MATHEMATICAL MODELLING IN RIVER POLLUTION CONTROL

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My utmost dedication to Mum and Dad. Thank you for always being there for me.

I love you.

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ABSTRACT

This study is conducted to determine the concentration of coliform bacteria along a river. Coliform bacteria are used as the indicator for the pollution level of a river because its concentration in wastewater discharges is much more compared to the concentration of other microorganisms. A mathematical model based on the convection reaction equation will be developed to determine the concentration of coliform bacteria along a river. Before studying the convection reaction equation, we will study the solutions of the simpler model based on the linear advection equation. The model based on the linear advection equation will be solved analytically using the method of characteristics. The model will also be solved numerically using the first order upwind scheme. The graphical outputs for the solution of the model will be presented using MATLAB. After analysing the linear advection equation, we will move on to the convection reaction equation. This equation will be solved analytically using the method of variable change and integrating factor. Once the equation is solved, the solution is plotted using Maple for an easier analysis of the result. The result suggests that the concentration of coliform bacteria is the highest at the source of wastewater discharges.

ABSTRAK

Kajian ini dilakukan untuk menentukan kepekatan bakteria koliform sepanjang sungai. Bakteria koliform digunakan sebagai penunjuk tahap pencemaran sungai kerana kepekatannya dalam pelepasan air sisa adalah lebih berbanding dengan kepekatan mikroorganisma lain. Satu model matematik berdasarkan persamaan tindak balas perolakan akan dibentuk untuk menentukan kepekatan bakteria koliform di sepanjang sungai. Sebelum mengkaji persamaan perolakan tindak balas, kita akan mengkaji penyelesaian model yang lebih mudah berdasarkan persamaan olahan linear. Model berdasarkan persamaan olahan linear akan diselesaikan secara analitik menggunakan kaedah ciri-ciri. Model tersebut juga akan diselesaikan secara berangka menggunakan skim "*First Order Upwind*". Output grafik untuk penyelesaian model akan dibentangkan menggunakan MATLAB. Selepas menganalisis persamaan olahan linear, kita akan menyelesaikan persamaan tindak balas perolakan. Persamaan ini akan diselesaikan secara analitik menggunakan kaedah pertukaran pembolehubah dan faktor integrasi. Setelah persamaan ini diselesaikan, penyelesaian untuk persamaan ini akan diplot menggunakan Maple untuk analisis keputusan yang lebih mudah. Hasilnya menunjukkan bahawa kepekatan bakteria koliform adalah tertinggi pada sumber pelepasan air sisa.

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LISTS OF SYMBOLS

A	-	Area of section occupied by water
e_j	-	Point where the *j*-th wastewater discharge is located
$\mathbf{f}$	-	Flux function
H	-	Height of the water
$H(x)$	-	Heaviside step function
I_0	-	Surface light energy
k	-	Loss rate for total coliform bacteria
k_1	-	Mortality rate
k_e	-	Extinction coefficient
k_i	-	Bacterial loss caused by the effect of light
k_s	-	Settling loss rate
$m_j(t)$	-	Mass coliform flow rate at the *j*-th wastewater discharge
P_s	-	Sea water's percentage
$u(x,t)$	-	Coliform concentration
v	-	Average velocity in the river
β	-	Proportionality constant close to unity
$\delta(x-b)$	-	Dirac measure at point *b*
$L_x(\Delta t)$	-	Differential marching operator
θ	-	Temperature
$\Im$	-	Symmetric positive definite matrix of diffusion coefficients

CHAPTER 1

INTRODUCTION

1.1 Background of the Study

Since the beginning of time, people have always used rivers as garbage disposal sites. Due to the rapid development of industries and populations, wastewater discharges in our rivers have increased at a rapid rate. As the problem of water pollution becomes more chronic, various developed countries have created stringent laws concerning wastewater disposal in rivers.

Wastewater in river can be classified into two types, which are domestic wastewater and industrial wastewater. Domestic wastewater refers to wastewater which comes from a purifying plant where water is collected from a sewer system. On the other hand, industrial wastewater refers to wastewater which comes from an industrial plant.

