water along the river, σ represent the rate of transfer of oxygen from the air into water, S represent the saturated oxygen concentration (kgm^{-3}) and z represent net oxygen decay rate in the presence of biological pollutants ($kgm^{-1}day^{-1}$). Other symbols are as defined in Equation (2.2). Since the advection term is much smaller as compared to diffusion term, the term $\frac{\partial(vAC)}{\partial x}$ along the river, is neglected. Thus, Equation (2.3) becomes:

$$\frac{\partial(AC)}{\partial t} = \beta\frac{\partial^2(AC)}{\partial x^2} - \sigma(S - C) - z; 0 \leq x < L, t > 0. \quad (2.4)$$

The term $\sigma(S - C)$ represent oxygen deficit. The method of lines was employed to solve Equation (2.4) subject to Dirichlet boundary condition. They investigated the effect of the pollutant on the concentration of DO where it was found that if the stream is unpolluted originally, the dissolved oxygen level remains near saturation, but in the presence of pollutant, oxygen level drops and the natural aeration through atmosphere becomes active which helps oxygen to regain its normal value.

In model, Jain et al. (2021), the influence of temperature has not been considered on the rate of oxygen transfer from the air into the river, σ in $\sigma(S - C)$ and temperature plays a crucial role in determining the rate of oxygen transfer into the water. If temperature is considered, a more comprehensive model of river pollution can be developed.

Hussain et al. (2012) considered the model

$$\frac{\partial(AP)}{\partial t} = D_k \frac{\partial^2(AP)}{\partial x^2} - \frac{\partial(vAP)}{\partial x} + zP, \tag{2.5}$$

$$\frac{\partial(AX)}{\partial t} = D_y \frac{\partial^2(AX)}{\partial x^2} - \frac{\partial(vAX)}{\partial x} + \alpha(S - X), \tag{2.6}$$

where $P := P(x,t)$ is the pollutant concentration ($kg\ m^{-3}$), $X := X(x,t)$ is the dissolved oxygen concentration ($kg\ m^{-3}$), D_y represent dispersion coefficient of dissolved oxygen along the river ($m^2 day^-1$), D_k represent dispersion coefficient of pollutant along the river ($m^2 day^-1$), A represents cross-sectional area of the river (m^2), α represent rate of transfer of oxygen from air to water ($m^2 day^-1$), z represent mass transfer of solids (solutes). Other symbols are as defined in Equation (2.2). Equation (2.5) represent pollutant concentration and includes the mass transfer of solids (solute) to the river while Equation (2.6) is a mass balance for dissolved oxygen. It is assumed that the river has a uniform cross-sectional area and is one dimensional.

They used separation of variables method to determine the steady state, where, the steady state solution for Equations (2.5) using the boundary conditions $P(0) = \frac{q}{kA}$, and $D_k = 0$ was found to be $P(x) = \frac{q}{kA} e^{\frac{z}{vA}x}$ and the steady state solution for Equation (2.6) subject to boundary condition $X(0) = S + \frac{q}{kA}$ and $D_y = 0$ was found to be $X(x) = \frac{q}{kA} e^{-\frac{\alpha}{vA}x} + S$, where $X(x)$ is the dissolved oxygen concentration downstream of the river. It was found that pollutant concentration and dissolved oxygen concentration level remain within the critical values of the parameters and approximately consistent with the values measured for different stations. This model provide a foundation for understanding the dynamics of pollutant and dissolved oxygen concentrations.

The effect of temperature on the rate of oxygen transfer from the air into water is not considered.

Manitcharoen and Pimpunchat (2020) considered the model,

$$\frac{\partial(AP_1)}{\partial t} = D_p\frac{\partial^2(AP_1)}{\partial x^2} - \frac{\partial(vAP_1)}{\partial x} - K_1AP_1 + qH(x), \quad (2.7)$$

$$\frac{\partial(AP_2)}{\partial t} = D_x\frac{\partial^2(AP_2)}{\partial x^2} - \frac{\partial(vAP_2)}{\partial x} - K_1AP_2 + q(1 - e^{(-\lambda x)})H(x), \quad (2.8)$$

where, H(x) is the Heaviside function given by

$$H(x) = \begin{cases} 1, & \text{if } 0 < x \leq L \\ 0, & \text{if otherwise.} \end{cases}$$

The distance down stream from its source is described by x, $P_1 := P_1(x,t)$ and $P_2 := P_2(x,t)$ represent concentration of pollutant which is assumed to be varying with time t(days). Sources of pollution were considered in two cases, P_1 increasing uniformly and P_2 increasing exponentially as demonstrated in Equations (2.7) and (2.8) respectively. The constant λ represent exponential pollution constant term, q is the constant rate of pollutant addition into the river and v is the velocity of the river in ($m\ day^{-1}$).

They used the Laplace transform method to obtain analytical solutions for Equations(2.7) and (2.8) and then applied finite difference technique to obtain numerical solutions. The steady-state solution of Equations (2.7) and (2.8) were obtained as:

$$P_1(x) = \frac{q}{AK_1} + (P_0 - \frac{q}{AK_1})e^{(-(\gamma - \frac{\beta}{\sqrt{D_P}})x)}, \quad (2.9)$$

$$P_2(x) = \frac{q}{AK_1} - \frac{q}{AK_3}e^{-\lambda x} + (P_0 - \frac{q}{AK_1} + \frac{q}{AK_3})e^{(-(\gamma - \frac{\beta}{\sqrt{D_p}})x)},$$

$$(2.10)$$

where, $\gamma = \frac{v}{2D_p}$, $\beta = \sqrt{\frac{v^2}{4D_p} + K_1}$, $K_3 = K_1 - v\lambda - D_p\lambda^2$ and P_0 represent source concentration at the origin. Upon introducing limits as $x \to \infty$ yields $P_1(x) = P_2(x) = \frac{q}{AK_1}$. It can be seen that, the trend of concentrations along the river varies with time and space and is affected by the rate of pollutant addition. The concentration of the pollutant vary with q along the river. This model is useful since it helps us understand how pollutant disperse in a river over a time.

Pimpunchat et al. (2009) considered

$$\frac{\partial(AP)}{\partial t} = D_p\frac{\partial^2(AP)}{\partial x^2} - \frac{\partial(vAP)}{\partial x} - K_1\frac{X}{X+k}AP + qH(x), \tag{2.11}$$

$$\frac{\partial(AX)}{\partial t} = D_x\frac{\partial^2(AX)}{\partial x^2} - \frac{\partial(vAX)}{\partial x} - K_2\frac{X}{X+k}AP + \sigma(S-X), \tag{2.12}$$

where, $0 < x < L < \infty, t > 0$. The rate at which pollutant is added in to the river is represented by q, the parameter k represents half saturated oxygen demand concentration for pollutant decay (kgm^{-3}), D_p represents dispersion coefficient of pollutant in the x direction (m^2day^{-1}), K_1 represents degradation rate coefficient for pollutant (day^{-1}), K_2 is the rate at which oxygen is being consumed by the pollutant (day^{-1}), D_x represent dispersion coefficient of dissolved oxygen (m^2day^{-1}), other symbols are as defined in Equation (2.2) and Equation (2.8). It was assumed that the pollutants are largely biological wastes and undergo various biochemical and biodegradation process using oxygen.

They considered the variation to be only in the downstream of the river where they used variation-of-parameters method and applied the boundary conditions

$P(0) = 0$, $X(0) = 0$ to determine the steady state solutions, where they found pollutant concentration downstream is $P(x) = \frac{q}{K_1 A}(1 - e^{\frac{-K_1 x}{v}})$ which upon taking limits as $x \to \infty$ yields $P(x) = \frac{q}{K_1 A}$ and for upstream where there is no dispersion since there is no pollution upstream, it was found that, the dissolved oxygen requirement for survival of aquatic animals such as fish is 30% of the saturated values S and therefore, q is required to be such that, $q < 0.7\sigma\frac{K_1 S}{K_2}$. They also investigated for $k \neq 0$, where they concluded that the steady state solution depends on parameters k and q downstream such that if $q \geq \frac{\sigma K_1 S}{K_2}$, downstream solution does not exist. In this model, the effect of temperature on the rate of oxygen transfer from the air into the water has not been considered.

Although mathematical models for determining oxygen concentration and pollutant concentration in a river exist, see for instance Pimpunchat et al. (2009) and Manitcharoen and Pimpunchat (2020), for the equations governing the concentration of pollutant, the models considered pollutant addition along the river. For the equation governing concentration of oxygen, the models considered the rate of transfer of oxygen through the surface of the water from the air but did not consider the effect of temperature on such transfer. None of these studies has incorporated temperature in the model.

Dissolved oxygen and temperature have an inverse relationship, see for instance (Rajwa-Kuligiewicz et al., 2015) which can be described using the term $e^{-\lambda\theta}$ since it captures the gradual changes over time and the asymptotic behavior of dissolved oxygen as temperature, θ, increases, where $\lambda > 0$, determines the strength of the effect of temperature θ.

Therefore, the formulation of the model in this research is similar to that proposed by Pimpunchat et al. (2009) but with the inclusion of temperature. This is what we do in the next Chapter.

