# SOLUTION OF BACTERIA- SURFACE DECONTAMINATION MODEL BY USING SEPARATION OF VARIABLES

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A dissertation submitted in partial fulfilment of the
requirements for the award of the degree of
Master of Science

Faculty of Science
Universiti Teknologi Malaysia

MARCH 2019

## DEDICATION

To my wife Zaleika and my children Mohammed, Tamim and Fatima

# ACKNOWLEDGEMENT

I would like to thank all who in one way or another contributed in the completion of this thesis. First, I give thanks to God for protection and ability to do work. I would like to my sincere appreciation to my supervisor, Prof. Dr. Ali Hassan Mohamed Murid for his guidance, advice, patience, encouragement and support to complete this work.

I would also like to thank my parents for their wise counsel and sympathetic ear. You are always there for me. Finally, there are my friends. We were not only able to support each other by deliberating over our problems and findings, but also happily by talking about things other than just our papers.

My sincere appreciation also to my fellow postgraduate student Abdullah Dahawi for his support and useful tips.

# ABSTRACT

The aim of this study is to investigate the application of the Fourier series method to solve a known mathematical model of surface disinfection and in order to determine its effectiveness. The mathematical model is based on the reaction-diffusion partial differential equation due to the diffusion of the bacteria into the disinfectant solution when the decontamination process begins and the reaction of the disinfectant killing effect on the bacteria. Analytical and approximate solution for the model is carried out using Fourier series. The infinite Fourier series is approximated twice by choosing finite terms of the series and by approximating some of the eigenvalues of the solution. Mathematica programming software is selected to execute the numerical computations. The obtained results are compared with the exact initial condition and a previous study. Simulation of the results demonstrate that the Fourier series method is able to approximate the solution of the surface disinfection model.

# ABSTRAK

Tujuan kajian ini adalah untuk mengkaji penggunaan kaedah siri Fourier untuk menyelesaikan model pembasmian kuman permukaan yang diketahui dan untuk menentukan keberkesanannya. Model matematik tersebut adalah berdasarkan persamaan pembezaan separa reaksi-difusi akibat penyebaran bakteria ke dalam larutan disinfektan apabila proses dekontaminasi bermula dan tindak balas kesan membunuh disinfektan pada bakteria. Penyelesaian analitik dan anggaran untuk model itu telah dijalankan menggunakan siri Fourier. Sisi Fourier tak terhingga telah dianggarkan dua kali dengan memilih terma siri terhingga dan dengan anggaran beberapa nilai eigen penyelesaiannya. Selain itu, perisian pengaturcaraan Mathematica dipilih untuk melaksanakan pengiraan berangka. Hasil yang diperoleh dibandingkan dengan syarat awal tepat dan kajian lepas. Hasil simulasi menunjukkan bahawa kaedah siri Fourier mampu menyelesaikan secara hampir model pembasmian kuman permukaan.

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# LIST OF ABBREVIATIONS

| | | |
|---|---|---|
| DOPRI | - | Dormand-Prince |
| E. *coli* | - | Escherichia coli |
| FDM | - | Finite Difference Method |
| FEM | | Finite Element Method |
| MOL | - | Method of Lines |
| ODE | - | Ordinary Differential Equation |
| PDE | - | Partial Differential Equation |
| RK4 | - | Fourth-Order Runge-Kutta Method |
| UTM | - | Universiti Teknologi Malaysia |
| UTM-CIAM | - | UTM Centre for Industrial and Applied Mathematics |

# LIST OF SYMBOLS

| | | |
|---|---|---|
| $\hat{x}$ | - | Region thickness |
| $\hat{t}$ | - | Time duration of the decontamination process |
| $\hat{b}(\hat{x},\hat{t})$ | - | Concentration of the microorganisms |
| $b_0$ | - | Initial concentration |
| $D$ | - | Microorganisms diffusion coefficient |
| $\hat{C}$ | - | Disinfectant concentration |
| $\hat{\theta}$ | - | Disinfectant killing effect |
| $\beta(\hat{t})$ | - | Surface concentration |
| $\hat{\gamma}$ | - | Microorganisms growth rate |
| $K$ | - | Partition coefficient |
| $\delta$ | - | Microorganisms' region thickness |
| $h$ | - | Total thickness |

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# CHAPTER 1

# INTRODUCTION

## 1.1 Introduction

Disinfection is a process of cleaning contaminated surface. It is indeed a less lethal process than sterilization. Most of the microorganisms on the surface can be eliminated like microbial forms such as bacterial spores by disinfection. It does not ensure an "overkill'' and therefore lacks the margin of safety achieved by sterilization procedures. Besides, there are some factors that can effect on the performance of the disinfection procedure and control it significantly (Favero and Arduino, 2006). Some of these factors are microorganisms' nature and number, the amount of organic matter present, the type and condition of instruments, devices, and materials to be disinfected and the temperature (Alhashmi, 2018).

