NUMERICAL SOLUTION OF KELLER-SEGEL EQUATION USING FINITE DIFFERENCE METHOD AND METHOD OF LINES

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DEDICATION

This dissertation is dedicated to my beloved family especially to my parents, siblings, supervisor, lecturers and all my friends who always supported me.

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ABSTRACT

Keller-Segel equation is a nonlinear partial differential equation (PDE) that modelled the movement of cells and organisms in response to chemical attractants, which is known as chemotaxis process. In this study, Keller-Segel (KS) equation is solved numerically by explicit finite difference method (FDM) and method of lines (MOL). The finite difference method is performed forward in time and centered in space meanwhile in the method of lines the solution will incorporate with Euler's method. Results of numerical experiments are presented and the accuracy of the numerical scheme is investigated by comparing the results with the exact solutions. The computational experiment is conducted using MS Visual C++ and results are presented graphically by MATLAB software. The result from both numerical methods shows good agreement with the exact solutions. From the comparison, both methods are shown to be good numerical approximations as the results obtained show closeness to the exact solution.

ABSTRAK

Persamaan Keller-Segel adalah persamaan pembezaan separa bukan linear (PDE) yang menggambarkan pergerakan sel dan organisma sebagai tindak balas kepada penarik kimia, yang dikenali sebagai proses chemotaxis. Dalam kajian ini, persamaan Keller-Segel (KS) diselesaikan secara berangka dengan kaedah perbezaan terhingga (FDM) yang jelas dan kaedah garis penyelesaian (MOL). Kaedah perbezaan terhingga dilakukan secara ke hadapan dalam masa dan pusat bagi jarak sementara kaedah garis penyelesaian akan dimasukkan dengan kaedah Euler. Keputusan eksperimen berangka dibentangkan dan ketepatan skema berangka diselidiki dengan membandingkan keputusan dengan penyelesaian yang tepat. Eksperimen pengkomputeran dilakukan menggunakan MS Visual C ++ dan keputusannya dibentangkan secara grafik oleh perisian MATLAB. Keputusan dari kedua-dua kaedah berangka menunjukkan persetujuan yang baik dengan penyelesaian yang tepat. Daripada perbandingan, kedua-dua kaedah ditunjukkan sebagai penghampiran berangka yang baik kerana hasilnya diperolehi hampir dengan penyelesaian yang tepat.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

PDE	-	Partial Differential Equations
FDM	-	Finite Difference Method
MOL	-	Method of Lines
FVM	-	Finite Volume Method
FEM	-	Finite Element Method
ODE	-	Ordinary Differential Equation
K-S	-	Keller-Segel
LHS	-	Left Hand Side
RHS	-	Right Hand Side
FTCS	-	Forward Time-Central Space
FD	-	Finite Difference

LIST OF SYMBOLS

k	-	Rate constant
D	-	Diffusivity
u	-	Microorganism Concentration
v	-	Attractant Concentration
x	-	Space
t	-	Time
c	-	Velocity

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Problem Background

In recent years, the number of mathematicians studying biological and medical phenomena’s are expanding. Hence the mathematical analysis of biological phenomena has turned out to be increasingly important in understanding these complex processes. Investigating the bacteria movement has been perceived as one of the biological experiments that have been led by various scientists.

Bacteria movement also known as chemotaxis is defined as any process that causes the oriented movement of a cell or an organism relative to chemical stimulus (Hulzebos, 2017). Expressed in (Hillen and Painter, 2009), chemotaxis is just a unique type of movement. For example, the organism can sense a chemical field leading to food sources and move according to it (Ciegis, R., & Bugajev, 2012).

The chemical stimuli for bacteria are diverse. The stimuli can be divided into (as shown in Figure 1.1);

(a) Positive chemotaxis: the movement is toward a higher concentration of the chemical (move to attractants; nutrient).

(b) Negative chemotaxis: the movement is in the inverse direction (move away from repellent).