CHAPTER 3

FORMULATION OF THE MODEL

3.1 Introduction

In this chapter, we develop a model that describes the dynamics of the concentration of pollutant and oxygen in a river using systems of advection-diffusion reaction partial differential equations. We start by stating the underlying assumptions in section 3.2 and then derive the model with the inclusion of temperature variation.

3.2 Assumptions of the model

We make the following plausible assumptions:

(i) The river is divided into sections where each section flows with uniform velocity v;

(ii) The flow is considered to be in one dimensional with a uniform cross-sectional area in each section;

(iii) The concentration of oxygen in the river depend on temperature gradient of the water;

(iv) The concentration of pollutant is primarily influenced by factors other than temperature, such as the rate of pollutant input into the river.

Let the concentration of pollutant at (x, t) be denoted by $P := P(x, t)$ and that of oxygen be denoted by $X := X(x, t)$. Let R define a region in space through which the water flows, known as control volume which extends from the water surface to the bottom, A to be the cross-sectional area and $\vec{n}$ to represent the outward unit normal vector to the control volume's boundary as illustrated in Figure 3.1.

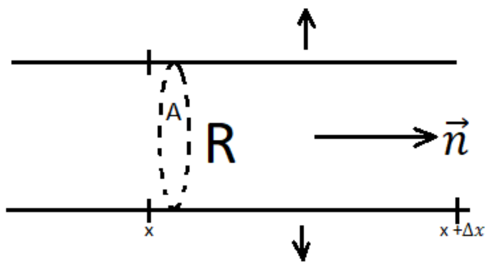

Figure 3.1: Schematic Diagram of a river cross section

By conservation of mass principle,

$$\begin{aligned} Net\ change\ of\ pollutant\ inside\ R &= The\ net\ flux\ across\ the\ boundaries \\ &\quad +net\ pollutant\ generated; \\ &= Net\ flux\ across\ the\ boundaries + Net \\ &\quad pollutant\ added + Advection \\ &\quad +Removal \end{aligned} \tag{3.1}$$

$$Total\ concentration\ of\ pollutant = \int_R P(s, t)ds, \tag{3.2}$$

where $R = [x, \ \ x + \Delta x]$.

Rate of net change of pollutant inside $R = \frac{d}{dt} \int_R P(s,t)ds$. Next, we show how the flux of pollution is obtained.

Let the flux of pollution, $P(x,t)$ in the river at a point (x,t) be represented by $J_p := J_p(x,t)$. The total flux J_p is a combination of convection and diffusion, and is given by

$$J_p = J_pc + J_pd = vP - D_p \nabla P, \tag{3.3}$$

where the convection component J_pc represent the transport of a pollutant due to fluid's bulk motion (how the river flows) and is given by the expression $J_pc = vP$. The diffusion component is represented by $J_pd = -D_p \nabla P$ where D_p is the dispersion coefficient and ∇P is the gradient of pollution concentration. The negative sign means that, the flux is from the side of higher concentration to that of lower concentration.

The Pollutant and Oxygen interact with each other, such that both the concentration of pollutant and dissolved oxygen change with time in response to each other's presence such that

$$F_1(X,P) := -K_1 \frac{X}{X+k} P, \tag{3.4}$$

where K_1 is the pollutant degradation rate coefficient which indicates how fast pollutants are broken down in the presence of dissolved oxygen and k denotes the half saturation oxygen demand concentration for pollutant decay. Equation (3.4) represents how concentration of pollutants changes with time in response to the presence of dissolved oxygen, and as the concentration of oxygen increases, the concentration of pollutants decreases. Similarly, the concentration of oxygen decreases, as pollutant concentration increases. Since pollutants use up oxygen during decomposition, we represent this by

$$F_2(X, P) := -K_2 \frac{X}{X+k} P. \tag{3.5}$$

Equation (3.5) describes how the concentration of dissolved oxygen decreases in response to increase in pollutants. K_2 is the de-aeration rate coefficient for dissolved oxygen which indicates how fast dissolved oxygen depletes in the presence of pollutants.

Equation (3.4) takes the indicated form to show the change in oxygen consumption is not constant but varies depending on the levels of available oxygen and the half saturation constant and to reflect the system's sensitivity to changes in both oxygen and pollutant concentration.

We consider a water body with cross-sectional area A, depth h and volume V; that is, $V = Ah$. We then assume that the reactions in the water body is influenced by several factors including pollutant addition, thus the reaction in the water body is

$$\frac{d(PV)}{dt} = -K_1 \frac{X}{X+k}(PV) + Q \tag{3.6}$$

where $Q = qAh$. Thus, the expression becomes

$$\frac{d(PAh)}{dt} = -K_1 \frac{X}{X+k}(PAh) + qAh \tag{3.7}$$

Dividing Equation (3.6) by Ah, we obtain

$$\frac{dP}{dt} = -K_1 \frac{X}{X+k} P + q. \tag{3.8}$$

By applying the mass conservation principle, we have:

Net change of pollutant inside R = $-$ what is disappearing over the boundary of R per unit time +what is produced in R per unit time,

$$\frac{d}{dt}\int_R PdV = -\int_{\partial R} J_p \cdot n d\sigma + \int_R r dV.$$

Here $d\sigma$ is an element of area on the control surface ∂R, dV is the element of volume within the control volume R, $\vec{n}$ is the outward unit normal vector to the control volume's boundary, $r := r(x,t)$ is the source term which includes both interaction term and the pollutant input.

Thus, from Equations (3.2), (3.3) and (3.8) and by the general mass conservation law, we have

$$\frac{d}{dt}\int_R P(s,t)ds + \int_{\partial R} J_p \cdot n d\sigma = \int_R (-K_1 \frac{X}{X+k} P + q)dx, \tag{3.9}$$

Applying Leibniz rule and the Divergence theorem, we obtain

$$\int_R (\frac{\partial P}{\partial t} + \nabla \cdot (vP - D_p \nabla P))dx = \int_R (-K_1 \frac{X}{X+k} P + q)dx \tag{3.10}$$

Since Equation (3.10) holds for any control region R and by the homogeneity of X, P and continuity, we have

$$\frac{\partial P}{\partial t} - D_p \nabla^2 P + \nabla \cdot vP = -K_1 \frac{X}{X+k} P + q, \; 0 < x < L, t > 0 \tag{3.11}$$

Re-arranging, we have

$$\frac{\partial P}{\partial t} \;=\; D_p \nabla^2 P - \nabla \cdot vP - K_1 \frac{X}{X+k} P + q, \tag{3.12}$$

for $0 < x < L, t > 0$. We see from Equation (3.12) that,

$$\frac{\partial P}{\partial t} = D_p \frac{\partial^2 P}{\partial x^2} - \frac{\partial (vP)}{\partial x} - K_1 \frac{X}{X+k} P + q, \tag{3.13}$$

for $0 < x < L, t > 0$.

In an analogous manner, if we let $X := X(x,t)$ denote oxygen concentration at x at time t, and apply the conservation of mass principle, then we have:

Net change of DO concentration inside R is = the net flux across the boundaries + net oxygen generated.

$$\begin{aligned} Net\ change\ of\ DO\ inside\ R &= Net\ flux\ across\ the\ boundaries \\ &\quad +Net\ oxygen\ added + Advection \\ &\quad +Removal \end{aligned}$$

Total concentration of oxygen in R = $\int_R X(s,t)ds$.
Net change of oxygen inside $R = \frac{d}{dt}\int_R X(s,t)ds$.

The derivation of the equation for oxygen concentration is similar to that of pollutant concentration apart from the last term for rate of oxygen transfer from air into the water. This is because if the water in the river is in contact with open air, oxygen enters the water through the water surface and it is assumed that the rate of increase in concentration of oxygen by movement from the surrounding air into the river is proportional to the saturated concentration S less the concentration X.

Let the rate at which oxygen is transfered into water from the air through the water surface, per unit area and time be given by β. Thus, the mass of oxygen that is transfered through the water surface per unit area and per unit time from the air is given by $\beta(S - X)$, where S is the saturation value for oxygen concentration in water and X is the dissolved oxygen concentration in the water. The term

$\beta(S-X)$ is the flux term for the transport of oxygen through the open-water surface which shows how much oxygen is transferred from the air into the water per unit area and time. If we consider a water body with cross-sectional area A, then, for $0 < x < L, t > 0$, we have:

$$\frac{\partial(AX)}{\partial t} = D_x\frac{\partial^2(AX)}{\partial x^2} - \frac{\partial(vAX)}{\partial x} - K_2\frac{X}{X+k}AP + A\beta(S-X) \quad (3.14)$$

Thus, from Equation (3.13) and (3.14), for $0 < x < L, t > 0$, we obtain

$$\frac{\partial P}{\partial t} = D_p\frac{\partial^2 P}{\partial x^2} - \frac{\partial(vP)}{\partial x} - K_1\frac{X}{X+k}P + q, \quad (3.15)$$

$$\frac{\partial X}{\partial t} = D_x\frac{\partial^2 X}{\partial x^2} - \frac{\partial(vX)}{\partial x} - K_2\frac{X}{X+k}P + \beta(S-X). \quad (3.16)$$

Since pollutants are only discharged for $x > 0$, we include the Heaviside function H(x) in Equation (3.15) which captures the fact that pollutants are only discharged for $x > 0$.