An example of disinfectant is clay solution. Clay is a finely-grained natural rock or soil material that combines one or more minerals. It includes hydrated aluminium silicate, quartz and some natural fragments. Further, many researchers have found that it is very beneficial to use the natural products like clay in the disinfection process because it displays antibacterial properties. Williams *et al.* (2008) reported that the healing skin and gastrointestinal ailments can be treated by using absorptive properties of clay minerals.

Practically, the antibacterial activity of the disinfection is reaction-diffusion process because the bacteria diffuse into the disinfectant, interact with disinfectant and killed due to the killing effect of the disinfectant. This interaction process between disinfectant solution and contaminant can be modelled, mathematically, in terms of reaction- diffusion equation which is one of the well-known partial differential equations.

## 1.2 Background of Problem

A study on formulating and solving a mathematical model for the effectiveness of the disinfectant on harmful bacteria reduction on a surface has been presented by Ockendon *et al.* (2016). The governing equations have been formulated as a second order reaction-diffusion parabolic partial differential equation (PDE). They have used Laplace transform method (LTM) and finite difference method (FDM) to achieve an analytical and numerical solutions, respectively, for the problem over the infinite interval $0 < x < \infty$. Later on, a numerical approach has been performed by Chai (2017) to solve the model over the finite interval $0 \leq x \leq h$ based on FDM and method of lines (MOL) with fourth-order Runge-Kutta method (RK4). Recently, Alhashmi (2018) utilized the Laplace transform method to solve the same model for only $x = 0$ and finite element method (FEM) over $0 \leq x \leq h$. Therefore, the studies mentioned above did not give an analytical approach for the problem over $0 \leq x \leq h$. This study presents a general and approximate solutions on solving the model based on Fourier series method.

Figure 1.1 demonstrates the disinfectant solution and bacteria interaction on a hard-contaminated surface. The bacteria will be killed when it diffuse into the disinfectant solution region.

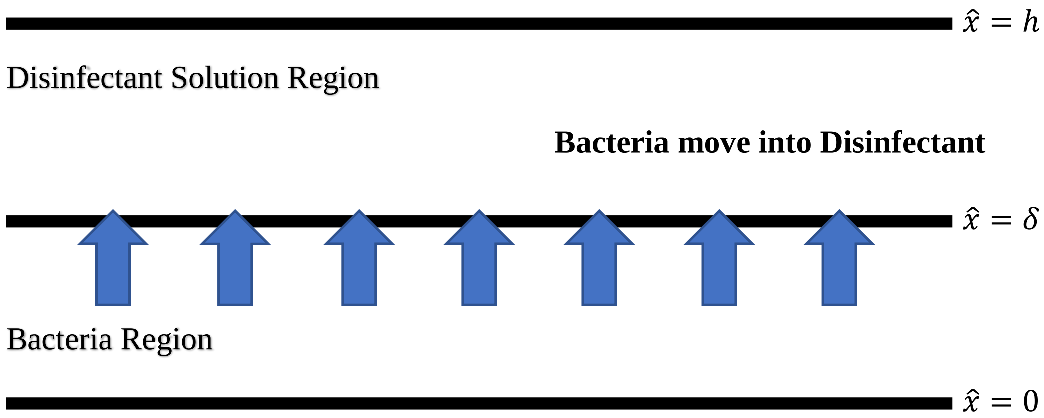


**Figure 1.1** The interaction between disinfectant solution and bacteria on the surface.

According to Ockendon *et al.* ( 2016), the mathematical model of the problem can be described as reaction-diffusion equation is

$$\frac{\partial \hat{b}}{\partial \hat{t}} = D\frac{\partial^2 \hat{b}}{\partial \hat{x}^2} - \hat{\theta}\hat{b} \quad ,0 < \hat{x} < h, \quad \hat{t} > 0 \tag{1.1}$$

where $\hat{b}$ is bacteria concentration, $\hat{t}$ is the time, $D$ is bacteria diffusion coefficient, $\hat{x}$ is region thickness, $\hat{\theta}$ disinfectant killing effect and $h$ is the total thickness of microorganisms and disinfectant solution regions.

