ANALYTICAL SOLUTION AND NUMERICAL SIMULATION OF ADVECTION-DIFFUSION EQUATION RELATED TO FUMIGATION PROBLEM

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To my beloved Ma and Abah, for your love and care,

to my siblings, Gee, Wani, Kak Elly and Abang Li for your support and concern,

and,

to my very best friend, Bella for your motivation, intelligence and guidance in life.

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ABSTRACT

The dissertation reports the analytical approach and numerical simulation of a transport phenomenon which is governed by the advection-diffusion equation. The main objective is to solve this governing equation by both analytical and numerical methods. One-dimensional advection-diffusion equation is solved by using Laplace Transformation method. Then, the solution is interpreted in two-dimensional graph of solute mass concentration over the distance. The graph is plotted using a mathematical tool i.e. MATLAB software. On the other hand, the numerical simulation is performed by using Computational Fluid Dynamics (CFD) software, ANSYS Fluent. In ANSYS Fluent, the solver discretizes the transport equation using Finite Volume Method where the computational flow domain is divided into control volumes. The transport model is partly adapted based on a phenomenon of solute mass concentration distribution in mixture with air in the flow domain of the cylindrical silo during fumigation. Based on this applications, the initial and boundary conditions are defined similar to the ones in analytical approach. From this simulation, data is obtained in form of graphical distribution profile of solute mass which can be compared against the works from analytical approach, hence, the verification is achieved. The verification demonstrates the accuracy of numerical solution on this transport phenomena, thus, it can be used for various experimental applications.

ABSTRAK

Disertasi ini melaporkan pendekatan analitik dan simulasi berangka terhadap fenomena angkutan yang diwakili oleh persamaan aliran-resapan. Objektif utama adalah untuk menyelesaikan persamaan ini dengan kedua-dua kaedah analitik dan berangka. Persamaan aliran-resapan berdimensi satu diselesaikan dengan menggunakan kaedah Transformasi Laplace. Kemudian, penyelesaian ditafsirkan dalam bentuk graf dua dimensi di mana kepekatan jisim bahan terlarut dicatat mengikut jarak. Graf diplot dengan menggunakan perisian MATLAB. Sebaliknya, simulasi berangka dilakukan dengan menggunakan perisian Pengiraan Dinamik Bendalir (CFD), iaitu ANSYS Fluent. Dalam ANSYS Fluent, teknik pendiskretan pada persamaan angkutan adalah menggunakan Kaedah Isipadu Terhingga di mana domain aliran pengiraan dibahagikan kepada isipadu terkawal. Model angkutan direka berdasarkan fenomena taburan kepekatan jisim bahan terlarut dalam campuran dengan udara di dalam domain aliran silo silinder semasa pengasapan. Berdasarkan aplikasi ini, syarat awal dan sempadan ditakrifkan sama seperti yang ditakrifkan di dalam pendekatan analitik. Dari simulasi ini, data diperolehi dalam bentuk grafik profil taburan jisim bahan terlarut di mana ianya boleh dibandingkan dengan kerja-kerja dari pendekatan analitik, dengan itu, pengesahan dicapai. Pengesahan menunjukkan ketepatan penyelesaian berangka pada fenomena angkutan, dengan itu, ia boleh digunakan untuk pelbagai aplikasi eksperimen.

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LIST OF SYMBOLS / ABBREVIATIONS

ρ	Density
c	Solute mass concentration
t	Time
δt	Time interval
x, y, z	Cartesian coordinates
$\delta x, \delta y, \delta z$	Space volume
q_x	Diffusive mass flux in x-direction
J_x	Total mass flux in x-direction
$\frac{\partial m_{CV}}{\partial t}$	Net change of mass within the Control Volume (CV) during time interval
$\sum \dot{m}_{in}$	Total mass entering the CV during time interval
$\sum \dot{m}_{out}$	Total mass leaving the CV during time interval
D	Solute dispersion coefficient
$\boldsymbol{u} = (u, v, w)$	Velocity components
$\dot{m}$	Mass flow rate
∇	Del operator
A	Input concentration
∞	Infinity

K	Diffusion dependent variable
$\mathcal{L}$	Laplace Transformation
$\mathcal{L}^{-1}$	Inverse Laplace Transformation
$\widehat{K}$	Laplace transformed diffusion dependent variable
s	Laplace transformed time
m_1, m_2	Roots of the characteristic equation
c_1, c_2	Arbitrary constants
exp	Exponential
erfc	Error function
CFD	Computational Fluid Dynamics
FDM	Finite Difference Method
FEM	Finite Element Method
FVM	Finite Volume Method

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CHAPTER 1

INTRODUCTION

1.1 Background of the Study

In our daily life, there are so many phenomena occurring in and within the surrounding environment. These phenomena are taking place right in front of our eyes and in fact, within human body. From movement of surrounding fluids to blood flow inside the blood veins, these are among many examples of transport phenomena.