Thus, Equation (3.15) becomes

$$\frac{\partial P}{\partial t} = D_p\frac{\partial^2 P}{\partial x^2} - \frac{\partial(vP)}{\partial x} - K_1\frac{X}{X+k}P + qH(x), \quad (3.17)$$

where, $0 < x < L, t > 0$ and

$$H(x) = \begin{cases} 1, & \text{if } 0 < x \leq L, \\ 0, & \text{if otherwise.} \end{cases}$$

In Equation (3.17), the influence of temperature has not been taken into account, since it is assumed that the concentration of pollutant is primarily influenced by factors other than temperature, such as the rate of pollutant input into the river. This is because the pollutant may be a run off from agricultural fields, where temperature is not the driving factor of the concentration of the pollutant.

We incorporate the effect of temperature in Equation (3.16) because it has a direct impact on dissolved oxygen.

Increase in temperature increases rate of respiration which leads to increased oxygen consumption. Dissolved oxygen concentration vary by season, depth and time of the day. Cold weather seasons are characterized by low temperatures while in hot seasons are characterized by high temperature. A narrow, deep, well shaded river reduces the impact of warming by the sun hence holding more dissolved oxygen while wide and shallow river would have high temperatures due to solar heating which lowers the amount of dissolved oxygen. Warmer air temperature affects water-temperature in a river.

If we consider the influence of temperature on the rate of oxygen transfer from the surrounding air into the water, Equation (3.16) becomes,

$$\frac{\partial X}{\partial t} = D_x \frac{\partial^2 X}{\partial x^2} - \frac{\partial (vX)}{\partial x} - K_2 \frac{X}{X+k} P + \beta(S-X)e^{-\lambda\theta}, \tag{3.18}$$

where $0 < x < L, t > 0$ and $e^{-\lambda\theta}$ indicate how the rate of oxygen transfer changes as temperature changes. The term $e^{-\lambda\theta}$ is used because it captures the gradual changes over time and the asymptotic behavior of dissolved oxygen as temperature, θ, increases. The rate of oxygen transfer from the air to water decreases with the increase in water-temperature and vice-versa and dissolved oxygen and temperature have an inverse relationship, see for instance (Rajwa-Kuligiewicz et al., 2015). The term $\beta(S-X)e^{-\lambda\theta}$ takes the indicated form since the rate of oxygen transfer from the air into the water depends on the gradient of its concentration.

Therefore, the two coupled advection-dispersion reaction equations, which accounts for the evolution of pollutant and dissolved oxygen concentrations are thus obtained from Equation (3.17) and Equation (3.18) and are represented as shown in Equation (3.19).

$$
\begin{aligned}
\frac{\partial P}{\partial t} &= D_p \frac{\partial^2 P}{\partial x^2} - \frac{\partial (vP)}{\partial x} - K_1 \frac{X}{X+k} P + qH(x), \\
\frac{\partial X}{\partial t} &= D_x \frac{\partial^2 X}{\partial x^2} - \frac{\partial (vX)}{\partial x} - K_2 \frac{X}{X+k} P + \beta (S - X) e^{-\lambda \theta}, \\
& \quad 0 < x < L, t > 0.
\end{aligned} \tag{3.19}
$$

For easy of analysis of Equation (3.19), we do non-dimensionalization, to reduce the number of parameters and group them in a meaningful way. For this purpose, we define

$$
\bar{t} := \frac{v}{L} t, \bar{x} := \frac{x}{L}, \bar{X} := X, \bar{P} := \frac{P}{S}, \bar{k} := \frac{k}{S} \tag{3.20}
$$

and assume that the length per unit time is equal to one, since it can be expressed per day, that is $\frac{L}{v} = 1$. We drop the bars for notational brevity and thus obtain;

$$
\begin{aligned}
\frac{\partial P}{\partial t} &= \epsilon_p \frac{\partial^2 P}{\partial x^2} - \frac{\partial P}{\partial x} - K_1 \frac{X}{X+k} P + \gamma_p, \\
\frac{\partial X}{\partial t} &= \epsilon_x \frac{\partial^2 X}{\partial x^2} - \frac{\partial X}{\partial x} - K_2 \frac{X}{X+k} P + \alpha_x (1 - X) e^{-\lambda \theta},
\end{aligned} \tag{3.21}
$$

for $0 < x < 1, t > 0$

where, $\epsilon_p := \frac{D_p}{L^2}$, $\epsilon_x := \frac{D_x}{L^2}$, $\gamma_p := \frac{q}{S}$, $\alpha_x := \beta$

system (3.21) is now the simplified form for the model of our interest that we shall analyse in Chapter 4.

CHAPTER 4

ANALYSIS AND RESULTS

4.1 Introduction

In this chapter, we wish to show that when a river is highly polluted, a slight change in temperature leads to a catastrophe or hypoxia. For this purpose, we shall need to determine the long-term solutions and analyse their respective stability/instability.

In section 4.2 we analyse the steady-state solution for zero dispersion, while in section 4.3 we shall show the relationship between a critical temperature and pollutant concentration and in section 4.4 we provide an analytic steady-state solutions for the model including dispersion.

We determine the long-term solution; that is, the steady-state solution and show that this solution is asymptotically stable. We will show how the long-term solution is related to temperature.

4.2 Long-term Solution without Dispersion

Long-term solution are contained in the steady-state which are attained when $\frac{\partial(P)}{\partial t} = \frac{\partial(X)}{\partial t} = 0$. With the assumption that the speed of the water is very high and dispersion coefficient are very small compared to speed of the water, we ignore the dispersion coefficient; that is, $D_p = 0$ and $D_x = 0$, and the system of partial differential Equations (3.21) then become a system of ordinary differential equations given in Equations (4.1) and (4.2).

$$\begin{aligned} \frac{dP}{dx} + K_1 \frac{X}{X+k} P - \gamma_p &= 0, & (4.1) \\ \frac{dX}{dx} + K_2 \frac{X}{X+k} P - \alpha_x (1-X) e^{-\lambda\theta} &= 0. & (4.2) \end{aligned}$$

Upon re-arranging, we obtain;

$$\begin{aligned} \frac{dP}{dx} &= -K_1 \frac{X}{X+k} P + \gamma_p, & (4.3) \\ \frac{dX}{dx} &= -K_2 \frac{X}{X+k} P + \alpha_x (1-X) e^{-\lambda\theta}. \end{aligned}$$

To find the asymptotic solutions of Equations (4.3), we shall state the following elementary and useful lemma.

Lemma 4.2.1. *Let $x \in (0, \infty)$ and $f : [x, \infty) \to \mathbb{R}$ be a differentiable function. If the $\lim_{x\to\infty} f(x)$ exists and the derivative of the function $f(x)$, $\dot{f}(x)$ is uniformly continuous on (x, ∞), then $\lim_{x\to\infty} \dot{f}(x) = 0$*

This lemma will be useful throughout our analysis and is motivated by the fact that the variables in the model are continuous and differentiable and the solution is bounded. Its proof can be found in Coppel (1965) and Gopalsamy (1992).

We wish to obtain the asymptotic solutions of the Equations (4.3). We look at the eventual solution; that is, when $x \to \infty$, by Lemma 1, since (P, X) is bounded as $x \to \infty$, we have,

$$\begin{aligned} 0 &= -K_1 \frac{X}{X+k} P + \gamma_p, & (4.4) \\ 0 &= -K_2 \frac{X}{X+k} P + \alpha_x (1-X) e^{-\lambda\theta}. & (4.5) \end{aligned}$$

From Equation (4.4),

$$\frac{X}{X+k}P = \frac{\gamma_p}{K_1}, \tag{4.6}$$

substituting in Equation (4.5), we obtain:

$$\frac{\gamma_p}{K_1} = \frac{\alpha_x}{K_2}(1-X)e^{-\lambda\theta}, \tag{4.7}$$

which yields

$$X^\star := 1 - \frac{\gamma_p}{K_1}\frac{K_2}{\alpha_x}e^{\lambda\theta}. \tag{4.8}$$

Using Equation (4.8) in Equation (4.6), we get

$$P^\star := \frac{\gamma_p}{K_1}\Big(\frac{X^\star + k}{X^\star}\Big), \tag{4.9}$$

Thus, the solution when $x \to \infty$ is

$$(P^\star, X^\star) = \Big(\frac{\gamma_p}{K_1}\Big(\frac{X^\star + k}{X^\star}\Big), 1 - \frac{\gamma_p}{K_1}\frac{K_2}{\alpha_x}e^{\lambda\theta}\Big). \tag{4.10}$$

The solution of Equations (4.3) as $x \to \infty$, $(P^\star, X^\star)$ is independent of x.