with boundary conditions

$$\hat{x} = 0: \quad \frac{\partial \beta}{\partial \hat{t}} = D\frac{\partial \hat{b}}{\partial \hat{x}} + \hat{\gamma}\beta\left(\hat{t}\right), \qquad \hat{t} > 0 \tag{1.2}$$

$$\hat{x} = 0: \quad \beta\left(\hat{t}\right)\delta^{-1} = K\ \hat{b}\left(0,\hat{t}\right), \qquad \hat{t} > 0 \tag{1.3}$$

$$\hat{x} = h: \quad \hat{b}\left(h,\hat{t}\right) = 0 \ \text{ or } \ \frac{\partial \hat{b}}{\partial \hat{x}} = 0, \qquad \hat{t} > 0 \tag{1.4}$$

where $K$ is the partition coefficient, $\hat{\gamma}$ is bacteria growth rate, $\beta\left(\hat{t}\right)$ is the surface concentration of the bacteria per area and $\delta$ bacteria region thickness.

The initial condition for the problem is assumed to be equally distributed and taking the value $b_0$ over bacteria region $0 \le \hat{x} \le \delta$ and no bacteria over the disinfection region (Ockendon *et al*., 2016).

Hence, from Figure 1.1, we have

$$\hat{b}\left(\hat{x},0\right) = \begin{cases} b_0 & , \quad 0 \le \hat{x} \le \delta, \\ 0 & , \quad \delta < \hat{x} \le h. \end{cases} \tag{1.5}$$

The previous model (model A) was formulated and modified by Ockendon *et al.* (2016) leading to three modified models B, C and D. In Chapter 2, a discussion on formulating all these models' cases is presented.

Unlike the previous studies in solving the governing equation presented by Ockendon *et al.* (2016), Chai (2017) and Alhashmi ( 2018), this research has utilized separation of variables and Fourier series methods to give analytical and approximate solutions for the model. These techniques are mostly being used to solve different type of PDEs like parabolic, hyperbolic and elliptic equations.

## 1.3 Problem Statement

A surface decontamination model has been proposed by Ockendon *et al.* (2016) and solved over the infinite interval $0 < x < \infty$ by means of Laplace transform method. Chai (2017) has solved the model over the finite interval $0 \le x \le h$ using finite difference method (FDM) and method of lines (MOL). Alhashmi (2018) has applied the Laplace transform method to solve the model over finite interval. These studies have led to the following questions:

a) Can the surface decontamination model equations (1.1) to (1.4) over the finite interval $0 \le \hat{x} \le h$ be solved using separation of variables and Fourier series method?
b) How will the results compared with the exact initial condition and the previous studies?

## 1.4 Research Objectives

The objectives of this research are:

a) To study a reaction-diffusion equation model for disinfectant solution of surface decontamination.
b) To apply the method of separation of variables and Fourier series method to solve a surface decontamination model.
c) To analyze the numerical results for various cases of the model's parameters.

## 1.5 Significance of the Study

The significant of this research is the new general and approximate solution for the surface decontamination model in terms of Fourier series. Thus, this study contributed in both knowledge and method of solving a surface decontamination model. Besides, solving the surface decontamination model will help relevant industries in optimising their decontamination products as well as the customers to save cost and the effort for the cleansing process.

## 1.6 Scope of the Study

In this research, the one-dimensional linear time dependent reaction-diffusion equation which formulates the disinfectant solution process is considered. The Fourier series method to solve the mathematical model is considered to obtain the analytical and approximate solutions on the domain of interest. To execute the mathematical code of the disinfectant solution model, Mathematica software is utilized.

## 1.7 Organization of Dissertation

This dissertation consists of five chapters. Chapter 1 introduces the main concepts and objectives of the research. In Chapter 2, the related literatures are presented and evaluated. Chapter 3 discusses the research methodology and provides the analytical approximate solutions of disinfectant solution model using Fourier series method. The analysis of the results and comparisons using different values of the model parameters are analysed in Chapter 4. Finally, Chapter 5 gives a conclusion and some recommendations for the future studies.

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