HYBRID LAPLACE TRANSFORM SOLUTION FOR COUPLED PARTIAL DIFFERENTIAL EQUATION OF FUMIGANT TRANSPORT IN STORED GRAIN

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DEDICATION

My humble effort dedicates to my beloved

FATHER: Late Alhaji.Muhammad Lukunti Koko

MOTHER: Late Hajiya.Aisha Muhammad

Siblings and friends.

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ABSTRACT

The research presented in this dissertation is a mathematical solution of hybrid analytical and numerical simulation approach to the model of coupled partial linear differential equations of grain stored fumigation. The model is partly adopted based on phenomena of advection-diffusion transport process of solute mass for the fumigation distribution of phosphine gas concentration in a cylindrical silo containing grain. One dimensional advection diffusion coupled of partial linear differential equation is solved using Laplace transform by applied numerical simulation of Week's method of Laplace inverse (WLI) and finite difference method (FDM) while Octave software is used in the simulation. The developed WLI algorithm results verified using Cauchy test for convergence on FDM error results. However, the FDM error shows that to have better results of FDM, need a smaller step size increment Δx. The error results also showed that the higher fumigant concentration (C_s=10 mg/L) injected to the silo, the higher relative error in the solution of concentration of phosphine gas and concentration in the grain obtained, when compared with C_s=5 mg/L. Furthermore, the investigation on efficiency of phosphine gas concentration during fumigation based on graph of the results showed that, the length of the time phosphine gas concentration could be taken for covering the silo is independent of the amount of boundary fumigant concentration (BFC) injected to the silo. While for concentration in the grain inside the silo, the time is depending on the BFC, where the higher fumigant concentration in the silo, the higher concentration received by the grain. Besides that, when the velocity of the model increase, the time taking for phosphine gas concentration during fumigation is reduced. In addition, the higher the velocity of the model and less amount of BFC, then the least amount of concentration the grain absorbs during the fumigation processes.

ABSTRAK

Penyelidikan yang disampaikan dalam disertasi ini adalah penyelesaian matematik menggunakan analisis hibrid analitik dan simulasi berangka kepada model persamaan terbitan separa linear bagi pengasapan penyimpanan bijirin. Model ini diadaptasi berdasarkan fenomena proses pengangkutan-penyebaran jisim larut untuk pengedaran pengasapan kepekatan gas phospine dalam silo berbentuk silinder yang mengandungi bijirin. Pengangkutan- penyebaran satu dimensi persamaan terbitan separa linear diselesaikan menggunakan transformasi Laplace dan menggunakan kaedah simulasi berangka iaitu laplace songsang Week (WLI) dan kaedah pembezaan terhingga (FDM) manakala perisian Octave digunakan untuk simulasi. Keputusan yang diperoleh menunjukkan algoritma WLI adalah menumpu di mana hasilnya telah disahkan dengan FDM melalui ujian ralat penumpuan pada FDM, dan ia menunjukkan bahawa ralat dikurangkan jika Δx adalah lebih kecil. Keputusan ralat juga menunjukkan bahawa kepekatan fumigant yang lebih tinggi (C_s=10 mg/L) disuntik ke silo, ralat relatif juga lebih tinggi dalam penyelesaian kepekatan gas phosphine dan kepekatan dalam bijirin yang diperoleh, jika dibandingkan dengan C_s=5 mg/L. Selain itu, penyiasatan terhadap tingkah laku kepekatan gas fosfin semasa pengasapan berdasarkan graf keputusan menunjukkan bahawa tempoh masa yang diambil oleh gas phosphine untuk memenuhi semua ruang adalah tidak bergantung kepada kepekatan fumigant yang disuntik ke silo manakala untuk kepekatan dalam bijirin di dalam silo, masa bergantung kepada kepekatan fumigant di dalam silo, dimana jika kepekatan yang lebih tinggi, kepekatan yang diterima oleh bijirin akan lebih meningkat. Selain itu, apabila halaju meningkat, pengambilan masa bagi kepekatan gas fosfin semasa pengasapan dikurangkan. Di samping itu, semakin tinggi halaju, jumlah kepekatan fumigant lebih rendah, maka jumlah kepekatan juga rendah yang akan diserap oleh bijirin semasa proses pengasapan.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