Proposition 4.2.1. *If* $\alpha_x > \frac{\gamma_p K_2 e^{\lambda\theta}}{K_1}$, *then* $(P^\star, X^\star)$ *is asymptotically stable.*

Proof. The Jacobian matrix from Equation (4.3) is:

$$J(P, X) := \begin{pmatrix} -K_1\frac{X}{X+k} & -K_1\frac{Pk}{(X+k)^2} \\ -K_2\frac{X}{X+k} & -K_2\frac{Pk}{(X+k)^2} - \alpha_x e^{-\lambda\theta} \end{pmatrix} \tag{4.11}$$

which at $(P^\star, X^\star)$, yields:

$$J(P^\star, X^\star) = \begin{pmatrix} -K_1\sigma_1 & -K_1\sigma_2 \\ -K_2\sigma_1 & -K_2\sigma_2 - \alpha_x e^{-\lambda\theta} \end{pmatrix}, \tag{4.12}$$

where, $\sigma_1 := \left(\frac{\alpha_x K_1 - \gamma_p K_2 e^{\lambda\theta}}{\alpha_x K_1 - \gamma_p K_2 e^{\lambda\theta} + \alpha_x k K_1}\right)$, $\sigma_2 := \left(\frac{k{\alpha_x}^2 K_1 \gamma_p}{(\alpha_x K_1 - \gamma_p K_2 e^{\lambda\theta})(\alpha_x K_1 - \gamma_p K_2 e^{\lambda\theta} + \alpha_x k K_1)}\right)$. The matrix in Equation (4.12) can be written as;

$$J(P^\star, X^\star) := \begin{pmatrix} m_1 & m_2 \\ m_3 & m_4 \end{pmatrix}, \tag{4.13}$$

where $m_1 = -K_1\sigma_1$, $m_2 = -K_1\sigma_2$, $m_3 = -K_2\sigma_1$, and $m_4 = -K_2\sigma_2 - \alpha_x e^{-\lambda\theta}$. The eigenvalues of $J(P^\star, X^\star)$ are given by;

$$\mu_1 := \frac{(m_1 + m_4) + \sqrt{(m_1 + m_4)^2 - 4(m_1 m_4 - m_2 m_3)}}{2}, \tag{4.14}$$

$$\mu_2 := \frac{(m_1 + m_4) - \sqrt{(m_1 + m_4)^2 - 4(m_1 m_4 - m_2 m_3)}}{2}. \tag{4.15}$$

For stability, the real part of the eigenvalues should be negative; that is, $-K_1\sigma_1 - K_2\sigma_2 - \alpha_x e^{-\lambda\theta} < 0$ hence for asymptotically stability, we have; $\alpha_x > \frac{\gamma_p K_2 e^{\lambda\theta}}{K_1}$. $\square$

If $\alpha_x > \frac{\gamma_p K_2 e^{\lambda\theta}}{K_1}$, it implies that the river maintains a sustainable DO concentration which provides a more favorable habitat for aquatic life.

In section 4.3, we show how a critical temperature is obtained and how it relates with pollutant concentration. For simplicity, we use γ_p and α_x such that, $\gamma_p := \frac{q}{S}$, $\alpha_x := \beta$, as defined in Equation (3.21).

4.3 Relationship between critical temperature and pollutant concentration

In this section, we wish to show that there exist critical temperature, θ_c, beyond which oxygen concentration will approach zero; that is, $X(x) = 0$ as $x \to \infty$. Let $X^\star$ be the positive deviation of concentration from the hypoxia level, which for simplicity we shall take it as 0. Critical temperature is defined as the temperature beyond which oxygen levels in a river tend to zero. We show that there is a temperature, θ_c for which we shall have a catastrophe, obtained as follows;

$$X^\star := 1 - \frac{K_2 q}{\beta S K_1} e^{\lambda\theta}. \tag{4.16}$$

Oxygen concentration approaches zero at a temperature θ_c, thus we have;

$$X^\star = 0 = 1 - \frac{K_2 q}{\beta S K_1} e^{\lambda\theta_c}, \tag{4.17}$$

$$\frac{\beta S K_1}{K_2 q} = e^{\lambda\theta_c}. \tag{4.18}$$

Which upon simplification yields

$$\theta_c := \frac{1}{\lambda}\ln\Big(\frac{K_1 \beta S}{q K_2}\Big), \tag{4.19}$$

where, θ_c is the critical temperature. Since $\theta_c > 0$, $\left(\frac{K_1 S \beta}{q K_2}\right) > 1$.
If $\theta \geq \theta_c$, then oxygen levels becomes too low making the river incapable of supporting aquatic life.

We wish to show the relationship between θ_c and the rate of pollutant addition,

θ_c and the degradation rate coefficient for pollutant. When the rate of pollutant addition is high, a slight change in critical temperature have a catastrophic effects, leading to oxygen depletion rendering the river ecologically dead. The relationship between critical temperature, θ_c, and rate of pollutant addition, q, can graphically be as shown in Figure 4.1

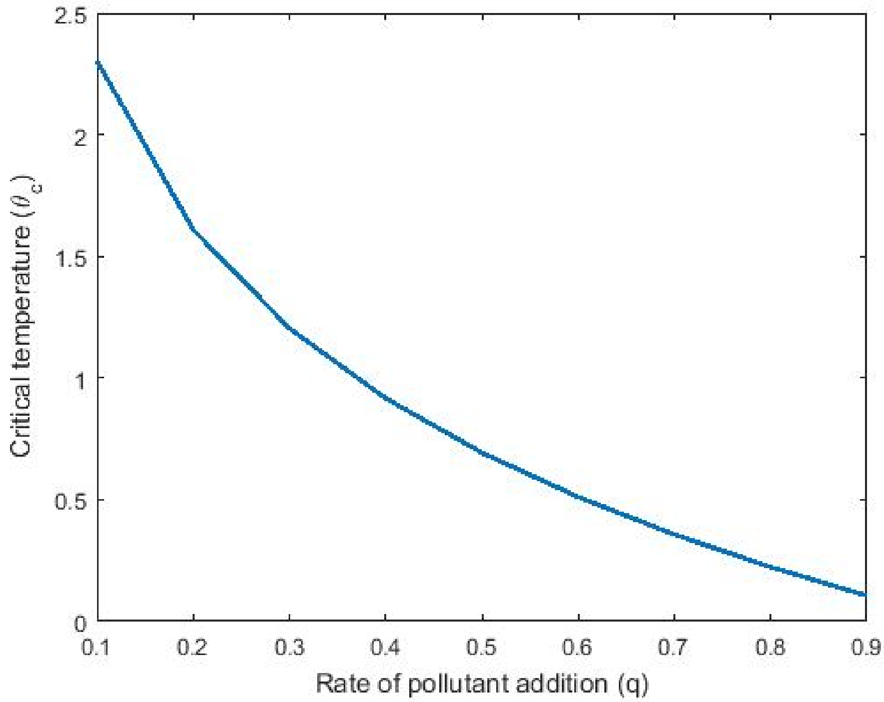

Figure 4.1: Critical temperature, θ_c vs Rate of pollutant addition, q

When the rate of pollutant addition, q is high, as illustrated in Figure 4.1, less θ_c is required for the river to be ecologically dead. High influx of pollutants puts pressure on the river's ecosystem which implies even at relatively lower θ_c, the river's oxygen levels tend to zero due to the excessive demand for oxygen caused by the degradation rate of the pollutants making the river ecologically dead. Conversely, when the rate of pollutant addition, q, is low, a higher θ_c is required for the river to reach anoxic conditions. Therefore, Figure 4.1 illustrates that as the rate of pollutant addition increases, less critical temperature is required for the river to become ecologically dead.

Oxygen levels depletes fast when rate of pollutant degradation is high and the temperature is high. Therefore, when the concentration rate of the pollutant is high and the critical temperature is very high, then the levels of oxygen in a river depletes fast which makes the river logically not sustainable. The relationship between critical temperature, θ and rate of pollutant degradation, K_1 is as shown in Figure 4.2.

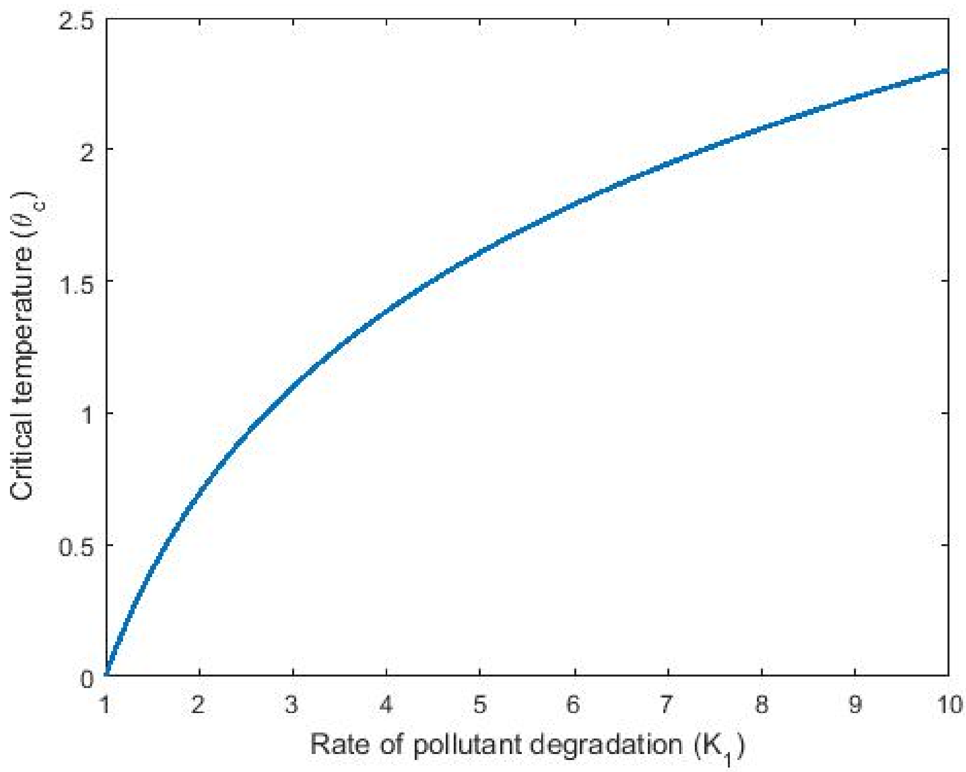

Figure 4.2: Critical temperature, θ vs Pollutant degradation rate, K_1

Figure 4.2 illustrates that, the rate of pollutant degradation increases as θ_c increases making the river to be in hypoxia levels. This is because, degradation of pollutants tends to increase with higher temperature. Therefore, a higher critical temperature is required, for the river to be ecologically dead. This is because a higher temperature accelerates biological activities and chemical processes, leading to a faster degradation rate of pollutants and as the degradation rate increases due to high temperature, the demand for oxygen also increases which leads to oxygen being depleted at a faster pace.