By choosing the proper indicators of pollution levels and designing a sampling technique which gives us the value of these indicators along the river, we are able to ensure that the river is absorbing the discharges. To control pollution caused by pathogenic microorganisms coming from domestic wastewater, one of the best indicators is the concentration (units m^{-3}) of the fecal coliform bacteria, due to the fact that its concentration in wastewater discharges is much more compared to the concentration of other microorganisms.

Fecal coliform bacteria are commonly found in faeces, or waste. They belong to a larger group of organisms known as coliform bacteria. In Standard Methods for the Examination of Water and Wastewater, 19^{th} Edition, coliform bacteria are classified as facultative anaerobes, which also mean that they can survive without oxygen and are rod-shaped bacteria that produce lactose, a type of sugar.

Figure 1.1: Fecal Coliform Bacteria

Fecal coliform bacteria can originate from various sources and it depends on the hydrologic conditions. The two main sources from which fecal coliform bacteria originate from are human sources and non-human sources.

Human sources can be divided into two categories, sewered watersheds and non-sewered watersheds. Sewered watersheds sources can be associated with combined sewer overflows, sanitary sewer overflows, illegal sanitary connections to storm drains, illegal disposal to storm drains and leaking sewer lines. Meanwhile, non-sewered watersheds can be related to failing septic systems, small, self-contained sewage-treatment systems and marinas and pumpout facilities.

On the other hand, non-human sources can also be split into two categories, which are domestic animals and urban wildlife, and livestock and rural wildlife. Dogs, cats, rats, pigeons and ducks are categorised in the domestic animals and urban wildlife section, whereas cattle, horse, poultry and deer are categorised in the livestock and rural wildlife section.

To control the concentration of coliform bacteria in rivers, we can divide the river into several sections with respect to the morphology of the river basin and the number, type and location of the discharges, and to obtain samples of water at each particular point of each section. The point at where the sampling station is located, also known as sampling point, is very important if we are looking for information about the pollution in the whole section of the river. (Alvarez-Vazquez L.J., Martinez A., Vazquez-Mendez M.E., Vilar M., 2006)

Thus, a further study on the mathematical model development for the transport of coliform bacteria along a river section is to be conducted. By using this model, we are able to determine the concentration of coliform bacteria along the river at any time.

Once we have obtained the knowledge on how the coliform bacteria are transported, we will be able to determine the point at which the concentration of coliform bacteria is highest. When the point has been determined, we are able to proceed with various ways to reduce the concentration, such as building wastewater treatment plant or sampling station at the particular point.

1.2 Statement of the Problem

To control pollution in a river, we must first determine the characteristics of the pollution in the river. This can be done by formulating a mathematical model to simulate the real life phenomenon. In this research, we will build a mathematical model to determine the concentration of coliform bacteria in a river. The model will then be solved via analytical and numerical methods. Once we have obtained the solution to the model, the solutions will be computed using MATLAB and Maple. Then, we will be able to identify the concentration level of coliform bacteria along a river at any time.

1.3 Objectives of the Study

The objectives of this study are:

a) To use mathematical modelling in determining the concentration of coliform bacteria in a river.

b) To solve the mathematical model based on the linear advection equation using analytical and numerical methods.

c) To study the effect of Dirac delta function in the mathematical model based on the convection reaction equation.

d) To present the results graphically using MATLAB and Maple.

1.4 Scope of the Study

This study emphasizes on the formulation of the mathematical model to determine the concentration of coliform bacteria based on the linear advection equation and convection reaction equation at a fixed initial condition.

We will also determine the best way to solve the complete mathematical model analytically and numerically. Once the mathematical model is solved, the result is presented in graphical outputs using MATLAB to observe the concentration of coliform bacteria at different points and also at different time.

We will also conduct a mathematical study on the mathematical model based on the convection reaction equation. The model will be solved analytically and the results will then be produced using the Maple software. Once the results have been obtained, we will interpret the results based on the graphical outputs.

1.5 Significance of the Study

The findings and discussions of this study are beneficial to several parties, including students taking Engineering Mathematics in Universiti Teknologi Malaysia (UTM) and also various water governing bodies.