BFC	-	Boundary fumigant concentration
CFD	-	Computational fluid dynamics
DE	-	Differential equation
FDS	-	Finite difference schemes
FDM	-	Finite difference method
ODE	-	Ordinary differential equation
PDE	-	Partial differential equation
WLI	-	Week’s method of Laplace inverse

LIST OF SYMBOLS

C_s - Boundary fumigant concentration
C_p - Concentration of phosphine gas in air
C_g - Concentration in grain
$J(x,t)$ - mass flux of the solute
$\mathcal{L}$ - Laplace transform
$\mathcal{L}^{-1}$ - Inverse Laplace transform
v - Velocity
t - Time
B_1,B_2,B_3,B_4 - Parameters
ε - Bulk porosity of the grain
$R_{filling}$ - Filling ratio
k_{fG} - Linear mass transfer coefficient of adsorbed liquid fumigant
k_{fA} - Linear mass transfer coefficient of gaseous fumigant
ρ_g - Density of the grain
F - Partition factor
S_{sorp} - Specific surface area for sorption
r_{fA} - First order reaction coefficient of gaseous fumigant in air
r_{fG} - First order reaction coefficient of adsorbed liquid fumigant
σ - Exponential factor
b - Time scale factor
E - Error
∞ - Infinity
h_1 - Increment in step size for time t
h_2 - Increment in step size for space x
Lt - Length of the time t
Lx - Length of the space x
Nt - Number of nodes for t
Nx - Number of nodes for x

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Introduction

The research work in this dissertation is to work out the solution to the model of coupled linear partial differential equation related to fumigation transport in stored grain. This chapter discusses the subject of the study begins with background of the research on general applications of transport phenomena and modelling, specifically on advection and diffusion, furthermore reduced to focus on the area of fumigation. The statement of the problem to conduct this research work is also presented in this introductory chapter, followed by the objectives, scope and the limitations of the study. Lastly the significant of the study and chapter by chapter dissertation structure are also presented in this chapter.

1.2 Research Background

Transport phenomena is the subject that deal with movement of different various entities such as mass, momentum and energy. Example of physical phenomenon, when a tea bag is place into cup of water, courses the chemicals that make a tea bag to diffuse into the water as showed in Figure 1.1. The tea bag content diffuses from it higher concentration to lower concentration. Another example is in phenomena of breathing; the diffusion in water surrounding a zebra fish embryo, the diffusion and reaction of oxygen in the fish embryo’s body is an example of transport phenomena and in this process the higher concentration of oxygen in the yolk, where there is hardly metabolism taking place, only energy storage. In the daily life of human body according to Enderle, John D. and Bronzino (2012), the gas exchange in the lungs, transport across capillaries and alveoli, transport across the kidneys, and transport across cell membranes. These mass transfer processes affect how oxygen and carbon dioxide are exchanged in your bloodstream, how metabolic waste products are removed from your blood, how nutrients are transported to tissues, and how all cells function throughout the body.