If $\frac{K_1}{K_2} << 1$, it indicates that the pollutant in a river is broken down or degraded at a slower rate as compared to the speed at which oxygen is being removed due to de-aeration process leading to a slower reduction in its concentration and oxygen essential for aquatic life is being depleted at a faster rate.

If $\frac{\beta}{q} << 1$, means that the river is receiving pollutants at a higher rate as compared to how the river is receiving oxygen from the air. This leads to insufficient oxygen levels in the river which adversely affects the ecosystem.

Next, we wish to show that there exist a temperature, θ, where θ is the temperature of the water in the river, that is favorable for supporting aquatic life; that is, there exist a non zero concentration of oxygen in the river. This occurs when $X^\star > 0$. Using Equation (4.16), we see that

If

$$\beta > \frac{qK_2 e^{\lambda\theta}}{SK_1},$$

then

$$\ln\beta > \ln(\frac{qK_2}{SK_1}) + \lambda\theta, \tag{4.20}$$

$$\ln\beta - \ln(\frac{qK_2}{SK_1}) > \lambda\theta. \tag{4.21}$$

Therefore from Equation (4.21),

$$\theta < \frac{1}{\lambda}\ln\Big(\frac{SK_1\beta}{qK_2}\Big). \tag{4.22}$$

Since $\theta < \frac{1}{\lambda}\ln\Big(\frac{SK_1\beta}{qK_2}\Big) := \theta_c$, the river environment remains conducive to supporting aquatic life. Clearly $q > 0$ and $\left(\frac{SK_1\beta}{qK_2}\right) > 1$.

We wish to show that if the rate of pollutant addition, is high, we shall require a smaller temperature change to lead to a catastrophe. This is contained in Proposition 2.

Proposition 4.3.1. *The function $\theta(q)$ is strictly decreasing with respect to q.*

Proof.

$$\begin{aligned}
\theta_c &= \frac{1}{\lambda}\ln\Big(\frac{SK_1\beta}{qK_2}\Big) && (4.23)\\
\theta_c &= \frac{1}{\lambda}\Big[\ln\Big(\frac{SK_1\beta}{K_2}\Big) - \ln q\Big] && (4.24)\\
\theta_c &= \frac{1}{\lambda}\Big[\ln\Big(\frac{SK_1\beta}{K_2}\Big) + \ln(\frac{1}{q})\Big] && (4.25)\\
\frac{\partial\theta_c}{\partial q} &= -\frac{1}{\lambda q} < 0. && (4.26)
\end{aligned}$$

□

The strictly decreasing relationship is significant in water quality management, as it provides insights into how pollutant addition affects the thermal dynamics of a river ecosystems.

Next, we wish to show that when the temperature of the water is equal to zero, then there is a certain amount of pollutant if added into the river will lead to a catastrophe. This is contained in Proposition 3.

Proposition 4.3.2. *If $\theta = 0$ and $\left(\frac{SK_1\beta}{K_2}\right) \geq q > 1$, then the river becomes ecologically dead when $\left(\frac{SK_1\beta}{K_2}\right) = q$.*

Proof. Let $X^\star$ be the positive deviation of concentration from the hypoxia level, which for simplicity we shall take it as 0.

$$X^\star = 1 - \frac{qK_2}{\beta SK_1}, \tag{4.27}$$

In this case, we have

$$0 = 1 - \frac{qK_2}{\beta S K_1}, \tag{4.28}$$

$$1 = \frac{qK_2}{\beta S K_1}, \tag{4.29}$$

hence,

$$\frac{\beta S K_1}{K_2} = q. \tag{4.30}$$

□

When $\frac{\beta S K_1}{K_2} = q$, it signifies a point where adding this specific amount of pollutant into the river leads to catastrophic consequences. This critical condition serves as a warning, indicating that surpassing a certain threshold could results in severe ecosystem damage. Lets now observe how the stability is affected by q and θ. For this purpose, we begin by considering θ and q being very small. Therefore if, θ and q are very small, $S\beta K_1 > K_2 q e^{\lambda\theta}$, which means $(m_1 + m_4) < 0$ and $(m_1 m_4 - m_2 m_3) > 0$. Thus, the fixed point $(P^\star, X^\star)$ remains stable.

If θ and q are very big, $K_2 q e^{\lambda\theta}$ becomes large. This means that $\beta < \frac{qK_2 e^{\lambda\theta}}{SK_1}$ due to high temperature and high pollutant input into the river. This affects the dissolved oxygen concentration and overall health of the habitat suitable for aquatic organisms, rendering the river incapable of supporting aquatic life. If $(1 + k) > \frac{K_2 q}{S\beta K_1} e^{\lambda\theta}$ this makes the system to have a saddle point. Thus, changes in θ and q, affect the stability and the overall behavior of the system.

We graphically show how θ and q affect the concentration of oxygen. This is as shown in Figure 4.3. Figure 4.3 shows the solution dynamics of the model when temperature is very small.

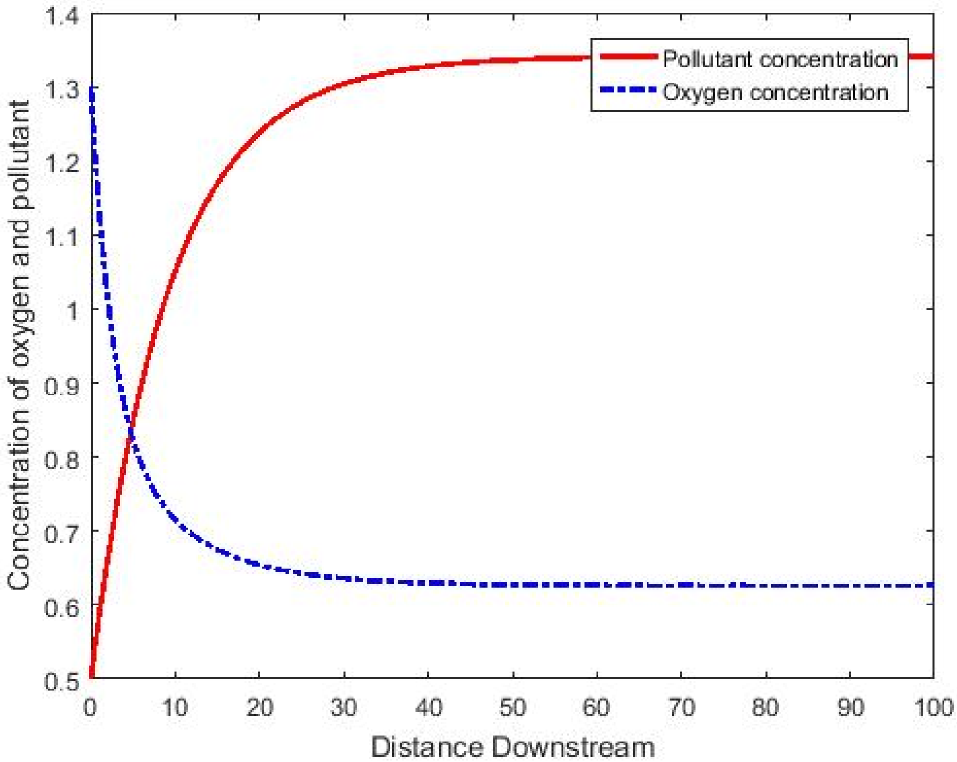

Figure 4.3: Oxygen and Pollutant concentration for small θ

From Figure 4.3, we observe that oxygen concentration is decreasing but pollutant concentration increases downstream.

If θ is big, oxygen concentration depletes resulting in ecologically dead river. This makes the river incapable of supporting aquatic life. Numerically, the results are as shown in Figure 4.4.