1. **Engineering Mathematics Student**

   Students taking Engineering Mathematics from Universiti Teknologi Malaysia would benefit from this study as they will learn and explore deeper on the application of their theoretical knowledge into real world scenarios. In this research, the theoretical knowledge is applied into determining the concentration of coliform bacteria along a river.

2. **Water Governing Bodies**

   Through the study conducted, the water governing bodies around the world will be able to determine where to build the sampling stations or wastewater treatment plant and obtain information regarding the characteristics of the pollution in the whole section of a river. With this knowledge, water pollution in a river can be controlled with the data obtained from the water pollution monitoring stations.

1.6 Outline of the Study

This study focuses on using mathematical modelling to model the concentration of coliform bacteria along a river and, analytical and numerical methods to solve the mathematical model. The first chapter includes the background of study, the statement of problem, objectives of study and scope of study, which is explained in details.

Chapter 2 discusses about the literature review. We will discuss on the reviews on previous researches conducted relating to the modelling of pollutant transport. An introduction to the mathematics of pollutant transport will also be included in this chapter. We will also take a look at the various models of pollutant transport based on the elliptic, parabolic and hyperbolic transport equations.

Chapter 3 will discuss on the methodology of the study. We will focus on how to obtain the mathematical model for determining the concentration of coliform bacteria along a river. Once the model has been obtained, the analytical and numerical methods used to solve the model will be discussed in depth.

Chapter 4 will discuss on the expected outcome of this research. The solutions obtained in Chapter 3 will be programmed using MATLAB and Maple to obtain the graphical outputs for a clearer understanding of the solution. The graphical outputs will be presented in this chapter, where we are able to interpret the concentration of coliform bacteria along a river.

Chapter 5 meanwhile discusses on the conclusion of this study based on the results obtained from Chapter 4. Recommendations relating to this study will also be included in this chapter to improve any future researches related to this field.

REFERENCES

Alvarez-Vazquez L.J., Martinez A., Vazquez-Mendez M.E., Vilar M. (2006). Optimal location of sampling points for river pollution control.*Mathematics and Computers in Simulation*, 71, 149-160. Elsevier.

Benedini M. (1998). Water quality in river systems management: application of risk and reliability analysis in: Computer methods and water resources: Water Quality, Planning and Management (D. Ouazar, C.A. Brebbia and G.E. Stout, ed.). 237-250. Springer.

Benedini M. (2011). Water quality models for rivers and streams. State of the art and future perspectives. *European Water,* 34**,** 27-40.

Bercovier M., Pironneau O., V Sastri. (1983). Finite elements and characteristics for some parabolic-hyperbolic problems. *Appl. Math. Modelling,* 7, 89-96. Butterworth & Co. Ltd.

Canale R.P., Auer M.T., Owens E.M., Heidtke T.M., Effler S.W. (1991). Modeling Fecal Coliform Bacteria-II. Model Development and Application. *Wat. Res*., 27, 703-714. Pergamon Press Ltd.

Causon D.M., Mingham C.G. (2010). *Introductory Finite Difference Methods for PDEs*. Ventus Publishing.

Chapra, S.C. (1997). *Surface Water Quality Modelling*. New York: McGraw-Hill.

Dixon W., Smyth G.K., Chiswell B. (1999). Optimized selection of river sampling sites. *Water Res.*, 33, 971-978. Elsevier.

I-Liang Chern. (2009). *Finite Difference Methods for Solving Differential Equations.* National Taiwan University.

Kuzmin D. (2010). *A Guide to Numerical Methods for Transport Equations*. Friedrich-Alexander-Universitat Erlangen-Nurnberg.

Sterck H.D., Ullrich P. (2009). *Introduction to Computational PDEs.* University of Waterloo.

Thomann R.V., Mueller J.A. (1987). *Principles of Surface Water Quality Modelling and Control*. New York: Harper & Row.

Wilkinson J., Jenkins A., Wyer M., Kay D. (1995). *Modelling faecal coliform concentrations in streams.* Institute of Hydrology.