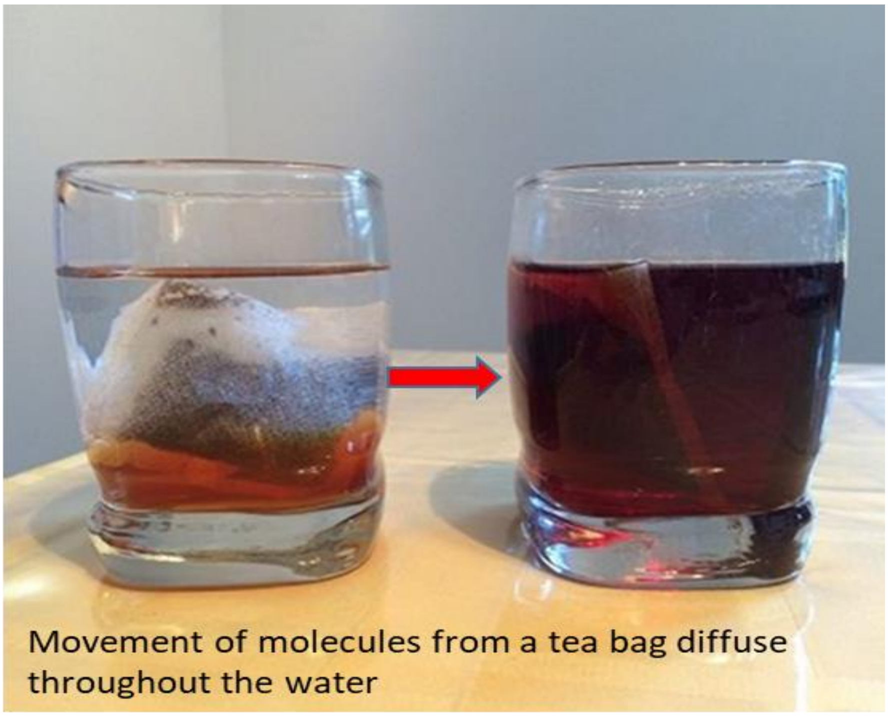

Figure 1.1: Example for transport phenomena involving diffusion process.

Evidently, there are many similarities in the mathematical descriptions of such transport phenomena which are essential for many processes in engineering, analytical chemistry, biology, agriculture, material science, metrology, pharmacy, physiology and other areas. According to Zoppou and Knight (1997) , the transport of pollutant occurs in a large variety of environmental and industrial processes can be adequately described by the advection and diffusion equation and such pollutant is vital to the effective management of these processes. By Athayde et al (2018), burning of fossil fuels, deforestation, manufacturing and use of vehicles pollute and influences in the quality of air especially in large urban centres which due to the influence of the industrial revolution, technological advances and population growth has degraded nature over the time. However today, technology is used to study the effects of pollution and to develop appropriate physical-mathematical models of advection-diffusion equation to predict damages to the environment. Similarly, there are many challenges in the environment of the presents insects in grain stored. With minimal changes occurring at the centre of large bulks for diurnal and seasonal, the store provides protection from the extremes of outside temperature and relative humidity fluctuations. However, in the grain bulk the presence of damaged grains, moisture and temperature gradients may act as rival attractants (Cox, P.D. and Collins 2002).

According to Darby (2008), the processes of exposure of the grain to use the gaseous chemical in order to kill all insects present is called grain fumigation and this processes refers to transport phenomena. Without harming the grain, such chemicals are usually applied as a dilute component in air that causes lethal responses in the insects. By the authors, Rajendran, S. and Sriranjini (2008) & Decker et al., (2010), fumigation plays a major role in insect pest elimination in stored products and phosphine gas is most widely used in grain fumigation, the ozone gas as fumigant used in controlling grain stored insects pests. However, modelling the behaviour of gas fumigants related to air volume of the stored grain mass is helpful in the finding out what factors may course fumigation failures and how this factors can be effected by environmental conditions due to limited information on fumigant activity within the commodity during the fumigation (Plumier, Schramm, and Maier 2018).

Today, for these multiple applications into various areas, researches conducted by many researchers experimentally to bring good management and better life to the society in general. Moreover, study grain fumigation is important roles in food commodities which is helpful to the environments. In this research work, advection and diffusion transport process is applied to the approach of mathematical modelling of grain fumigation in finding alternative techniques for the solution.