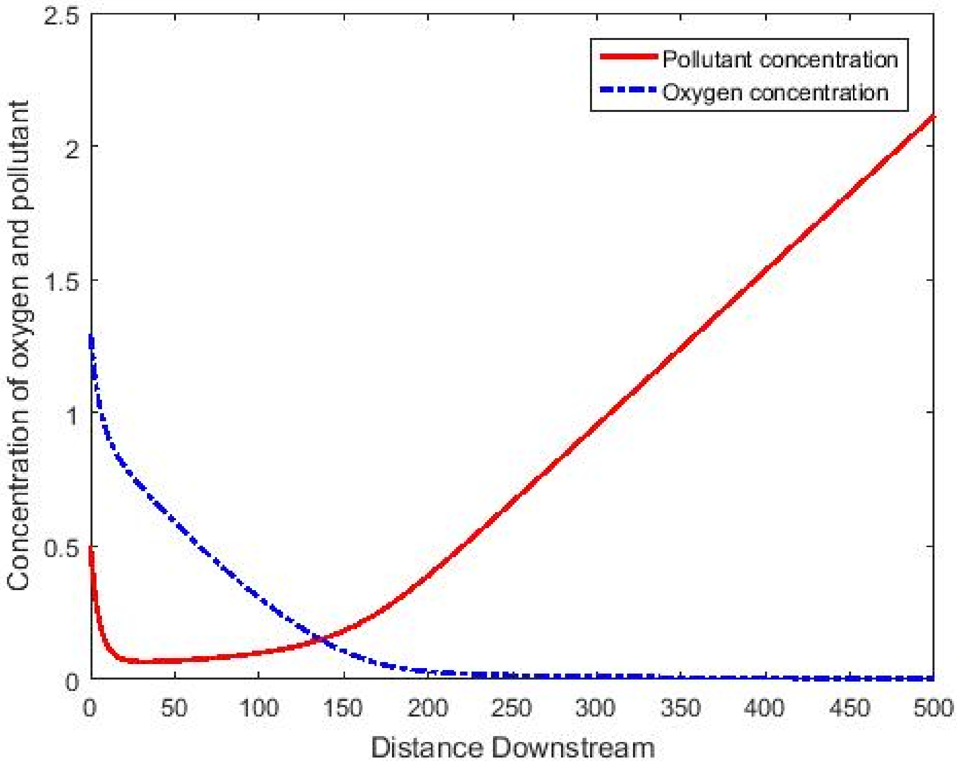

Figure 4.4: Oxygen and Pollutant concentration as θ varies

From Figure 4.4, we observe that when θ is large, the concentration of oxygen depletes very fast.

For small values of q and θ, there will be adequate oxygen concentration as illustrated in Figure 4.5.

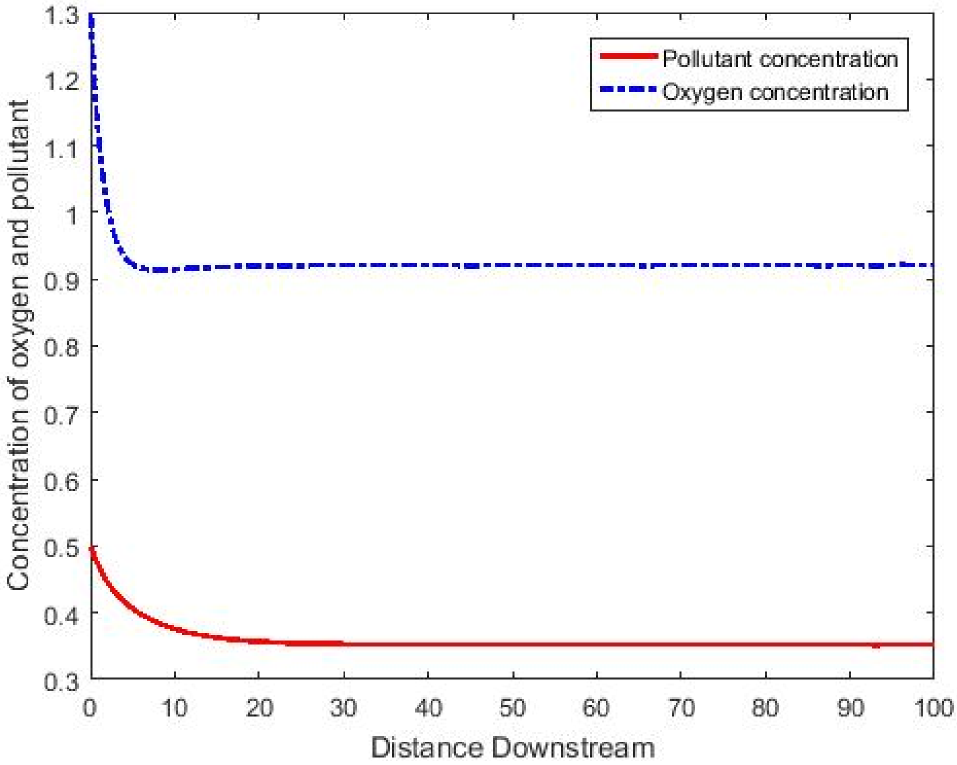

Figure 4.5: Oxygen and Pollutant concentration when θ and q are small

From Figure 4.5, we observe that the concentration of oxygen reaches equilibrium point faster. The concentration of pollutant reaches its equilibrium faster when the rate of pollutant addition is low.

4.4 Analytic steady-state solution for the model including dispersion

At steady state when the dispersion coefficient are included, that is $D_p \neq 0$ and $D_x \neq 0$, the system of partial differential equation in Equation (3.21) become a system of second order ordinary differential equations, since that involve x as the only independent variable. This results into Equations (4.31) and (4.32).

$$\epsilon_p \frac{d^2P}{dx^2} - \frac{dP}{dx} - K_1 \frac{X}{X+k} P + \gamma_p = 0; \quad x > 0, t > 0 \tag{4.31}$$

$$\epsilon_x \frac{d^2X}{dx^2} - \frac{dX}{dx} - K_2 \frac{X}{X+k} P + \alpha_x (1-X) e^{-\lambda\theta} = 0 \tag{4.32}$$

Equation (4.31) and (4.32) becomes,

$$\frac{d^2P}{dx^2} = \frac{1}{\epsilon_p}\frac{dP}{dx} + \frac{K_1}{\epsilon_p}\frac{X}{X+k}P - \frac{\gamma_p}{\epsilon_p}, \tag{4.33}$$

$$\frac{d^2X}{dx^2} = \frac{1}{\epsilon_x}\frac{dX}{dx} + \frac{K_2}{\epsilon_x}\frac{X}{X+k}P - \frac{\alpha_x}{\epsilon_x}(1-X)e^{-\lambda\theta}. \tag{4.34}$$

Since Equation (4.31) and (4.32) are second order ODES, we can transform them to first order ODES, to obtain,

$$\begin{aligned} \frac{dP_1}{dx} &= P_2, \\ \frac{dP_2}{dx} &= \alpha_1 P_2 + \alpha_2 \frac{X_1}{X_1+k} P_1 - \omega, \\ \frac{dX_1}{dx} &= X_2, \\ \frac{dX_2}{dx} &= \alpha_3 X_2 + \alpha_4 \frac{X_1}{X_1+k} P_1 - \rho(1-X_1). \end{aligned} \tag{4.35}$$

where $\alpha_1 = \frac{1}{\epsilon_p}$, $\alpha_2 = \frac{K_1}{\epsilon_p}$, $\alpha_3 = \frac{1}{\epsilon_x}$, $\alpha_4 = \frac{K_2}{\epsilon_x}$, $\omega = \frac{\gamma_p}{\epsilon_p}$, $\rho = \frac{\alpha_x}{\epsilon_x}e^{-\lambda\theta}$.

For asymptotic solutions, $P_2 = 0$, and $X_2 = 0$, thus we obtain.

$$\frac{X_1}{X_1+k}P_1 = \frac{\omega}{\alpha_2} \tag{4.36}$$

$$\frac{X_1}{X_1+k}P_1 = \frac{\rho}{\alpha_4}(1-X_1) \tag{4.37}$$

which upon simplification yields:

$$X_1^\star := 1 - \frac{\gamma_p}{K_1}\frac{K_2}{\alpha_x}e^{\lambda\theta} \tag{4.38}$$

$$P_1^\star := \frac{\gamma_p}{K_1}\Big(\frac{X^\star + k}{X^\star}\Big)\Big) \tag{4.39}$$

$$(P_1^\star, P_2^\star, X_1^\star, X_2^\star) = \Big(\frac{\gamma_p}{K_1}\Big(\frac{X^\star + k}{X^\star}\Big), 0, 1 - \frac{\gamma_p}{K_1}\frac{K_2}{\alpha_x}e^{\lambda\theta}, 0\Big) \tag{4.40}$$

We wish to show that the fixed point $(P_1^\star, P_2^\star, X_1^\star, X_2^\star)$ is always unstable. The instability implies that the river ecosystem is prone to fluctuations or disturbances which poses challenges to aquatic organisms, affecting their population and the overall ecosystem dynamics due to low oxygen. This is contained in Proposition 4

Proposition 4.4.1. *The fixed point* $(P_1^\star, P_2^\star, X_1^\star, X_2^\star)$ *is unstable whenever it exists.*