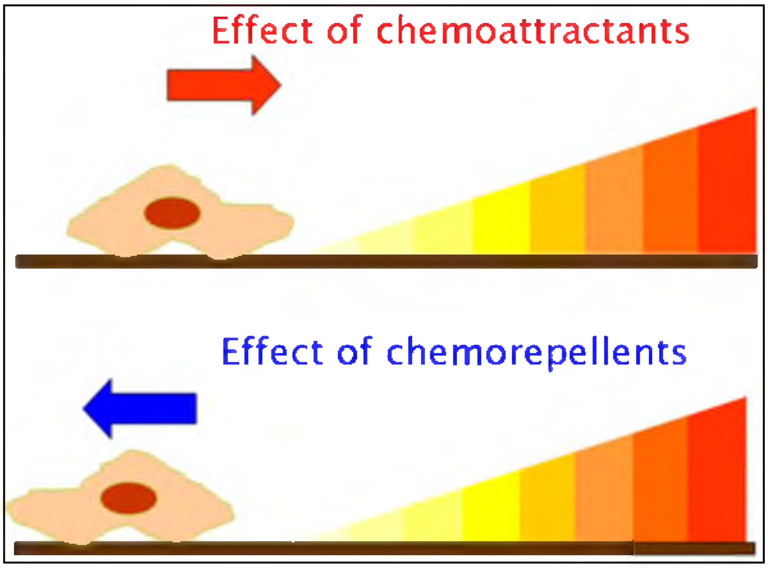

Figure 1.1 Positive and negative chemotaxis by Kohidal L. 2008.

Keller and Segel (Murray, 2013) created the first model to represent the biological phenomena of the bacteria observed in the experiments. The primary basis of the Keller-Segel model is that organisms or rather cells are moving in response to an external chemical concentration fields. Their model could replicate the traveling pulse of bacteria that was observed in the one dimensional experiment. The simple model is composed of two equations.

Keller–Segel equations have turned out to be generally used in models for chemotaxis, since of their capacity to seize key phenomena, instinctive nature and relative tractability (diagnostically and numerically) when contrasted with discrete or individual based methodologies (Roberts and Chung, 2012).

The Keller-Segel model is typically depicted by highly nonlinear time dependent systems in mathematical models for chemotaxis of partial differential equations (PDEs). Demonstrates in (Shubina, 2016) that this chemotaxis driven instability defined by the backward in time diffusion process with using method of lines to construct effective numerical approximations can be associated with the ill-posed problem.

Often, modelling of real biomedical issues needs to manage the complicated structure of the computational domains. Hence, there is a requirement for precise, quick, and computationally efficient numerical techniques for various chemotaxis models that can deal with arbitrary geometries (Murray, 2013).

In this study, the construction of numerical techniques are considered to solve Keller-Segel equations. The numerical results will be analysed, and will be able to describe the chemotaxis phenomenon. To achieve this goal, a finite difference method (FDM) and method of lines (MOL) are utilized. There are mathematical programming that can be utilized such as Visual Basic C++.

1.2 Problem Statement

The biological process, chemotaxis, can be described by the nonlinear DE, known as Keller–Segel equation, given by;

$$\frac{\partial u}{\partial t} = D\frac{\partial u}{\partial x}\left[\frac{\partial u}{\partial x} - 2\frac{u}{v}\frac{\partial v}{\partial x}\right]$$

$$\frac{\partial v}{\partial t} = -ku$$

where x and t stand for space and time, $u(x,\ t)$ is the microorganism concentration (cell density), $v(x,\ t)$ is the chemoattractant concentration, D and k are constants.

The aim for this study is to construct efficient numerical approximations to the above problem. The targeted numerical schemes are finite difference method and method of lines. In overall, the study will explore the following questions:

1. What is the suitable and efficient method to obtain good numerical approximation of Keller-Segel equation?
2. How to conduct the transformation of the nonlinear PDE into finite difference form?

3. How to calculate and analyze the error of the numerical approximation when compared with exact solutions?

1.3 Objectives of Study

The following objectives will be achieved from this project.

(a) To solve Keller-Segel equation using finite difference method.

(b) To solve Keller-Segel equation using method of lines.

(c) To explain the relationship between microorganism concentration and attractant concentration based on the numerical solutions.

(d) To analyze the performance of the numerical solutions by comparing with the exact solutions.

1.4 Scope of the Study

This study is focused on the one-dimensional Keller-Segel equation. The main numerical technique that is used are finite difference method and method of lines. The discretization is performed forward in time and centered in space, because it is easy to handle nonlinear PDE. Computer codes will be constructed using Visual Basic C++.

1.5 Significant of the Study

In recent years, the research of Keller-Segel equation had contributes various achievement especially in chemotaxis, biological field. Thus, the significant of this research are:

1. This research determined the accuracy of result obtained using numerical approach in Keller-Segel equation.
2. This research also provides information on the comparison between finite difference method and method of lines in Keller-Segel equation.
3. This research provides other alternative to solve Keller-Segel equation.by using two different approach of numerical methods, the PDE and the ODE solver.

1.6 Organization of the Research

The remaining parts are summarized as follows: Chapter 2 discussed briefly about Keller-Segel equation previous work and the minimum model used; Chapter 3 present the solution of the Keller-Segel equation using finite difference method and method of lines; Chapter 4 discussed the results and performance evaluation; and lastly Chapter 5 summarized and conclude the study.

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