1.3 Problem Statement

The applications of transport phenomena play an important role to various disciplines including engineering, pharmacy, biology, agriculture, biomedical and others. Transport phenomena describes the relations and similarities among different types of transport that may occur in any system which comprising of momentum, energy and mass transports. There are uncertainties flow and transport properties on that phenomena which could be investigate through the field of experiments. The best application methods of fumigation phosphine gas distribution in grain silos are needed for fumigation to works properly so that the adequate concentration can be maintained for an adequate exposure period. However, solving such problem through the field of experiments will involve a very high cost. Hence mathematical modelling and computer simulation are alternative to that experimentation method with wide range research areas.

Advection-diffusion transport process of solute mass distribution can be studied by mathematical modelling to work out the solution by analytical or numerical approach. The couple advection-diffusion linear partial differential equations (PDEs) of solute mass transport is considered to be solved in this research work. The basic idea relies on the coupled advection-diffusion equation and linear partial differential equations (PDEs) for storage grain fumigation.

Besides that, this study will begin with a problem involving a coupled partial differential equation (PDE). This coupled equation is expected to be solved by hybrid numerical analytic and also numerically. Furthermore, this study will provide information on behaviour of gas based on available mathematical modelling, and hence the lack of understanding regarding fumigation will reduce.

1.4 Research Objectives

The objectives of this research work are as follows:

a) To get a hybrid numerical analytic solution of couple advection-diffusion of partial differential equation (PDE) related to grain fumigation problem using Laplace transform with numerical Week’s method of Laplace inverse (WLI).

b) To find the numerical solution of couple advection-diffusion partial differential equation (PDE) related to grain fumigation using finite difference method (FDM).

c) To verify the current numerical Week’s method of Laplace inverse (WLI) algorithm.

d) To study the efficiency of phosphine gas concentration related to grain fumigation process.

1.5 Scope and Limitation of the study

Transport phenomena is useful in the wide range of related application. In transport process that are consists of advection and diffusion equation, many mathematical models of differential equations (ODEs and PDEs) developed as well as grain fumigation from various researchers. The transport model partly adapted from grain fumigation in stored grain is an advection-diffusion equation which is a coupled of linear PDE were considered in this research work. However, various mathematical methods of the solution analytically or numerically applied to the problem in order to work out the solution to the models. This research work is limited to hybrid numerical analytic solution using Laplace transform with numerical Week’s method of Laplace inverse (WLI) and numerical finite difference method (FDM).

1.6 Research Significance

The advection and diffusion processes occur in surrounding of human life. fumigation application in a silo is among the significant transport phenomena in which there are many uncertainties about how the fumigant gas is distributed in air within the flow domain of silo. The study will show whether the gas concentration is sometimes lost due to the surrounding chemical reaction or absorb into something during the transport process and developed an understanding the behaviour of phosphine gas distribution throughout the silo. Significantly, the results obtained from this study will gives insight and enhance knowledge of the of advection-diffusion equation behaviour, particularly advection-diffusion of one-dimensional linear PDE. In addition, this study will contribute to a new theoretical knowledge in fumigation processes.

1.7 Outline Report

This dissertation consists of five chapters. Firstly, chapter 1 which deal with an introduction to the whole work. This chapter contains subsections and includes all the important points such as research background, research objectives, problem statement, scope and limitation and the significance of the study. Secondly, Chapter 2 presents the literature review of this work. By different researchers, various works regarding transport phenomena, diffusion equation, advection diffusion equation, mathematical modelling of grain fumigation are discussed in details. In addition, the theory on Laplace transform as well as numerical Laplace inversion and numerical solution using FDM as it is the methodology were also presented in this dissertation.

The formulation of mathematical model as well as parameters values of the problem for this research work presented in Chapter 3. The algorithm solution to the model using Laplace transform with numerical Week’s method of Laplace inverse (WLI) and numerical technique of FDM are all discussed in chapter 4. Then followed by the results in chapter 5, based on the results of FDM, verification of the numerical Week’s method of Laplace inverse (WLI) algorithm and how the behaviour of a gas concentration related to grain fumigation process also briefly discusses. Lastly, the

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