Proof. The Jacobian matrix of the system (4.35) is;

$$J = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \alpha_2 \frac{X_1}{X_1+k} & \alpha_1 & \alpha_2 \frac{kP_1}{(X_1+k)^2} & 0 \\ 0 & 0 & 0 & 1 \\ \alpha_4 \frac{X_1}{X_1+k} & 0 & \alpha_4 \frac{kP_1}{(X_1+k)^2} + \rho & \alpha_3 \end{pmatrix} \tag{4.41}$$

Evaluating the Jacobian at $(P_1^\star, P_2^\star, X_1^\star, X_2^\star)$, yields;

$$J(P_1^\star, P_2^\star, X_1^\star, X_2^\star) := \begin{pmatrix} 0 & 1 & 0 & 0 \\ \alpha_2\sigma_1 & \alpha_1 & \alpha_2\sigma_2 & 0 \\ 0 & 0 & 0 & 1 \\ \alpha_4\sigma_2 & 0 & \alpha_4\sigma_2 + \rho & \alpha_3 \end{pmatrix}$$

$$ \tag{4.42} $$

where, $\sigma_1 = \left(\frac{\alpha_x K_1 - \gamma_p K_2 e^{\lambda\theta}}{\alpha_x K_1 - \gamma_p K_2 e^{\lambda\theta} + \alpha_x k K_1}\right)$, $\sigma_2 = \left(\frac{k {\alpha_x}^2 K_1 \gamma_p}{(\alpha_x K_1 - \gamma_p K_2 e^{\lambda\theta})(\alpha_x K_1 - \gamma_p K_2 e^{\lambda\theta} + \alpha_x k K_1)}\right)$

$$ J({P_1}^\star, {P_2}^\star, {X_1}^\star, {X_2}^\star) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ a & b & c & 0 \\ 0 & 0 & 0 & 1 \\ e & 0 & f & g \end{pmatrix} \tag{4.43} $$

where,$a = \alpha_2\sigma_1$, $b = \alpha_1$, $c = \alpha_2\sigma_2$, $e = \alpha_4\sigma_2$, $f = \alpha_4\sigma_2 + \rho$, $g = \alpha_3$

Thus, we have

$$ J(P_1^\star, P_2^\star, X_1^\star, X_2^\star) = \begin{vmatrix} -\mu & 1 & 0 & 0 \\ a & b-\mu & c & 0 \\ 0 & 0 & -\mu & 1 \\ e & 0 & f & g-\mu \end{vmatrix} = 0 \tag{4.44} $$

whose characteristic equation is

$$ \mu^4 + n_1\mu^3 + n_2\mu^2 + n_3\mu + n_4 = 0, \tag{4.45} $$

where $n_1 = -(\alpha_1 + \alpha_3)$, $n_2 = \alpha_3\alpha_1 - \alpha_4\sigma_2 - \rho - \alpha_2\sigma_1$, $n_3 = \alpha_1(\alpha_4\sigma_2 + \rho) + \alpha_2\sigma_1\alpha_3$, $n_4 = \alpha_2\sigma_1 - \alpha_2{\sigma_2}^2\alpha_4$.

By Routh-Hurwitz criteria, we shall have stability provided; $n_1 > 0, n_3 > 0, n_4 > 0$ and $(n_1n_2 - n_3)n_3 - {n_1}^2 n_4 > 0$. It is clear that $n_1 < 0$ since $\alpha_1 > 0$, $\alpha_3 > 0$ and $n_3 > 0$, if

$$ \alpha_1(\alpha_4\sigma_2 + \rho) + \alpha_2\sigma_1\alpha_3 > 0. \tag{4.46} $$

Equation (4.46) is satisfied when $\sigma_1, \sigma_2 > 0$ and is achieved when $\alpha_x > \frac{\gamma_p K_2}{K_1} e^{\lambda\theta}$.

Also $n_4 > 0$ if $\alpha_1\sigma(\alpha_4\sigma_2 + \rho) > \sigma_2{}^2\alpha_4$ and $\sigma_1, \sigma_2 > 0$. Since $n_1 < 0$, then the fixed point $(P_1^\star, P_2^\star, X_1^\star, X_2^\star)$ is unstable. $\square$

We wish to show that there exist a temperature, θ, where θ is the temperature of the water in a river, that is favorable for supporting aquatic life, that is there exist a non zero concentration of oxygen in the river. This occurs when $X^\star \geq 0$, where $X^\star$ is the positive deviation of concentration from the hypoxia levels as defined in (4.27). Without loss of generality, we take it to be 0. Thus, using Equation (4.38), we see that

$$X^\star := 1 - \frac{\gamma_p}{K_1}\frac{K_2}{\alpha_x}e^{\lambda\theta}. \tag{4.47}$$

Oxygen concentration approaches zero at a temperature θ_c, thus we have;

$$X^\star = 0 = 1 - \frac{K_2\gamma_p}{\alpha_x K_1}e^{\lambda\theta_c}, \tag{4.48}$$

$$\frac{\alpha_x K_1}{K_2\gamma_p} = e^{\lambda\theta_c}, \tag{4.49}$$

that upon simplification yields

$$\theta_c := \frac{1}{\lambda}\ln\Big(\frac{K_1\alpha_x}{\gamma_p K_2}\Big), \tag{4.50}$$

If $\theta < \frac{1}{\lambda}\ln\Big(\frac{K_1\alpha_x}{\gamma_p K_2}\Big)$ where, $\theta_c > 0$, $\Big(\frac{K_1\alpha_x}{\gamma_p K_2}\Big) > 1$, then the river environment remains conducive to supporting aquatic life and if $\theta \geq \theta_c$, then oxygen levels depletes making the river ecologically dead, rendering it incapable of supporting aquatic life.

CHAPTER 5

NUMERICAL SIMULATIONS

5.1 Introduction

In this chapter, we use Matlab software for numerical simulations to describe the theoretical results for Equation 3.21. We describe the variables and parameters values to enable us make numerical simulations.

Variables and Parameters	**values**	**Source**
K_1	8.27	(Pimpunchat et al., 2009)
γ_p	0.05-0.98	(Pimpunchat et al., 2009)
K_2	44.10	(Pimpunchat et al., 2009)
λ	0.2	Estimate
α_x	16.50	(Pimpunchat et al., 2009)
ϵ_x	0.000246	(Pimpunchat et al., 2009)
ϵ_p	0.000246	(Pimpunchat et al., 2009)
k	0.007	(Pimpunchat et al., 2009)
θ	$1^\circ - 45^\circ$	Estimate

For numerical simulation, we use the following initial conditions;

$$P_0 = 0.3,$$

$$X_0 = 4.$$

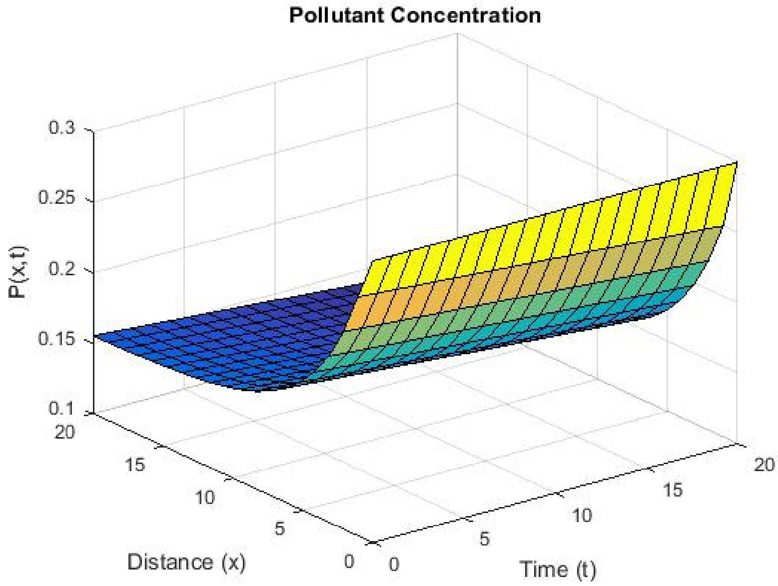

Figure 5.1: Pollutant concentration when $q = 0.05kgm^{-1}day^{-1}$

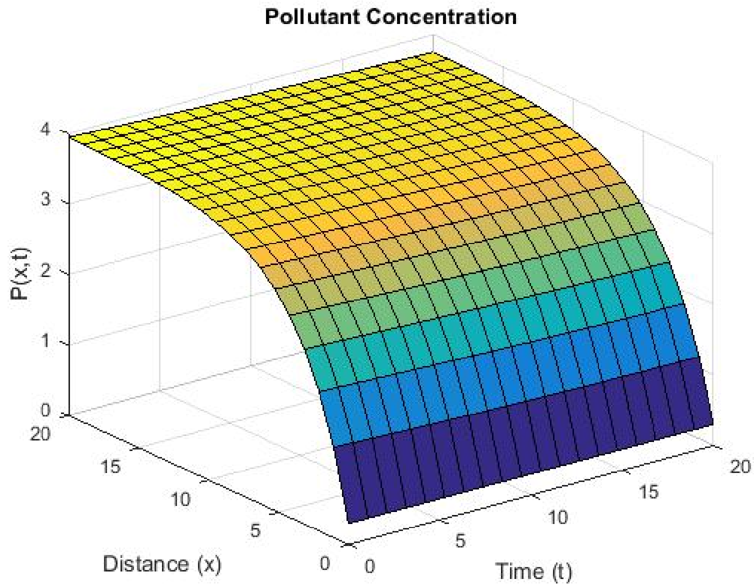

Figure 5.2: Pollutant Concentration when $q = 0.98kgm^{-1}day^{-1}$

Figure 5.1, show that when the rate of pollutant addition, q is small, the concentration of pollutant in the river is low and $P(x,t) \to 0.15$ as $x \to \infty$.