Through phenomena of breathing for example, air is inhaled into the lung. Within air, there is oxygen gas as one of the components. The molecules of oxygen are carried by air and moves around throughout the respiratory system until they reach the lung. Then, the oxygen molecules are carried by blood and moves around within the blood vessel system all the way through human body. This is happening right within human body in daily life, and indeed, every second of human life. This transport phenomena is known as advection and diffusion transport process (Quarteroni *et al.*, 2001). Advection denotes the oxygen gas is carried by air which is caused by pressure gradient when breathing (Beard and Bassingthwaighte, 2001). On the other hand, the natural tendency of oxygen molecules move around within air in human body system can be described by diffusion process (Beard and Bassingthwaighte, 2001).

Another example of transport phenomena also can be found in fabric manufacturing industry. In order to get the desired colour to dye the fabric, the concentrated colour dye is poured into a solvent. The mixing reaction between the liquid dye and the solvent involves diffusion process. At some point, the dye will stop spreading when its concentration is the same within the solvent or in other words, there is no more concentration gradient. These processes are illustrated in Figure 1.1.

Figure 1.1 Example of transport phenomena involving diffusion process.

There are many other example of real applications involving the advection and diffusion transport process. The ability to understand, predict and control such phenomena is essential. This ability offers substantial economic benefits and contributes for a better life to human being. Thus, through this work, an alternative approach of mathematical modelling is applied to study this advection and diffusion transport process.

1.2 Statement of the Problem

In the subject of transport phenomena, the transport process is full of uncertainty when it comes to real life examples in many industrial applications such as reactor design, multiphase flows in furnaces and heat exchangers, design of better inkjet printers, and grain fumigation in the silo. However, the conventional engineering methods through field experiments to investigate these uncertainties involve a very high cost. Thus, an alternative way is being considered in wide range of research area. Mathematical modelling is one of such alternative to experimental method.

Among many applications, the transport phenomena of solute mass distribution is an example of advection-diffusion transport process which can be studied by mathematical modelling, either by analytical or numerical approach. Hence, this work of solute mass transport process analysis is initiated to contribute to the subject of the transport phenomena. The one-dimensional advection-diffusion equation of solute mass transport is considered to be solved by both analytical approach and numerical simulation.

1.3 Objectives of the Study

The following are list of objectives defined for this study:

i. To solve the one-dimensional advection-diffusion equation by analytical approach.

ii. To perform numerical simulation for the one-dimensional advection-diffusion equation by using ANSYS Fluent software.

iii. To verify results of the numerical simulation against the analytical solution for one-dimensional problem of the advection-diffusion equation.

1.4 Scopes of the Study

The transport phenomena of phosphine gas particularly in grain fumigation application is considered to be studied. This transport process consists of both advection and diffusion reactions. Only movement of phosphine gas or its concentration (in terms of mass fraction) distribution in one-dimensional problem is considered. The transport model is partly adapted from grain fumigation application in the silo which it is assumed free from the grain and fully filled with air. This model is solved by both analytical and numerical works. The computational programming tool in MATLAB software is used to demonstrate the result of analytical work. On the other hand, ANSYS Fluent software is used to perform the numerical simulation. Then, the results from both works are compared for verification.

1.5 Significance of the Study

Advection and diffusion processes are indeed among interesting transport phenomena which occur in surrounding of human life. Fumigation application in a silo is among these significant phenomena in which there are many uncertainties about how the fumigant gas (i.e. phosphine gas) is distributed in air within the flow domain of silo. Thus, a study need to be developed in order to understand the behaviour of phosphine gas distribution throughout the silo. A mathematical modelling is applied as an alternative approach to conventional engineering method which is normally very costly. This study is expected to contribute to the answer of those uncertainties so that the outcomes can be useful in the wide range of related applications in various industries. In addition, this study is expected to encourage the academic community to explore further on the mathematical approach which can be applied in various phenomena of transport and fluid dynamics.

1.6 Dissertation Outline

This dissertation is structured in six chapters. Chapter 1 which consists of six sections, introduces the study frameworks. First section describes a brief background of this study. The second section explains the statement of problem, followed by a list of the objectives for this study. Scopes of the study are presented in the following section and significance of the study is described in the second last section. Lastly, in this section, the contents of this dissertation is briefly explained.

In Chapter 2, the literature review from previous and current researches are discussed. The advection-diffusion equation is introduced as a governing equation in transport phenomena and its principle of mass conservation and Fick's Law will be discussed in details. Subsequently, a brief background of the numerical simulation is discussed.

The analytical approach of this study will be discussed in Chapter 3. It consists of the derivation of advection-diffusion equation and finding its analytical solution by defining the initial and boundary conditions based on the transport model of grain fumigation. Then, the numerical simulation is discussed for which the step by step of transport model simulation procedures including the geometry design of flow domain, meshing, setup and solution procedures of ANSYS Fluent software are shown in Chapter 4.

In Chapter 5, the results of study are presented, compared and the verification is achieved. The results include the findings from both analytical and numerical works for which the comparison between both approaches can be performed. Finally, together with the summary of this study, the conclusion and few possible suggestions for further study are recommended in Chapter 6.

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