Figure 5.2 shows that when the rate of pollutant addition is high, the concentration of pollutant increases downstream as distance increases and $P(x,t) \to 4$ as $x \to \infty$.

Clearly, from Figures 5.1 and 5.2, we see that the pollutant concentration in a river depends on the rate of pollutant addition q.

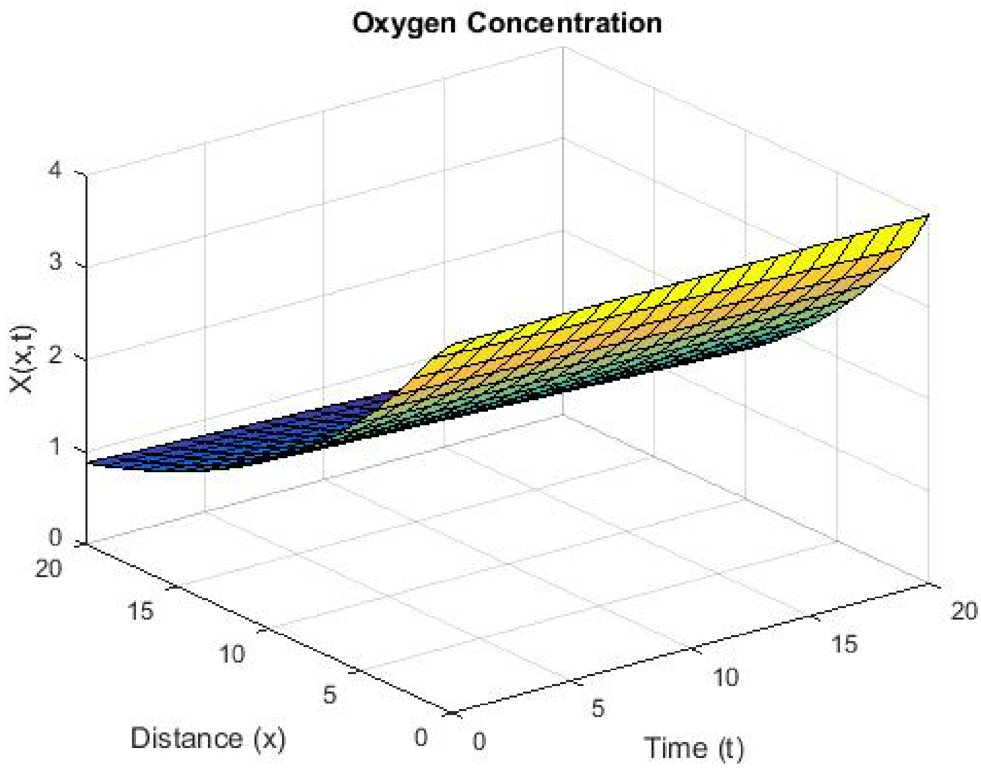

Figure 5.3: Oxygen Concentration when $\theta < \theta_c$

Figure 5.3 shows that when the distance x increases, the concentration of oxygen slightly decreases but remains high. In this case, we see that when the temperature of the water in a river is less than the critical temperature, that is, $\theta < \theta_c$, the concentration of oxygen is high and $X(x,t) \to 1$ as $x \to \infty$.

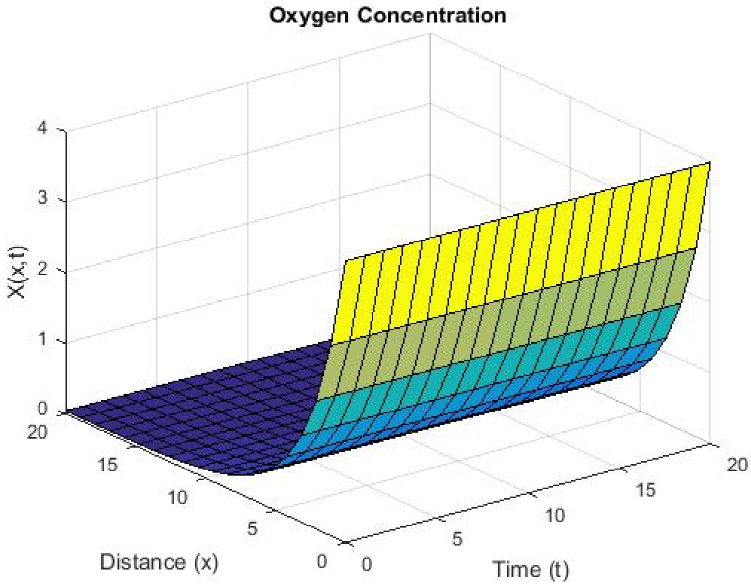

Figure 5.4: Oxygen concentration when $\theta_c = \theta$

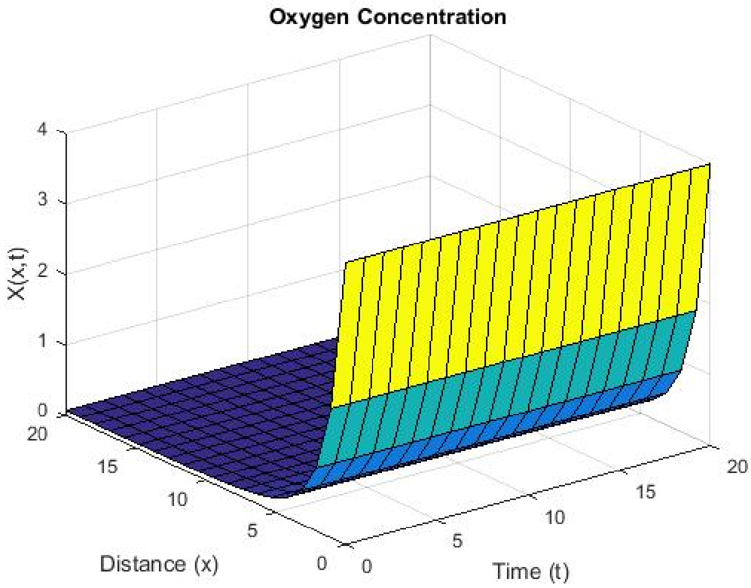

Figure 5.5: Oxygen concentration when $\theta > \theta_c$

Figures 5.4 and 5.5 show that when distance x increases, the concentration of oxygen approaches zero; that is, $X(x,t) \to 0$ as $x \to \infty$. In these two cases, oxygen concentration is not changing with distance as x increases as it goes to zero when $\theta \geq \theta_c$.

Thus, we can see from Figures 5.3, 5.4 and 5.5 that oxygen concentration in a river depends on temperature of the water. This results agrees with analytical results in the sense that, when $\theta \geq \theta_c$, $X \to 0$ as distance increases.

CHAPTER 6

CONCLUSION AND RECOMMENDATIONS

6.1 Introduction

In this chapter, we present a summary of what we have found in this research. Section 6.2 contains the conclusion while section 6.3 contains the recommendation.

6.2 Conclusion

We have formulated a model of temperature dependent dissolved oxygen and pollutant concentration in a river and found that the concentration of dissolved oxygen is dependent on rate of pollutant addition into the river and temperature of the water.

By using both the analytical and numerical results, we have shown that, there is a temperature, θ_c beyond which oxygen levels approach zero; that is, $X = 0$, as $x \to \infty$ and if $\theta \geq \theta_c$, then oxygen levels depletes making the river ecologically dead. We have also shown that if $\theta < \theta_c$, then the river remains conducive to supporting aquatic life.

Furthermore, from the stability analysis, we have shown that when the river is highly polluted, a slight change in temperature leads to catastrophe.

We have shown that when $\theta = 0$, there is certain amount of pollutant if added into the river leads to catastrophe; that is, if

$$\frac{\beta S K_1}{K_2} = q. \tag{6.1}$$

Therefore, it is important to monitor and manage the pollutant load, as well as temperature to ensure that oxygen concentration levels in the water remains above a critical threshold.

6.3 Recommendations

Water pollution remains a considerable problem in rivers for countries like Kenya for instance in Nairobi river. Though the establishment of a new strategies to curb pollution and enhance dissolved oxygen is still a problem, there is a need to strengthen control strategies at hand to decrease pollution.
We recommend adaptive strategies to address extreme temperature fluctuations and their effects and reduce river pollution.

We have considered a mathematical model, where we considered the effect of temperature on the rate of oxygen transfer from the air into the river, ignoring the effect of temperature on the rate of pollutants addition into the river under the assumption that pollutant addition into the river are influenced by other factors other than temperature. In future, temperature-dependent pollutant addition can be considered. In future also time lag for temperature variation to impact water-temperature can be considered, that is, consider the time it takes for temperature variation to impact water temperature.

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